



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 4, 2026 – 11:30 PM UTC

PDB ID : 9I50 / pdb_00009i50
Title : Crystal structure of feruloyl esterase from *Fusarium oxysporum* G122S variant
Authors : Karampa, P.; Dimarogona, M.; Topakas, E.; Makryniotis, K.; Nikolaivits, E.
Deposited on : 2025-01-27
Resolution : 1.90 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

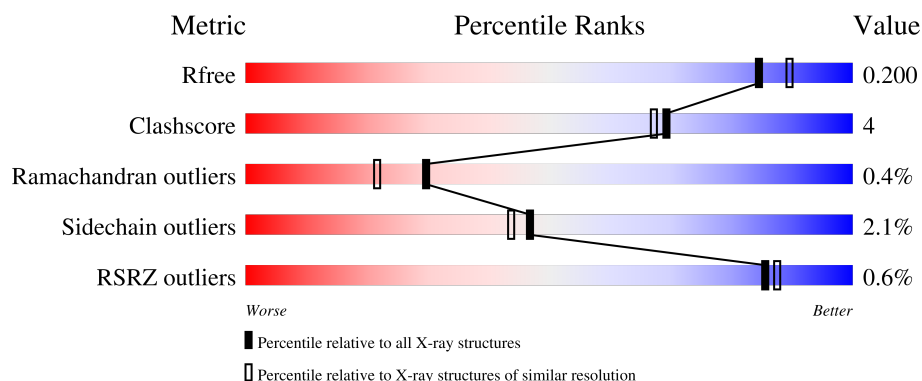
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



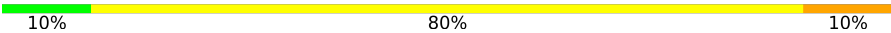
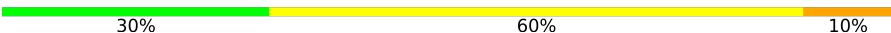
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	563	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 1%, yellow 84%, orange 5%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 84% 5% 10% </div> </div>
1	B	563	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 84%, yellow 6%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 84% 6% 10% </div> </div>
2	C	3	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 67%, orange 33%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 67% 33% </div> </div>
3	D	6	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 17%, yellow 67%, orange 17%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 17% 67% 17% </div> </div>
4	E	9	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 89%, orange 11%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 89% 11% </div> </div>

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Mol	Chain	Length	Quality of chain
5	F	10	 10%80%10%
5	G	10	 30%60%10%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17439 atoms, of which 8238 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.

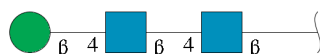
- Molecule 1 is a protein called Carboxylic ester hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	508	Total	C	H	N	O	S	112	4	0
			7806	2522	3814	696	753	21			
1	B	508	Total	C	H	N	O	S	116	5	0
			7792	2519	3803	691	758	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	122	SER	GLY	engineered mutation	UNP A0A1D3S5H0
B	122	SER	GLY	engineered mutation	UNP A0A1D3S5H0

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



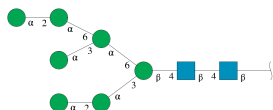
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	3	Total	C	H	N	O	7	0	0
			76	22	37	2	15			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



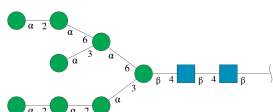
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	6	Total	C	H	N	O	14	0	0
			139	40	67	2	30			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	9	Total	C	H	N	O	20	0	0
			202	58	97	2	45			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



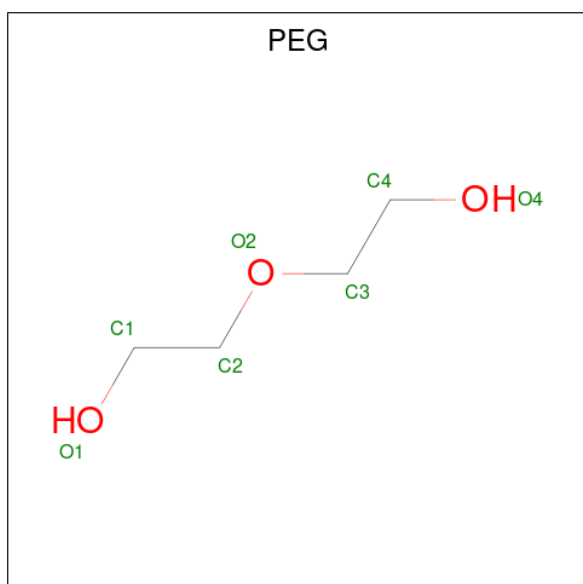
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	10	Total	C	H	N	O	23	0	0
			223	64	107	2	50			
5	G	10	Total	C	H	N	O	23	0	0
			223	64	107	2	50			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



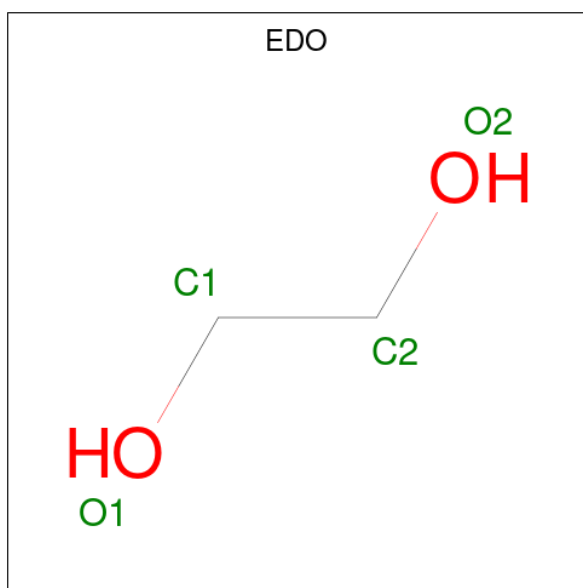
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
6	A	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
6	B	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
6	B	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
6	B	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C H O 17 4 10 3	1	0
7	A	1	Total C H O 17 4 10 3	1	0
7	A	1	Total C H O 17 4 10 3	1	0
7	A	1	Total C H O 17 4 10 3	1	0
7	B	1	Total C H O 17 4 10 3	1	0
7	B	1	Total C H O 17 4 10 3	1	0
7	B	1	Total C H O 17 4 10 3	1	0
7	B	1	Total C H O 17 4 10 3	1	0

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



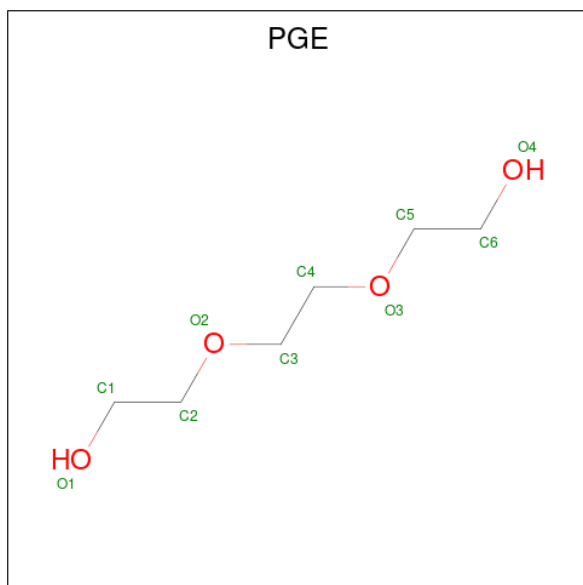
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C H O 10 2 6 2	1	0
8	A	1	Total C H O 10 2 6 2	1	0
8	B	1	Total C H O 10 2 6 2	1	0
8	B	1	Total C H O 10 2 6 2	1	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	H	O	1	0
			10	2	6	2		
8	B	1	Total	C	H	O	1	0
			10	2	6	2		
8	B	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	1	0
			24	6	14	4		

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	Ca	0	0
			1	1		
10	B	1	Total	Ca	0	0
			1	1		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	288	Total	O	0	0
			288	288		

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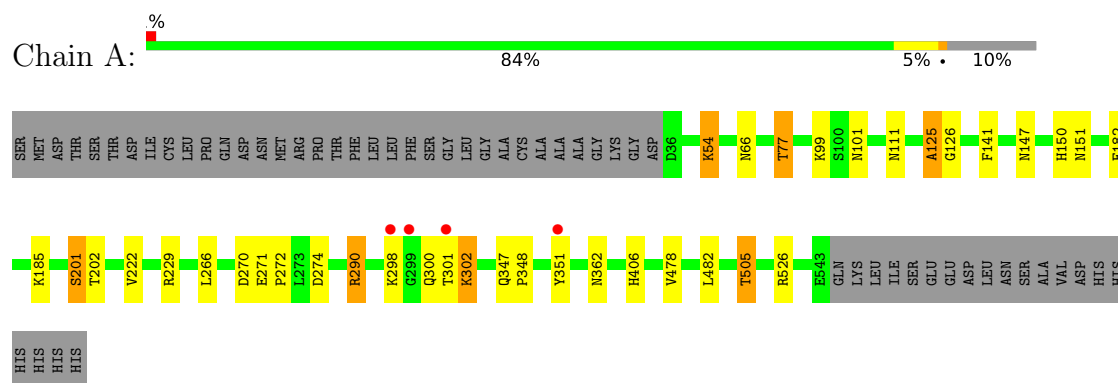
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	318	Total 318	O 318	0	0

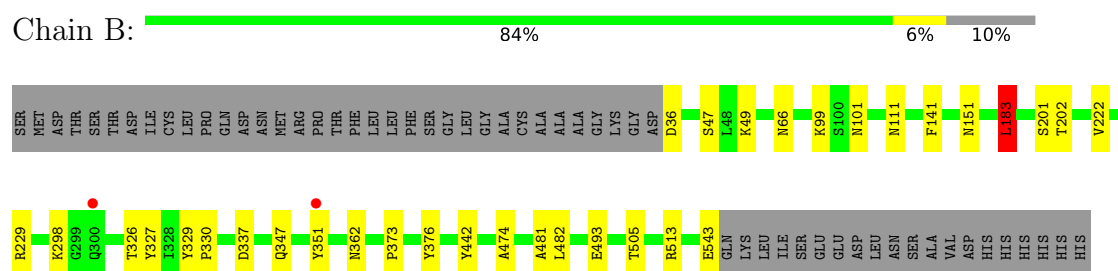
3 Residue-property plots [i](#)

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.

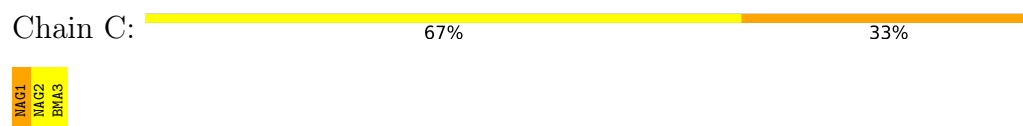
- Molecule 1: Carboxylic ester hydrolase



- Molecule 1: Carboxylic ester hydrolase

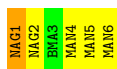


- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 89% 11%



- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 10% 80% 10%



- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 30% 60% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.56Å 89.26Å 116.48Å 90.00° 101.72° 90.00°	Depositor
Resolution (Å)	114.05 – 1.90 114.05 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (114.05-1.90) 98.9 (114.05-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.162 , 0.197 0.165 , 0.200	Depositor DCC
R_{free} test set	5438 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17439	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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: PGE, PEG, MAN, EDO, NAG, CA, BMA

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	0.56	0/4105	1.01	7/5576 (0.1%)
1	B	0.56	0/4102	0.99	5/5574 (0.1%)
All	All	0.56	0/8207	1.00	12/11150 (0.1%)

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	3
1	B	0	2
All	All	0	5

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	TYR	N-CA-CB	6.83	119.98	110.07
1	A	77	THR	CA-CB-OG1	-6.50	99.86	109.60
1	A	505	THR	CA-CB-OG1	-6.17	100.34	109.60
1	B	183	LEU	N-CA-CB	-6.12	101.10	110.16
1	B	141	PHE	CA-CB-CG	5.97	119.78	113.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	A	229	ARG	Sidechain
1	A	290	ARG	Sidechain
1	B	229	ARG	Sidechain
1	B	513	ARG	Sidechain

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	3992	3814	3801	32	0
1	B	3989	3803	3788	27	0
2	C	39	37	34	5	0
3	D	72	67	61	5	0
4	E	105	97	88	3	0
5	F	116	107	97	5	0
5	G	116	107	97	3	0
6	A	28	28	26	7	0
6	B	42	42	39	8	0
7	A	28	40	40	0	0
7	B	28	40	40	1	0
8	A	8	12	12	1	0
8	B	20	30	30	1	0
9	A	10	14	14	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	A	288	0	0	2	0
11	B	318	0	0	1	0
All	All	9201	8238	8167	59	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 4.

The worst 5 of 59 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:101:ASN:HD21	6:A:601:NAG:C1	1.00	1.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ASN:HD21	5:F:1:NAG:C1	0.99	1.59
1:B:101:ASN:HD21	6:B:601:NAG:C1	0.96	1.58
1:A:151:ASN:HD21	3:D:1:NAG:C1	0.94	1.58
1:A:362:ASN:HD21	4:E:1:NAG:C1	0.99	1.56

There are no symmetry-related clashes.

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	510/563 (91%)	495 (97%)	12 (2%)	3 (1%)	21	13
1	B	511/563 (91%)	499 (98%)	11 (2%)	1 (0%)	43	36
All	All	1021/1126 (91%)	994 (97%)	23 (2%)	4 (0%)	30	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	LYS
1	B	201	SER
1	A	201	SER
1	A	270	ASP

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	424/466 (91%)	412 (97%)	12 (3%)	38	32
1	B	425/466 (91%)	418 (98%)	7 (2%)	55	54
All	All	849/932 (91%)	830 (98%)	19 (2%)	47	42

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	202	THR
1	B	505	THR
1	B	543	GLU
1	B	493	GLU
1	A	302	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	66	ASN
1	B	101	ASN
1	B	502	ASN
1	B	147	ASN
1	B	151	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 ⓘ

38 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	2	14,14,15	0.41	0	17,19,21	1.31	3 (17%)
2	NAG	C	2	2	14,14,15	0.41	0	17,19,21	1.44	3 (17%)
2	BMA	C	3	2	11,11,12	0.48	0	15,15,17	0.81	1 (6%)
3	NAG	D	1	3	14,14,15	0.36	0	17,19,21	1.05	1 (5%)
3	NAG	D	2	3	14,14,15	0.41	0	17,19,21	1.29	2 (11%)
3	BMA	D	3	3	11,11,12	0.28	0	15,15,17	0.76	0
3	MAN	D	4	3	11,11,12	0.81	0	15,15,17	1.65	3 (20%)
3	MAN	D	5	3	11,11,12	0.53	0	15,15,17	1.63	3 (20%)
3	MAN	D	6	3	11,11,12	0.75	0	15,15,17	1.25	1 (6%)
4	NAG	E	1	4	14,14,15	0.50	0	17,19,21	1.12	1 (5%)
4	NAG	E	2	4	14,14,15	0.62	0	17,19,21	1.28	2 (11%)
4	BMA	E	3	4	11,11,12	0.86	1 (9%)	15,15,17	0.68	0
4	MAN	E	4	4	11,11,12	0.70	0	15,15,17	1.20	1 (6%)
4	MAN	E	5	4	11,11,12	0.88	1 (9%)	15,15,17	2.34	2 (13%)
4	MAN	E	6	4	11,11,12	0.75	0	15,15,17	1.57	2 (13%)
4	MAN	E	7	4	11,11,12	1.24	0	15,15,17	2.07	4 (26%)
4	MAN	E	8	4	11,11,12	0.53	0	15,15,17	2.44	3 (20%)
4	MAN	E	9	4	11,11,12	0.60	0	15,15,17	1.22	2 (13%)
5	NAG	F	1	5	14,14,15	0.41	0	17,19,21	1.10	1 (5%)
5	MAN	F	10	5	11,11,12	0.55	0	15,15,17	1.02	1 (6%)
5	NAG	F	2	5	14,14,15	0.56	0	17,19,21	1.10	2 (11%)
5	BMA	F	3	5	11,11,12	0.78	1 (9%)	15,15,17	0.92	1 (6%)
5	MAN	F	4	5	11,11,12	0.53	0	15,15,17	1.42	2 (13%)
5	MAN	F	5	5	11,11,12	0.65	0	15,15,17	1.39	2 (13%)
5	MAN	F	6	5	11,11,12	0.86	0	15,15,17	1.16	2 (13%)
5	MAN	F	7	5	11,11,12	0.60	0	15,15,17	1.27	2 (13%)
5	MAN	F	8	5	11,11,12	0.39	0	15,15,17	0.90	0
5	MAN	F	9	5	11,11,12	0.55	0	15,15,17	0.86	1 (6%)
5	NAG	G	1	5	14,14,15	0.62	0	17,19,21	1.20	1 (5%)
5	MAN	G	10	5	11,11,12	0.67	0	15,15,17	1.85	5 (33%)
5	NAG	G	2	5	14,14,15	0.46	0	17,19,21	1.00	0
5	BMA	G	3	5	11,11,12	0.52	0	15,15,17	0.41	0
5	MAN	G	4	5	11,11,12	0.63	0	15,15,17	1.36	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	G	5	5	11,11,12	0.55	0	15,15,17	1.61	4 (26%)
5	MAN	G	6	5	11,11,12	0.57	0	15,15,17	0.91	0
5	MAN	G	7	5	11,11,12	0.41	0	15,15,17	1.35	4 (26%)
5	MAN	G	8	5	11,11,12	0.40	0	15,15,17	1.44	2 (13%)
5	MAN	G	9	5	11,11,12	0.69	0	15,15,17	1.07	1 (6%)

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	2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	0/2/19/22	0/1/1/1
3	MAN	D	6	3	-	2/2/19/22	0/1/1/1
4	NAG	E	1	4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	2/2/19/22	0/1/1/1
4	MAN	E	5	4	-	0/2/19/22	0/1/1/1
4	MAN	E	6	4	-	0/2/19/22	0/1/1/1
4	MAN	E	7	4	-	0/2/19/22	0/1/1/1
4	MAN	E	8	4	-	2/2/19/22	0/1/1/1
4	MAN	E	9	4	-	0/2/19/22	0/1/1/1
5	NAG	F	1	5	-	0/6/23/26	0/1/1/1
5	MAN	F	10	5	-	0/2/19/22	0/1/1/1
5	NAG	F	2	5	-	1/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	MAN	F	4	5	-	2/2/19/22	0/1/1/1
5	MAN	F	5	5	-	0/2/19/22	0/1/1/1
5	MAN	F	6	5	-	0/2/19/22	0/1/1/1
5	MAN	F	7	5	-	0/2/19/22	0/1/1/1
5	MAN	F	8	5	-	0/2/19/22	0/1/1/1
5	MAN	F	9	5	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1	5	-	0/6/23/26	0/1/1/1
5	MAN	G	10	5	-	0/2/19/22	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
5	MAN	G	4	5	-	2/2/19/22	0/1/1/1
5	MAN	G	5	5	-	1/2/19/22	0/1/1/1
5	MAN	G	6	5	-	0/2/19/22	0/1/1/1
5	MAN	G	7	5	-	0/2/19/22	0/1/1/1
5	MAN	G	8	5	-	0/2/19/22	0/1/1/1
5	MAN	G	9	5	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	3	BMA	C4-C5	-2.41	1.47	1.53
5	F	3	BMA	C4-C5	-2.36	1.48	1.53
4	E	5	MAN	O2-C2	2.31	1.48	1.43

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5	MAN	C1-O5-C5	-7.79	101.75	112.19
4	E	8	MAN	C1-O5-C5	7.58	122.35	112.19
4	E	7	MAN	C1-O5-C5	4.69	118.47	112.19
3	D	5	MAN	C1-O5-C5	4.49	118.21	112.19
5	G	4	MAN	C1-O5-C5	4.14	117.74	112.19

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

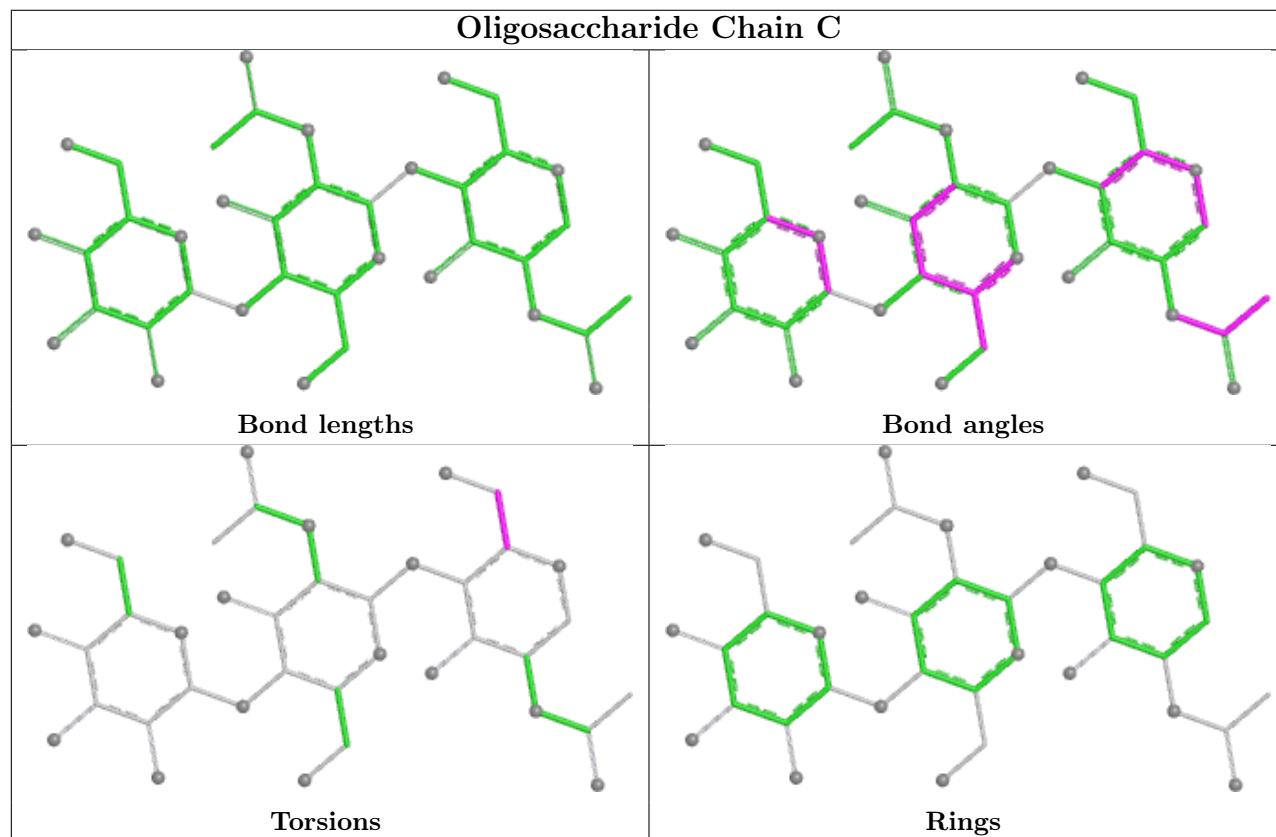
Mol	Chain	Res	Type	Atoms
5	F	9	MAN	O5-C5-C6-O6
4	E	8	MAN	C4-C5-C6-O6
4	E	8	MAN	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
5	F	9	MAN	C4-C5-C6-O6

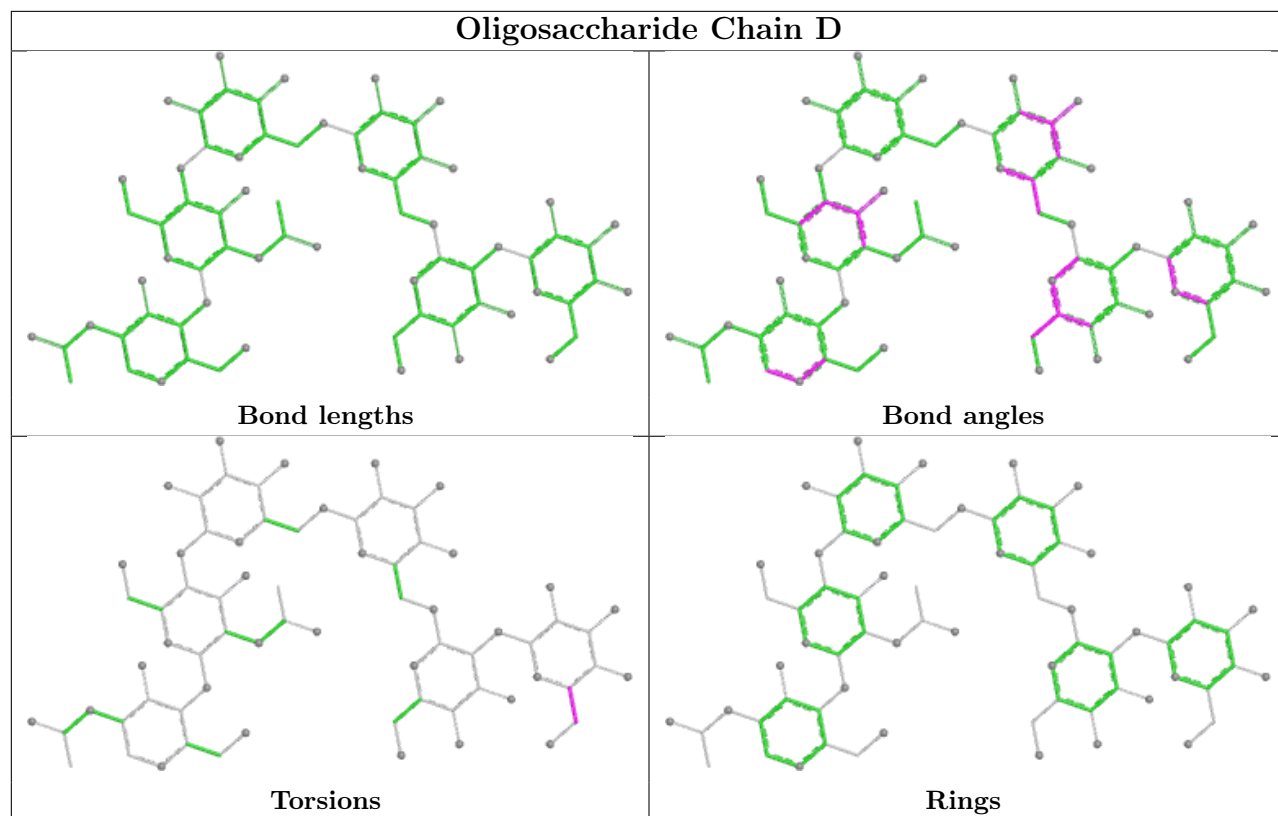
There are no ring outliers.

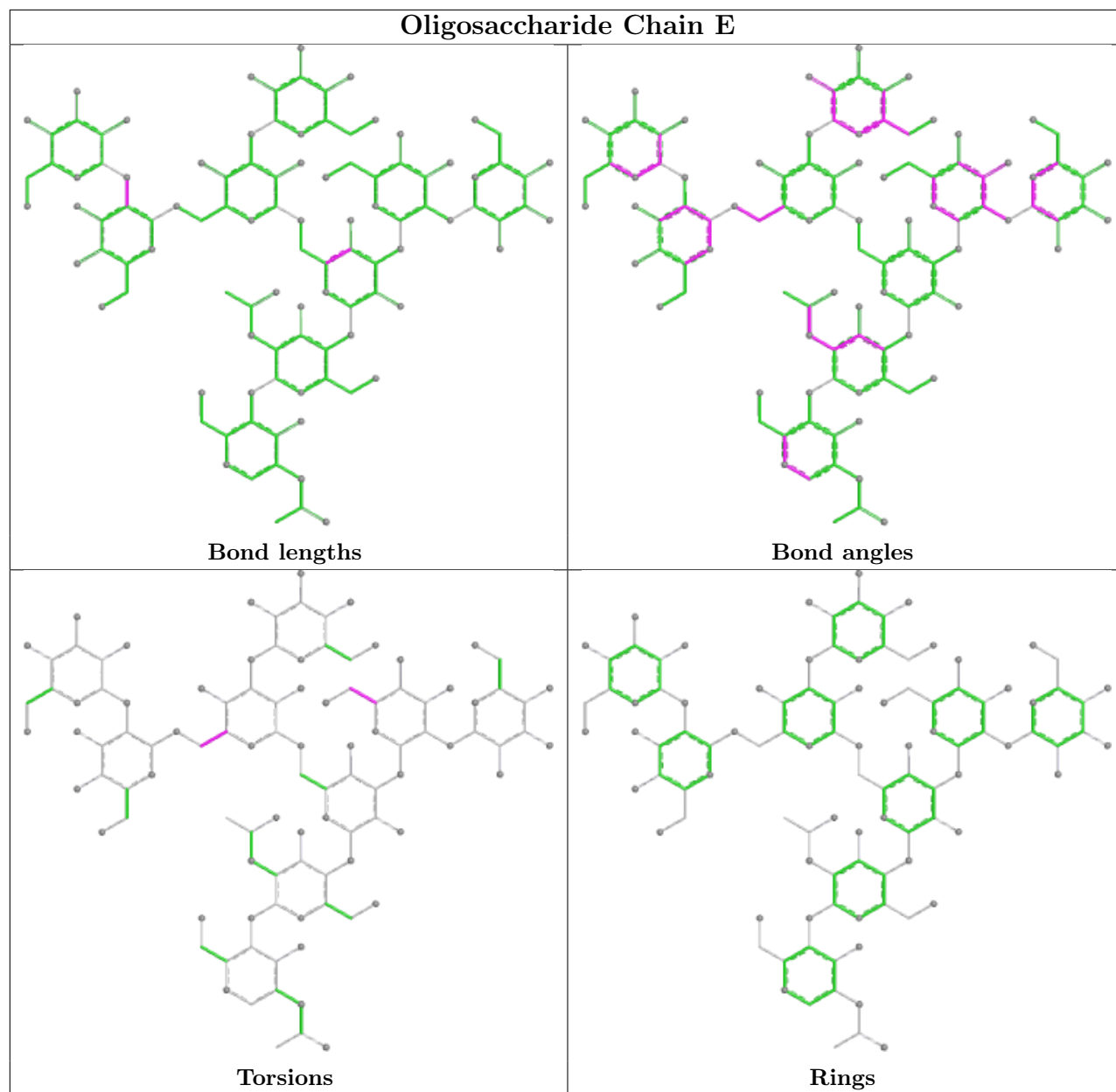
5 monomers are involved in 21 short contacts:

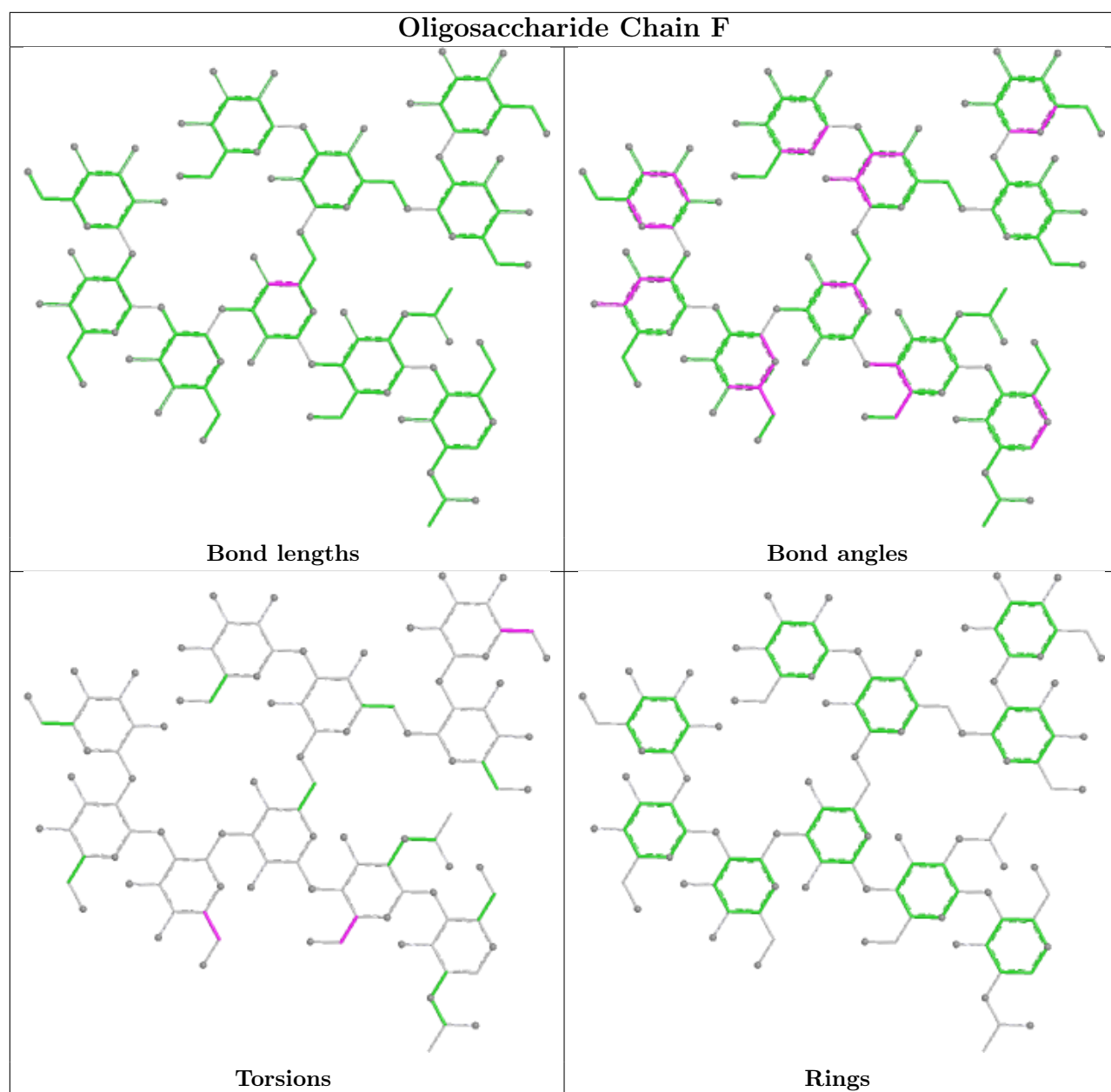
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1	NAG	5	0
4	E	1	NAG	3	0
5	G	1	NAG	3	0
2	C	1	NAG	5	0
3	D	1	NAG	5	0

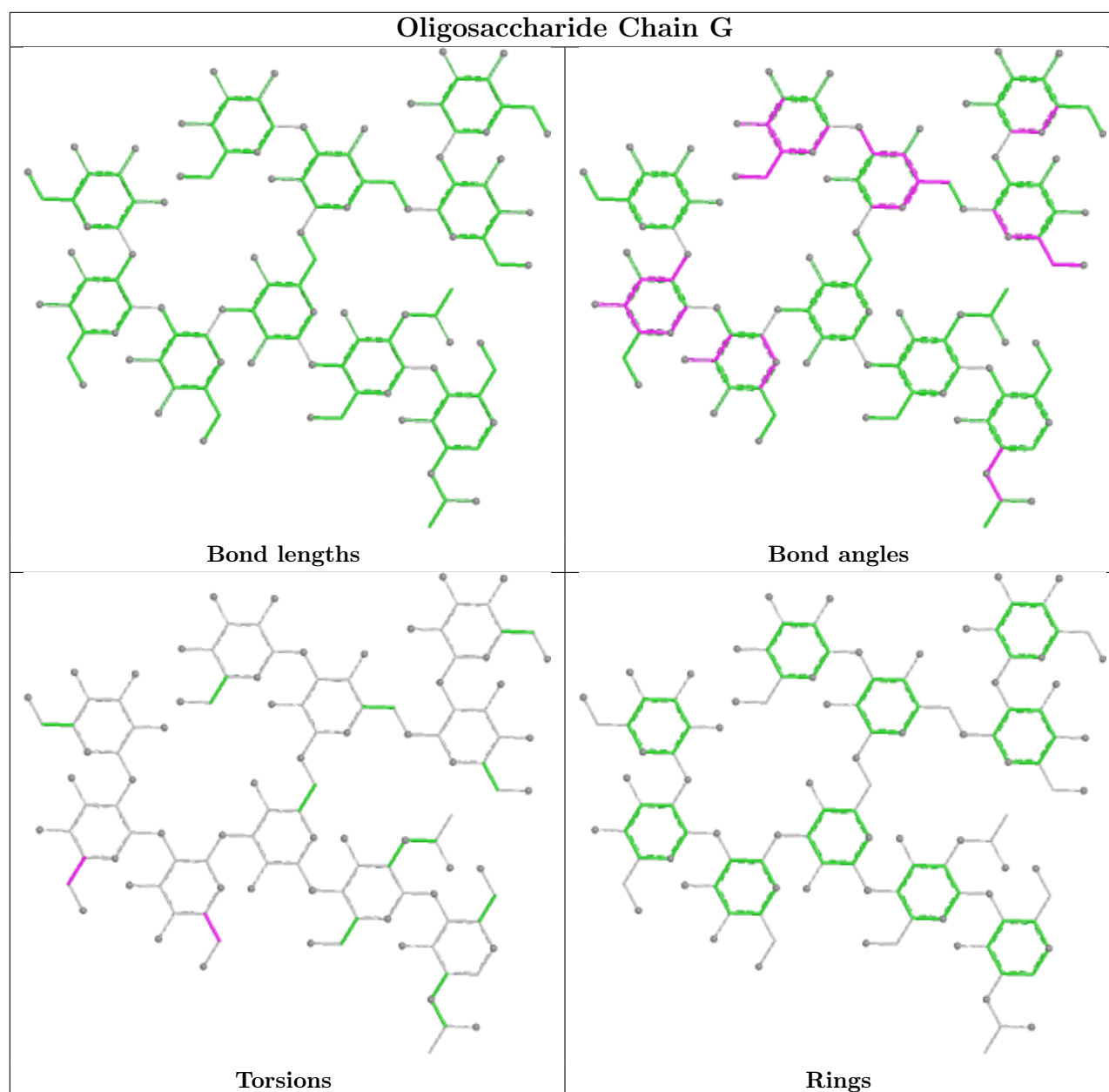
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 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
6	NAG	B	609	-	14,14,15	0.78	0	17,19,21	1.56	3 (17%)
7	PEG	A	603	-	6,6,6	0.14	0	5,5,5	0.16	0
7	PEG	B	612	-	6,6,6	0.20	0	5,5,5	0.18	0
7	PEG	A	602	-	6,6,6	0.10	0	5,5,5	0.12	0
6	NAG	B	608	-	14,14,15	0.65	0	17,19,21	1.14	2 (11%)
6	NAG	A	608	-	14,14,15	0.66	0	17,19,21	1.11	1 (5%)
8	EDO	A	604	-	3,3,3	0.12	0	2,2,2	0.38	0
8	EDO	B	603	-	3,3,3	0.14	0	2,2,2	0.32	0
9	PGE	A	607	-	9,9,9	0.24	0	8,8,8	0.14	0
7	PEG	A	605	-	6,6,6	0.14	0	5,5,5	0.13	0
8	EDO	B	604	-	3,3,3	0.27	0	2,2,2	0.45	0
7	PEG	A	610	-	6,6,6	0.14	0	5,5,5	0.09	0
6	NAG	B	601	-	14,14,15	0.49	0	17,19,21	1.07	1 (5%)
8	EDO	B	606	-	3,3,3	0.06	0	2,2,2	0.17	0
8	EDO	B	607	-	3,3,3	0.14	0	2,2,2	0.25	0
7	PEG	B	611	-	6,6,6	0.15	0	5,5,5	0.16	0
7	PEG	B	602	-	6,6,6	0.15	0	5,5,5	0.15	0
7	PEG	B	613	-	6,6,6	0.41	0	5,5,5	0.28	0
6	NAG	A	601	-	14,14,15	0.50	0	17,19,21	0.95	0
8	EDO	B	605	-	3,3,3	0.30	0	2,2,2	0.34	0
8	EDO	A	606	-	3,3,3	0.40	0	2,2,2	0.47	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
6	NAG	B	609	-	-	1/6/23/26	0/1/1/1
7	PEG	A	603	-	-	2/4/4/4	-
7	PEG	B	612	-	-	1/4/4/4	-
7	PEG	A	602	-	-	1/4/4/4	-
6	NAG	B	608	-	-	2/6/23/26	0/1/1/1
6	NAG	A	608	-	-	0/6/23/26	0/1/1/1
8	EDO	A	604	-	-	0/1/1/1	-
8	EDO	B	603	-	-	1/1/1/1	-
9	PGE	A	607	-	-	0/7/7/7	-
7	PEG	A	605	-	-	3/4/4/4	-
8	EDO	B	604	-	-	1/1/1/1	-
7	PEG	A	610	-	-	2/4/4/4	-
6	NAG	B	601	-	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	B	606	-	-	1/1/1/1	-
8	EDO	B	607	-	-	1/1/1/1	-
7	PEG	B	611	-	-	3/4/4/4	-
7	PEG	B	602	-	-	2/4/4/4	-
7	PEG	B	613	-	-	2/4/4/4	-
6	NAG	A	601	-	-	0/6/23/26	0/1/1/1
8	EDO	B	605	-	-	1/1/1/1	-
8	EDO	A	606	-	-	1/1/1/1	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	609	NAG	C1-C2-N2	-4.45	103.42	110.43
6	B	608	NAG	C2-N2-C7	3.09	127.04	122.90
6	B	609	NAG	C3-C4-C5	-2.77	105.20	110.23
6	B	609	NAG	O4-C4-C5	2.52	115.54	109.32
6	A	608	NAG	C2-N2-C7	2.44	126.17	122.90

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	608	NAG	O5-C5-C6-O6
6	B	608	NAG	C4-C5-C6-O6
7	A	603	PEG	O1-C1-C2-O2
7	A	605	PEG	O2-C3-C4-O4
7	B	602	PEG	O2-C3-C4-O4

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	609	NAG	2	0
6	B	608	NAG	3	0
6	A	608	NAG	4	0
8	B	604	EDO	1	0
6	B	601	NAG	3	0
7	B	613	PEG	1	0
6	A	601	NAG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	606	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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	508/563 (90%)	-0.31	4 (0%) 82 85	19, 42, 62, 99	4 (0%)
1	B	508/563 (90%)	-0.36	2 (0%) 88 90	15, 41, 62, 103	5 (0%)
All	All	1016/1126 (90%)	-0.33	6 (0%) 85 87	15, 41, 62, 103	9 (0%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	351	TYR	3.3
1	A	301	THR	2.8
1	A	351	TYR	2.8
1	A	298	LYS	2.3
1	A	299	GLY	2.1

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	BMA	C	3	11/12	0.67	0.11	30,93,97,99	3
4	MAN	E	9	11/12	0.78	0.13	30,82,86,87	3
3	MAN	D	4	11/12	0.80	0.13	30,67,70,76	3
5	MAN	F	9	11/12	0.80	0.14	30,68,78,87	3
4	MAN	E	8	11/12	0.81	0.12	30,72,77,87	2

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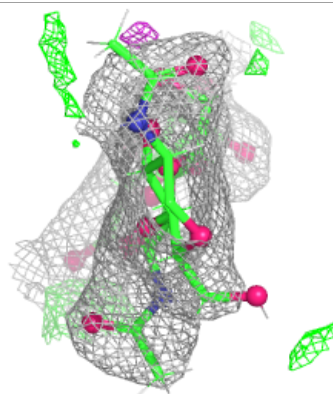
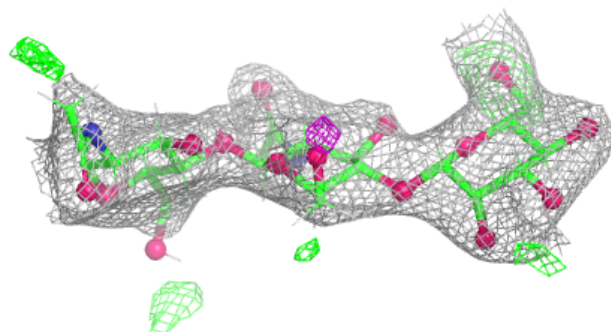
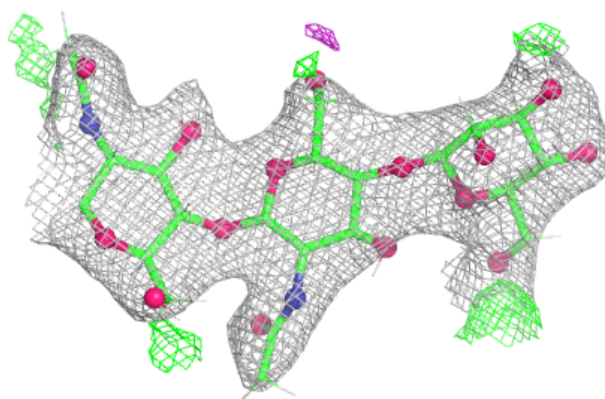
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	C	2	14/15	0.82	0.11	30,81,91,99	2
3	MAN	D	6	11/12	0.85	0.12	30,72,76,79	3
3	MAN	D	5	11/12	0.85	0.13	30,75,78,79	2
3	BMA	D	3	11/12	0.87	0.10	30,69,74,76	2
4	MAN	E	7	11/12	0.88	0.12	30,49,52,54	3
2	NAG	C	1	14/15	0.91	0.09	30,71,75,77	2
5	MAN	G	4	11/12	0.92	0.08	30,40,44,48	2
4	MAN	E	6	11/12	0.93	0.08	30,52,55,57	3
4	MAN	E	4	11/12	0.93	0.08	30,46,48,49	2
5	MAN	F	10	11/12	0.94	0.07	30,55,56,56	3
5	MAN	F	8	11/12	0.94	0.07	30,55,58,59	2
5	MAN	G	5	11/12	0.94	0.08	30,48,52,55	3
5	MAN	G	6	11/12	0.94	0.07	30,46,50,54	3
4	NAG	E	1	14/15	0.95	0.08	30,49,53,58	2
5	MAN	F	4	11/12	0.95	0.07	30,40,48,57	2
3	NAG	D	1	14/15	0.95	0.08	30,49,60,60	2
4	MAN	E	5	11/12	0.95	0.07	30,48,52,54	2
5	MAN	G	10	11/12	0.95	0.08	30,49,56,64	3
3	NAG	D	2	14/15	0.96	0.06	30,50,57,65	2
5	NAG	G	2	14/15	0.96	0.06	30,46,51,51	2
5	MAN	F	5	11/12	0.96	0.07	30,41,44,47	3
5	MAN	F	6	11/12	0.96	0.06	30,40,43,46	3
4	BMA	E	3	11/12	0.96	0.06	30,45,49,51	1
5	BMA	F	3	11/12	0.96	0.06	30,38,40,43	1
5	NAG	G	1	14/15	0.97	0.05	30,44,46,49	2
5	MAN	F	7	11/12	0.97	0.05	30,48,50,52	2
5	MAN	G	8	11/12	0.97	0.05	30,39,42,45	2
5	MAN	G	9	11/12	0.97	0.05	30,43,47,48	3
4	NAG	E	2	14/15	0.97	0.06	30,47,51,51	2
5	MAN	G	7	11/12	0.98	0.04	30,36,41,45	2
5	NAG	F	1	14/15	0.98	0.05	30,39,51,52	2
5	NAG	F	2	14/15	0.98	0.05	30,38,43,46	2
5	BMA	G	3	11/12	0.98	0.05	30,38,40,42	1

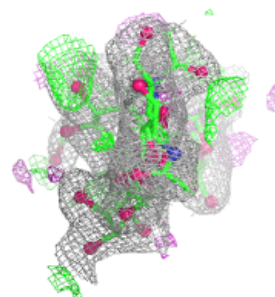
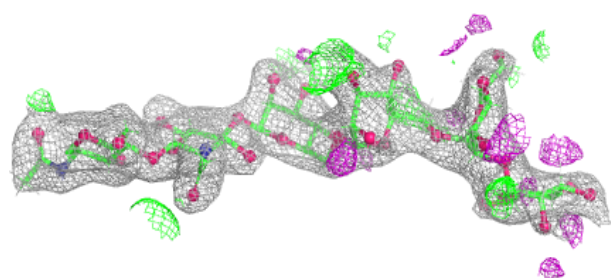
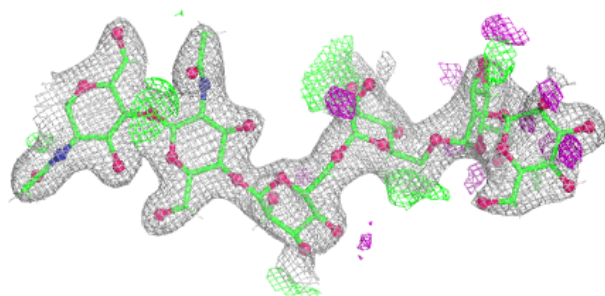
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

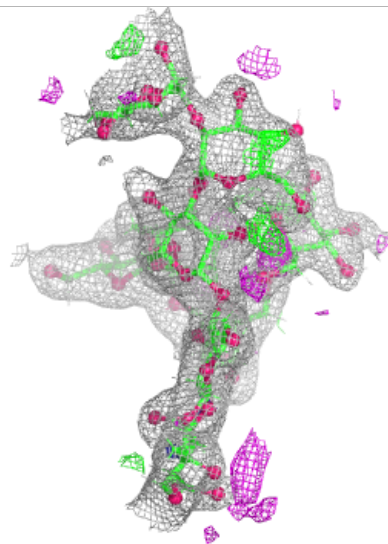
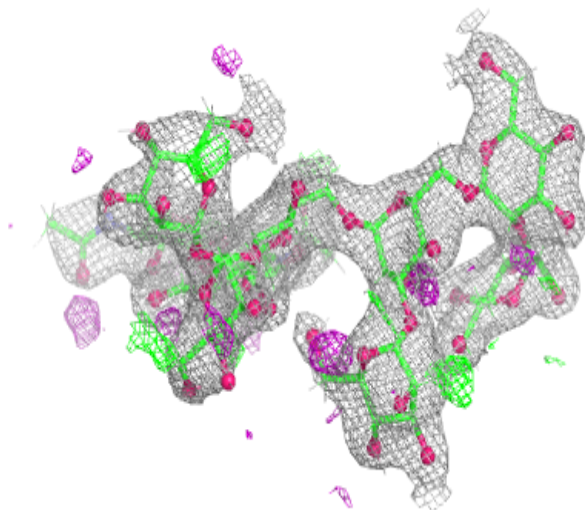
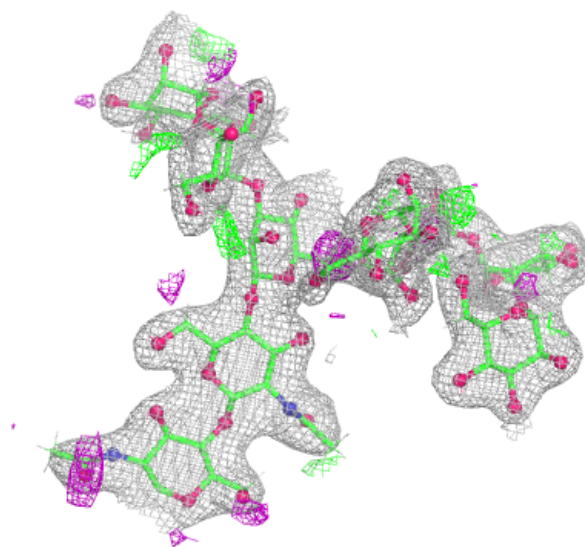
**Electron density around Chain D:**

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



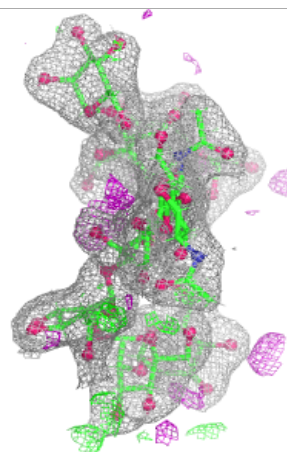
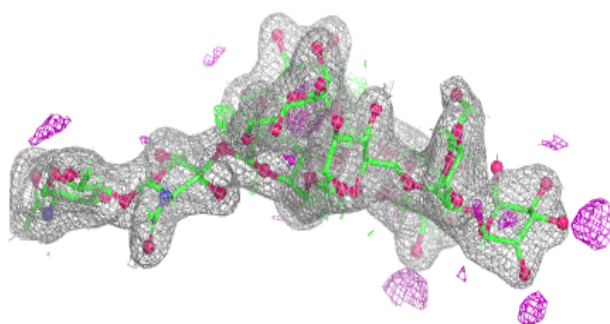
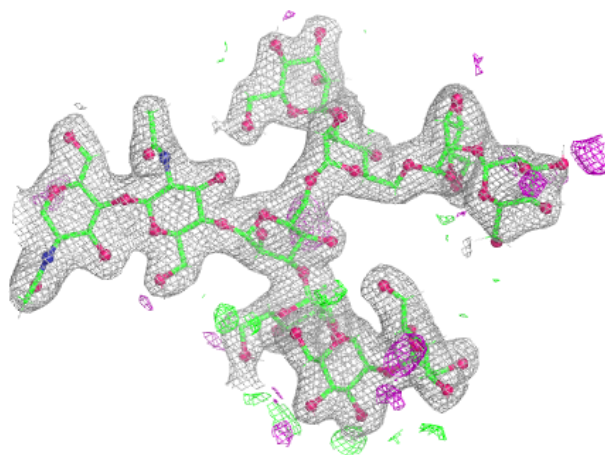
Electron density around Chain E:

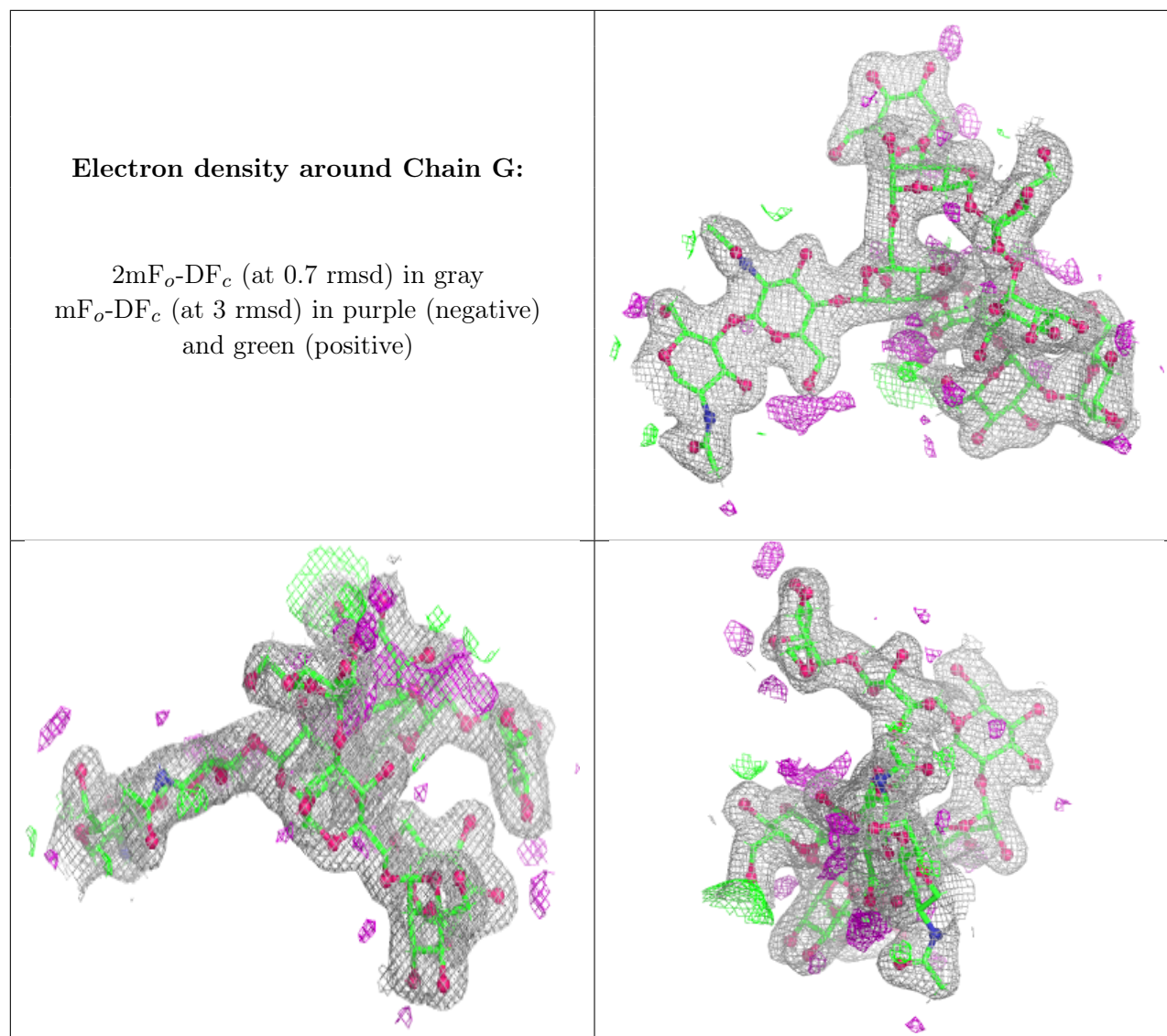
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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
6	NAG	A	608	14/15	0.79	0.12	30,83,87,88	3
6	NAG	B	608	14/15	0.81	0.13	30,81,86,89	3
7	PEG	B	613	7/7	0.81	0.15	35,69,76,79	1
7	PEG	A	605	7/7	0.82	0.16	30,75,82,85	1
9	PGE	A	607	10/10	0.85	0.14	30,80,86,86	1
8	EDO	A	606	4/4	0.86	0.16	30,59,61,62	1
6	NAG	A	601	14/15	0.87	0.11	30,65,70,70	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NAG	B	609	14/15	0.87	0.12	30,72,80,82	3
8	EDO	B	604	4/4	0.88	0.12	30,60,65,65	1
7	PEG	B	611	7/7	0.89	0.14	35,76,87,87	1
8	EDO	B	605	4/4	0.89	0.14	30,60,61,62	1
7	PEG	B	612	7/7	0.89	0.13	35,83,87,90	1
6	NAG	B	601	14/15	0.90	0.10	30,56,63,66	3
7	PEG	A	610	7/7	0.90	0.14	35,70,84,85	1
8	EDO	B	603	4/4	0.90	0.12	30,65,66,66	1
8	EDO	A	604	4/4	0.91	0.14	30,77,80,81	1
7	PEG	B	602	7/7	0.91	0.12	30,62,64,66	1
8	EDO	B	607	4/4	0.93	0.10	30,70,71,71	1
8	EDO	B	606	4/4	0.94	0.10	30,76,81,81	1
7	PEG	A	603	7/7	0.94	0.12	30,69,74,77	1
7	PEG	A	602	7/7	0.94	0.09	30,71,77,79	1
10	CA	B	610	1/1	0.99	0.02	38,38,38,38	0
10	CA	A	609	1/1	1.00	0.02	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.