



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 07:45 PM UTC

PDB ID : 4DHL / pdb_00004dhl
Title : Crystal structure of red kidney bean purple acid phosphatase in complex with Maybridge fragment MO07123
Authors : Feder, D.; Clayton, D.J.; Hussein, W.M.; Schenk, G.; McGeary, R.; Guddat, L.W.
Deposited on : 2012-01-29
Resolution : 2.30 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

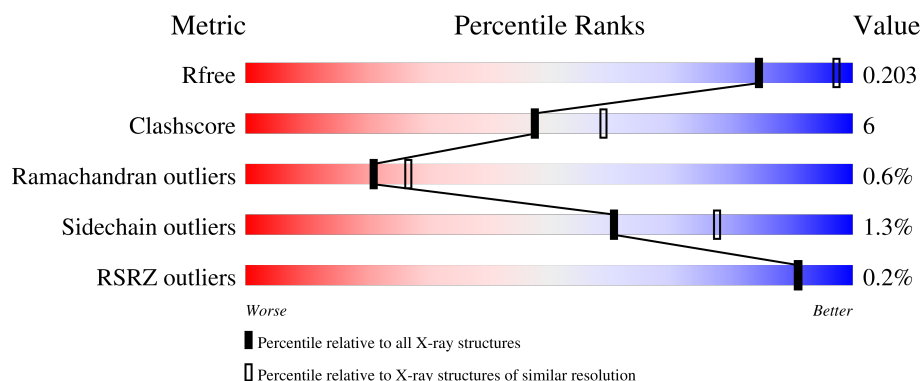
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

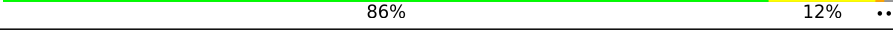
The reported resolution of this entry is 2.30 Å.

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.



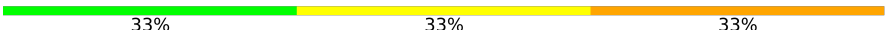
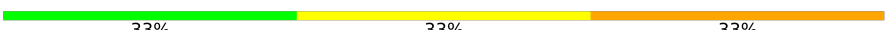
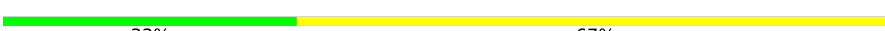
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	426	 87% 12% .
1	B	426	 85% 14% .
1	C	426	 87% 12% .
1	D	426	 86% 12% ..
2	E	3	 33% 67%

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Mol	Chain	Length	Quality of chain
2	F	3	
2	G	3	
2	I	3	
2	J	3	
2	M	3	
3	H	2	
3	K	2	
3	L	2	

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
6	0K7	D	503	-	X	-	-

2 Entry composition [i](#)

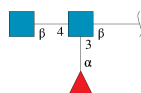
There are 11 unique types of molecules in this entry. The entry contains 16091 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Purple acid phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	1	0
			3502	2248	610	634	10			
1	B	425	Total	C	N	O	S	0	3	0
			3524	2260	612	641	11			
1	D	423	Total	C	N	O	S	7	1	0
			3495	2245	607	633	10			
1	C	424	Total	C	N	O	S	0	1	0
			3499	2248	606	634	11			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	F	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	G	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	I	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	J	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	M	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	K	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	L	2	Total	C	N	O	0	0	0
			24	14	1	9			

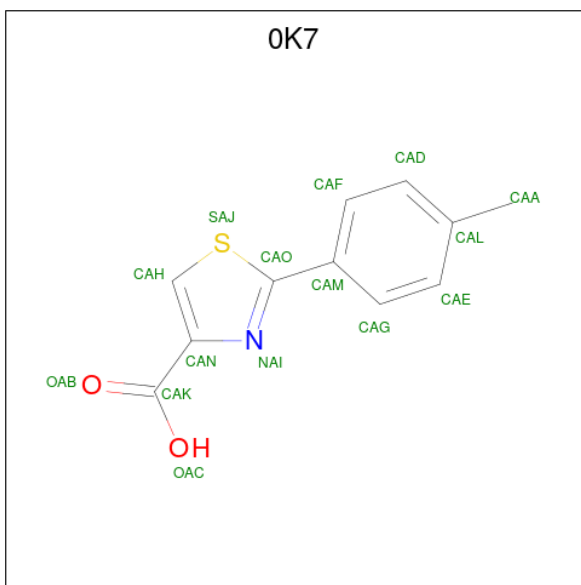
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		

- Molecule 5 is FE (III) ION (CCD ID: FE) (formula: Fe).

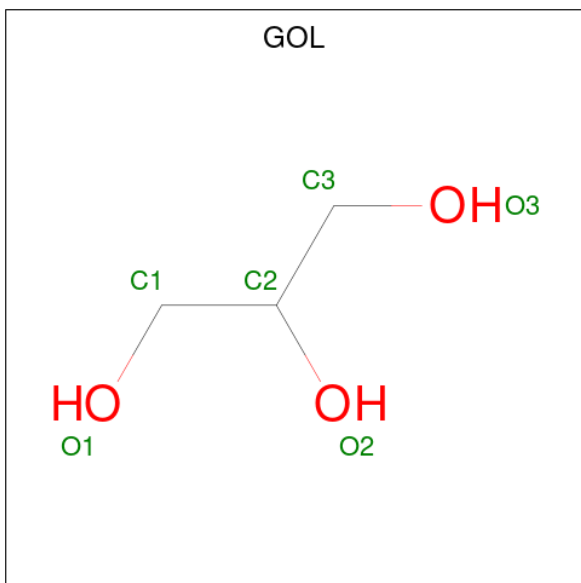
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Fe	0	0
			1	1		
5	B	1	Total	Fe	0	0
			1	1		
5	D	1	Total	Fe	0	0
			1	1		
5	C	1	Total	Fe	0	0
			1	1		

- Molecule 6 is 2-(4-methylphenyl)-1,3-thiazole-4-carboxylic acid (CCD ID: 0K7) (formula: C₁₁H₉NO₂S).



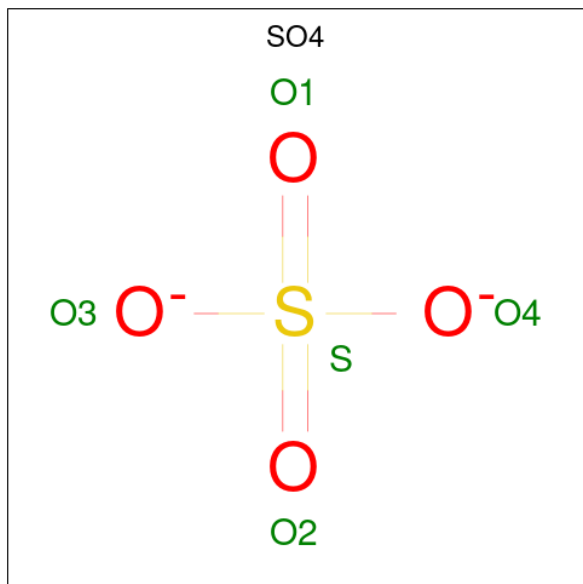
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			15	11	1	2	1		
6	B	1	Total	C	N	O	S	0	0
			15	11	1	2	1		
6	D	1	Total	C	N	O	S	0	0
			8	4	1	2	1		
6	C	1	Total	C	N	O	S	0	0
			15	11	1	2	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



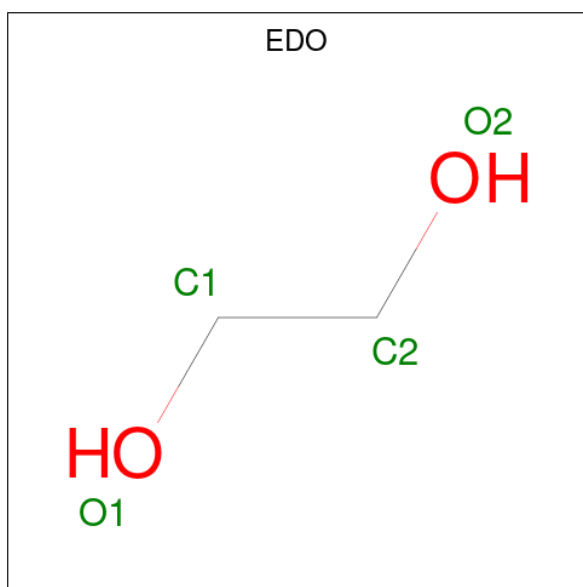
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



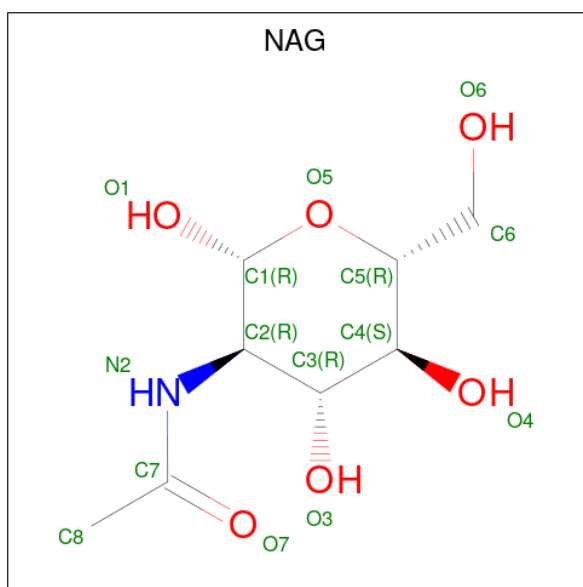
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	D	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	D	1	Total	C	O	0	0
			4	2	2		
9	D	1	Total	C	O	0	0
			4	2	2		
9	D	1	Total	C	O	0	0
			4	2	2		
9	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

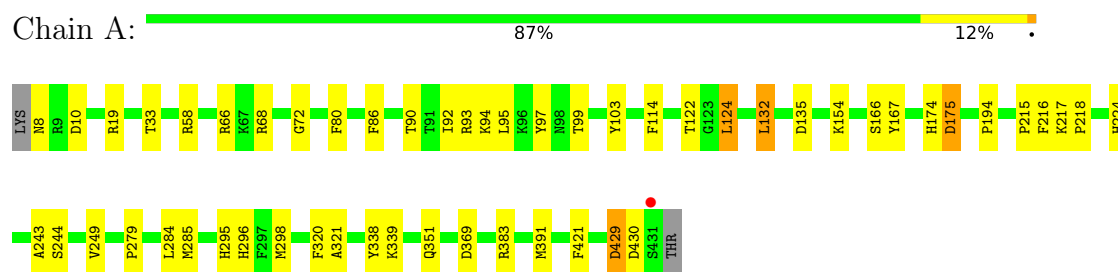
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	403	Total	O	0	0
			403	403		
11	B	378	Total	O	0	0
			378	378		
11	D	380	Total	O	0	0
			380	380		
11	C	384	Total	O	0	0
			384	384		

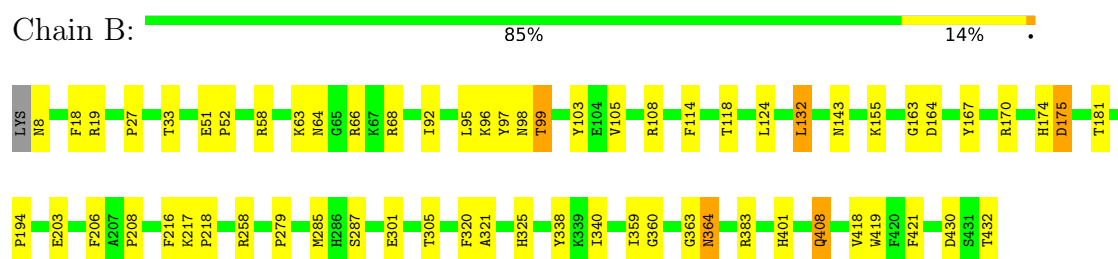
3 Residue-property plots

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.

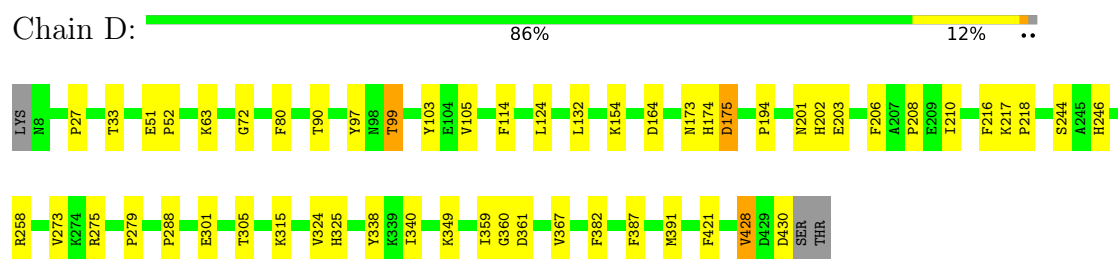
• Molecule 1: Purple acid phosphatase



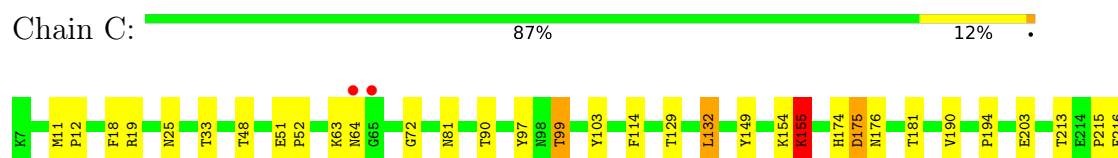
• Molecule 1: Purple acid phosphatase



• Molecule 1: Purple acid phosphatase

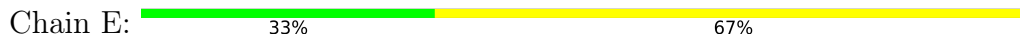


• Molecule 1: Purple acid phosphatase





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



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



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



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



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



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



- Molecule 3: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  50% 50%

NAG1
FUC2

- Molecule 3: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

NAG1
FUC2

- Molecule 3: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  50% 50%

NAG1
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	126.10Å 126.10Å 297.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.82 – 2.30 19.82 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.1 (19.82-2.30) 93.9 (19.82-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.30Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.158 , 0.206 0.154 , 0.203	Depositor DCC
R_{free} test set	5774 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16091	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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: GOL, NAG, FE, EDO, SO4, ZN, OK7, FUC

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	0.45	0/3624	0.75	1/4927 (0.0%)
1	B	0.44	0/3643	0.75	2/4953 (0.0%)
1	C	0.45	0/3618	0.75	0/4919
1	D	0.46	0/3614	0.76	1/4915 (0.0%)
All	All	0.45	0/14499	0.75	4/19714 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	PHE	CB-CA-C	-5.24	110.52	116.54
1	B	287	SER	CA-C-N	5.07	125.23	119.90
1	B	287	SER	C-N-CA	5.07	125.23	119.90
1	D	367	VAL	N-CA-C	5.03	115.16	108.11

There are no chirality outliers.

There are no planarity outliers.

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	3502	0	3321	39	0
1	B	3524	0	3334	42	0
1	C	3499	0	3312	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3495	0	3310	38	0
2	E	38	0	34	0	0
2	F	38	0	34	2	0
2	G	38	0	34	0	0
2	I	38	0	34	1	0
2	J	38	0	34	0	0
2	M	38	0	34	0	0
3	H	24	0	22	0	0
3	K	24	0	22	0	0
3	L	24	0	22	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	15	0	8	3	0
6	B	15	0	8	4	0
6	C	15	0	8	2	0
6	D	8	0	1	1	0
7	A	6	0	8	0	0
7	C	6	0	8	0	0
7	D	6	0	8	1	0
8	A	10	0	0	1	0
8	B	5	0	0	0	0
8	C	5	0	0	0	0
8	D	5	0	0	0	0
9	A	4	0	6	0	0
9	D	20	0	30	4	0
10	A	14	0	13	0	0
10	B	28	0	26	1	0
10	C	28	0	26	0	0
10	D	28	0	26	0	0
11	A	403	0	0	3	0
11	B	378	0	0	3	0
11	C	384	0	0	2	0
11	D	380	0	0	4	0
All	All	16091	0	13723	159	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 6.

The worst 5 of 159 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:D:173:ASN:H	9:D:510:EDO:H22	1.43	0.83
1:D:124:LEU:HD12	1:D:279:PRO:HG3	1.60	0.81
1:B:408[A]:GLN:HE21	1:B:408[A]:GLN:H	1.27	0.81
1:B:325:HIS:HE1	6:B:503:OK7:H8	1.50	0.77
1:A:217:LYS:HB3	1:A:218:PRO:HD3	1.67	0.75

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	423/426 (99%)	402 (95%)	19 (4%)	2 (0%)	24	31
1	B	426/426 (100%)	402 (94%)	19 (4%)	5 (1%)	10	12
1	C	423/426 (99%)	395 (93%)	26 (6%)	2 (0%)	24	31
1	D	422/426 (99%)	401 (95%)	20 (5%)	1 (0%)	43	55
All	All	1694/1704 (99%)	1600 (94%)	84 (5%)	10 (1%)	21	27

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	ASP
1	B	64	ASN
1	B	175	ASP
1	D	175	ASP
1	C	175	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	374/375 (100%)	370 (99%)	4 (1%)	65	81
1	B	377/375 (100%)	371 (98%)	6 (2%)	55	73
1	C	373/375 (100%)	367 (98%)	6 (2%)	55	73
1	D	373/375 (100%)	368 (99%)	5 (1%)	61	77
All	All	1497/1500 (100%)	1476 (99%)	21 (1%)	61	76

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	428	VAL
1	C	132	LEU
1	C	383	ARG
1	C	155	LYS
1	C	99	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	295	HIS
1	C	405	ASN
1	C	371	ASN
1	D	173	ASN
1	C	173	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

24 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	E	1	2,1	14,14,15	0.48	0	17,19,21	1.15	2 (11%)
2	FUC	E	2	2	10,10,11	0.65	0	14,14,16	0.54	0
2	NAG	E	3	2	14,14,15	0.48	0	17,19,21	1.13	2 (11%)
2	NAG	F	1	2,1	14,14,15	0.61	0	17,19,21	0.81	0
2	FUC	F	2	2	10,10,11	0.60	0	14,14,16	1.00	1 (7%)
2	NAG	F	3	2	14,14,15	0.51	0	17,19,21	0.76	0
2	NAG	G	1	2,1	14,14,15	0.57	0	17,19,21	1.12	2 (11%)
2	FUC	G	2	2	10,10,11	0.76	0	14,14,16	0.98	1 (7%)
2	NAG	G	3	2	14,14,15	0.57	0	17,19,21	0.81	0
3	NAG	H	1	1,3	14,14,15	0.57	0	17,19,21	0.96	1 (5%)
3	FUC	H	2	3	10,10,11	0.60	0	14,14,16	0.48	0
2	NAG	I	1	2,1	14,14,15	0.56	0	17,19,21	0.89	1 (5%)
2	FUC	I	2	2	10,10,11	0.75	0	14,14,16	0.76	0
2	NAG	I	3	2	14,14,15	0.50	0	17,19,21	0.68	0
2	NAG	J	1	2,1	14,14,15	0.64	0	17,19,21	0.71	0
2	FUC	J	2	2	10,10,11	0.65	0	14,14,16	0.53	0
2	NAG	J	3	2	14,14,15	0.59	0	17,19,21	1.08	1 (5%)
3	NAG	K	1	1,3	14,14,15	0.50	0	17,19,21	0.91	0
3	FUC	K	2	3	10,10,11	0.67	0	14,14,16	0.84	0
3	NAG	L	1	1,3	14,14,15	0.49	0	17,19,21	1.18	1 (5%)
3	FUC	L	2	3	10,10,11	0.64	0	14,14,16	0.55	0
2	NAG	M	1	2,1	14,14,15	0.60	0	17,19,21	1.23	2 (11%)
2	FUC	M	2	2	10,10,11	0.68	0	14,14,16	0.51	0
2	NAG	M	3	2	14,14,15	0.57	0	17,19,21	0.95	1 (5%)

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	E	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	E	2	2	-	-	0/1/1/1
2	NAG	E	3	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	FUC	F	2	2	-	-	0/1/1/1
2	NAG	F	3	2	-	4/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	FUC	G	2	2	-	-	0/1/1/1
2	NAG	G	3	2	-	0/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	FUC	H	2	3	-	-	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	FUC	I	2	2	-	-	0/1/1/1
2	NAG	I	3	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	FUC	J	2	2	-	-	0/1/1/1
2	NAG	J	3	2	-	2/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	K	2	3	-	-	0/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	L	2	3	-	-	0/1/1/1
2	NAG	M	1	2,1	-	0/6/23/26	0/1/1/1
2	FUC	M	2	2	-	-	0/1/1/1
2	NAG	M	3	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	1	NAG	C1-O5-C5	3.16	116.42	112.19
2	E	1	NAG	C2-N2-C7	-3.13	118.71	122.90
2	J	3	NAG	C2-N2-C7	-3.03	118.84	122.90
3	L	1	NAG	C1-O5-C5	2.96	116.16	112.19
2	M	1	NAG	C2-N2-C7	-2.95	118.94	122.90

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	3	NAG	O5-C5-C6-O6
2	J	3	NAG	O5-C5-C6-O6

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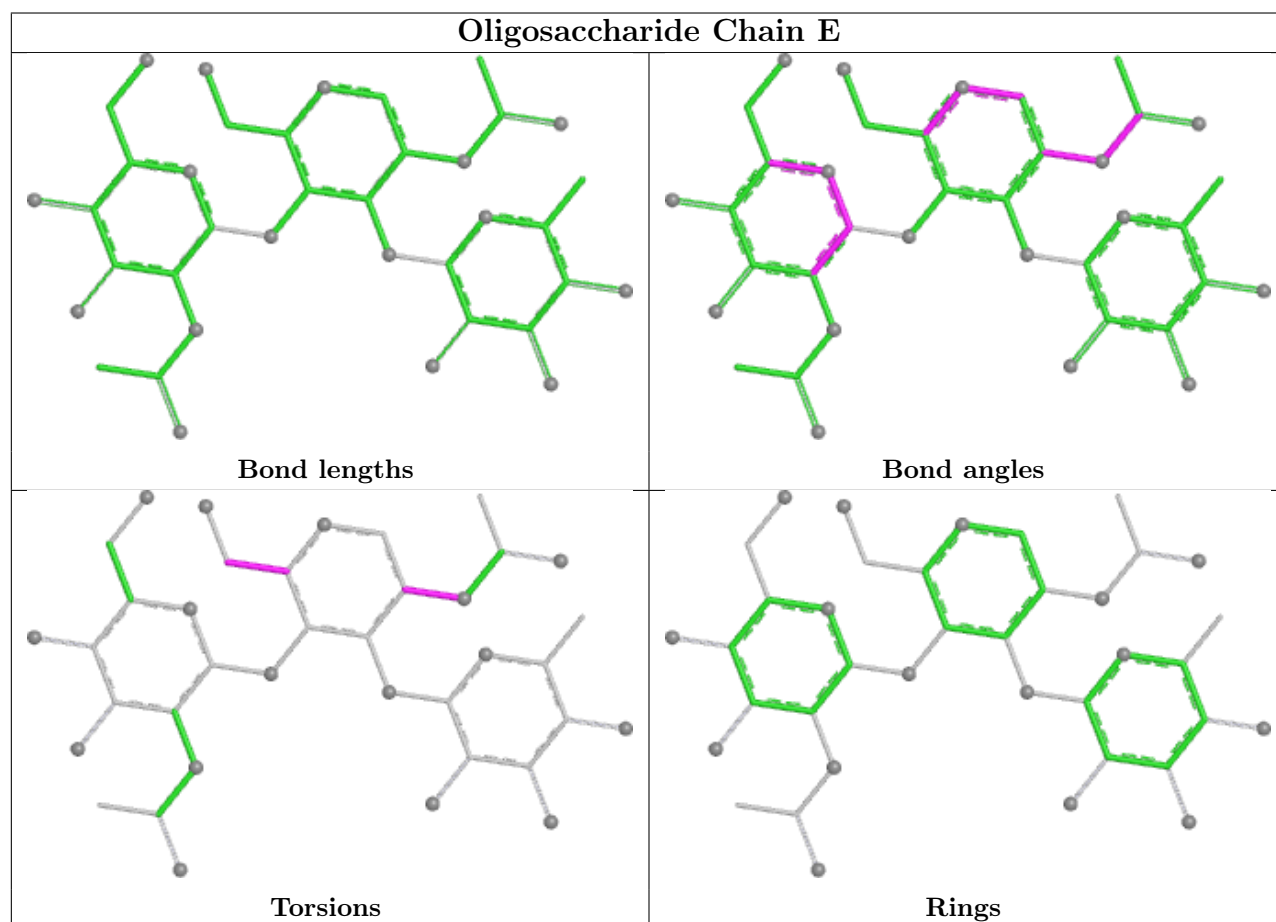
Mol	Chain	Res	Type	Atoms
2	F	3	NAG	C4-C5-C6-O6
2	J	3	NAG	C4-C5-C6-O6
2	F	3	NAG	C8-C7-N2-C2

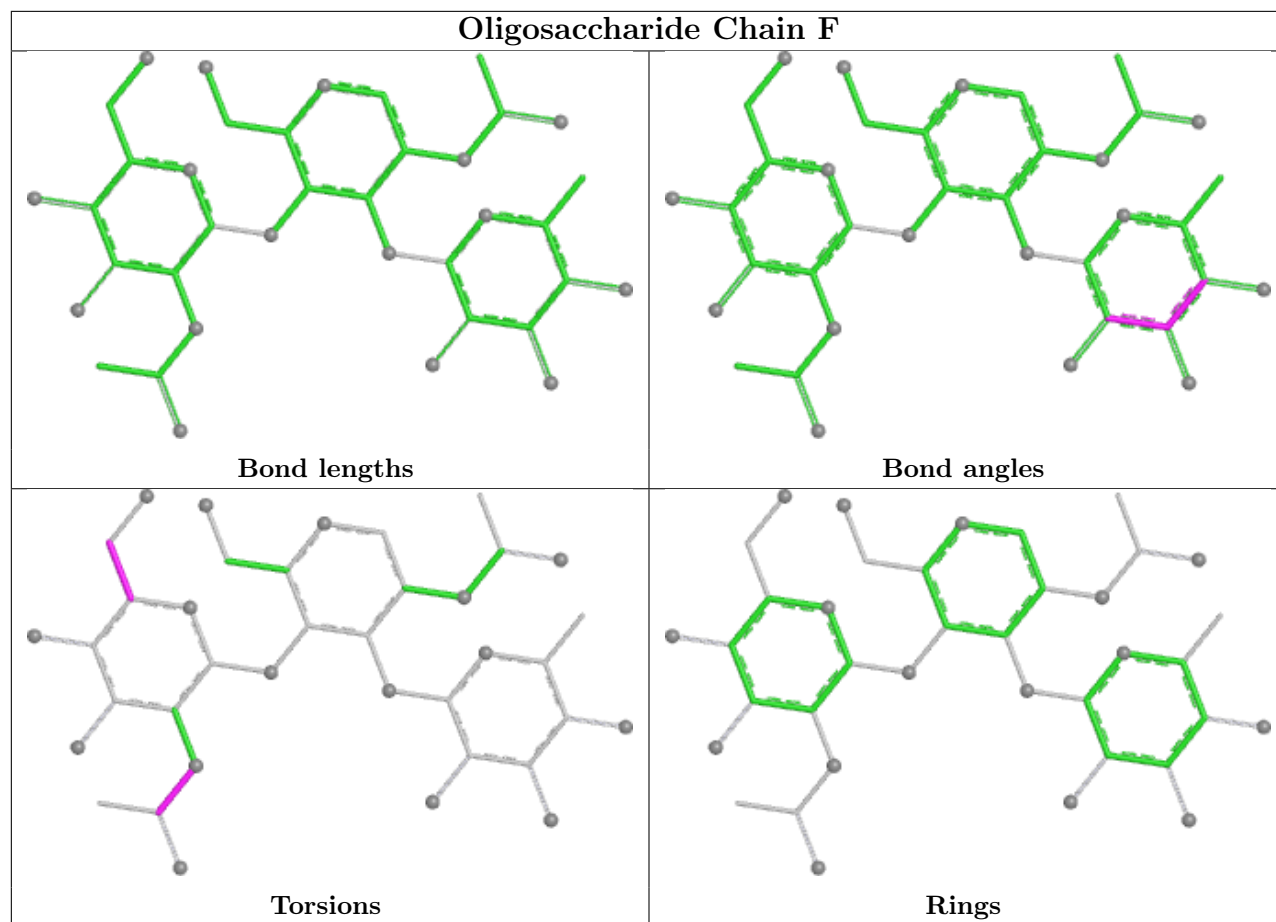
There are no ring outliers.

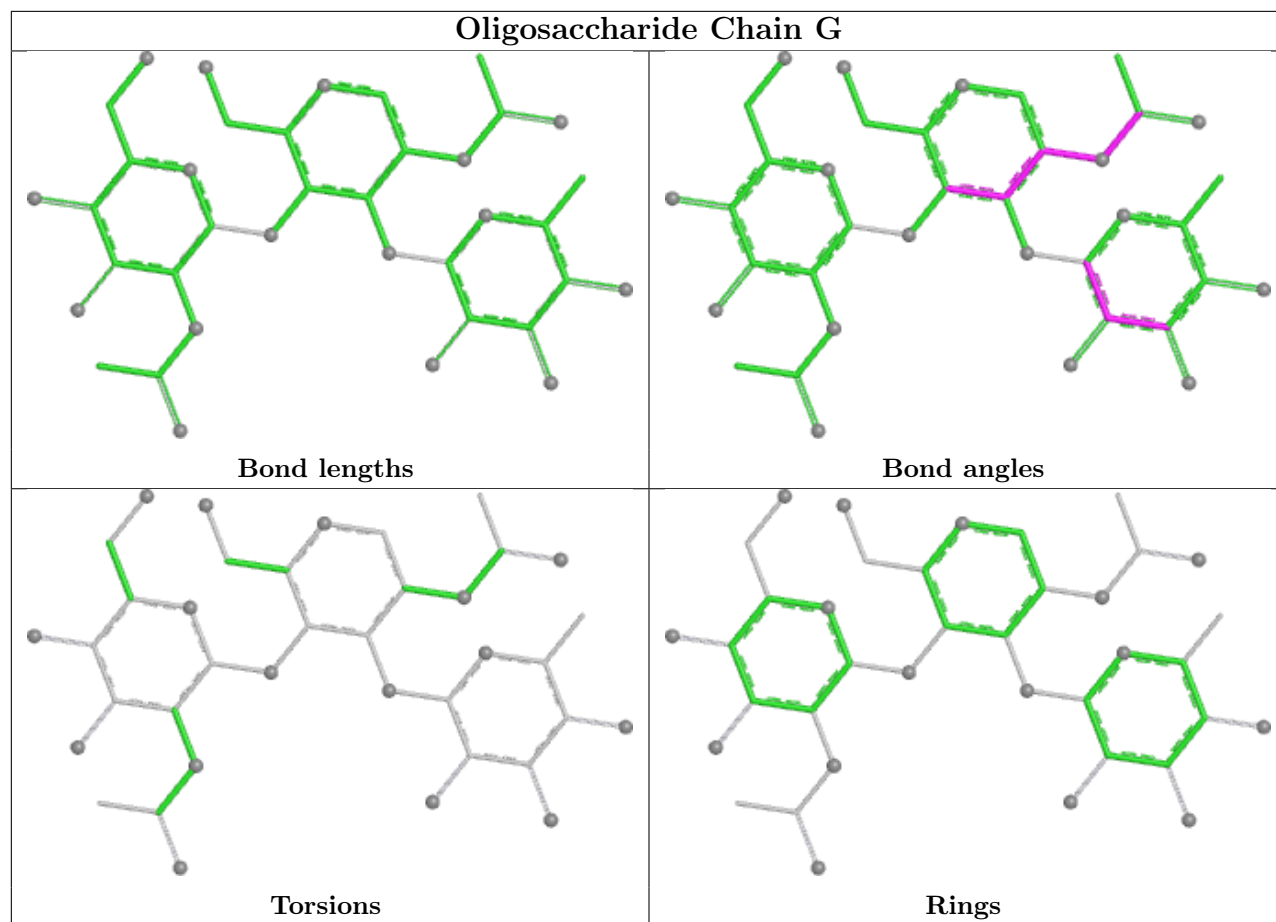
4 monomers are involved in 3 short contacts:

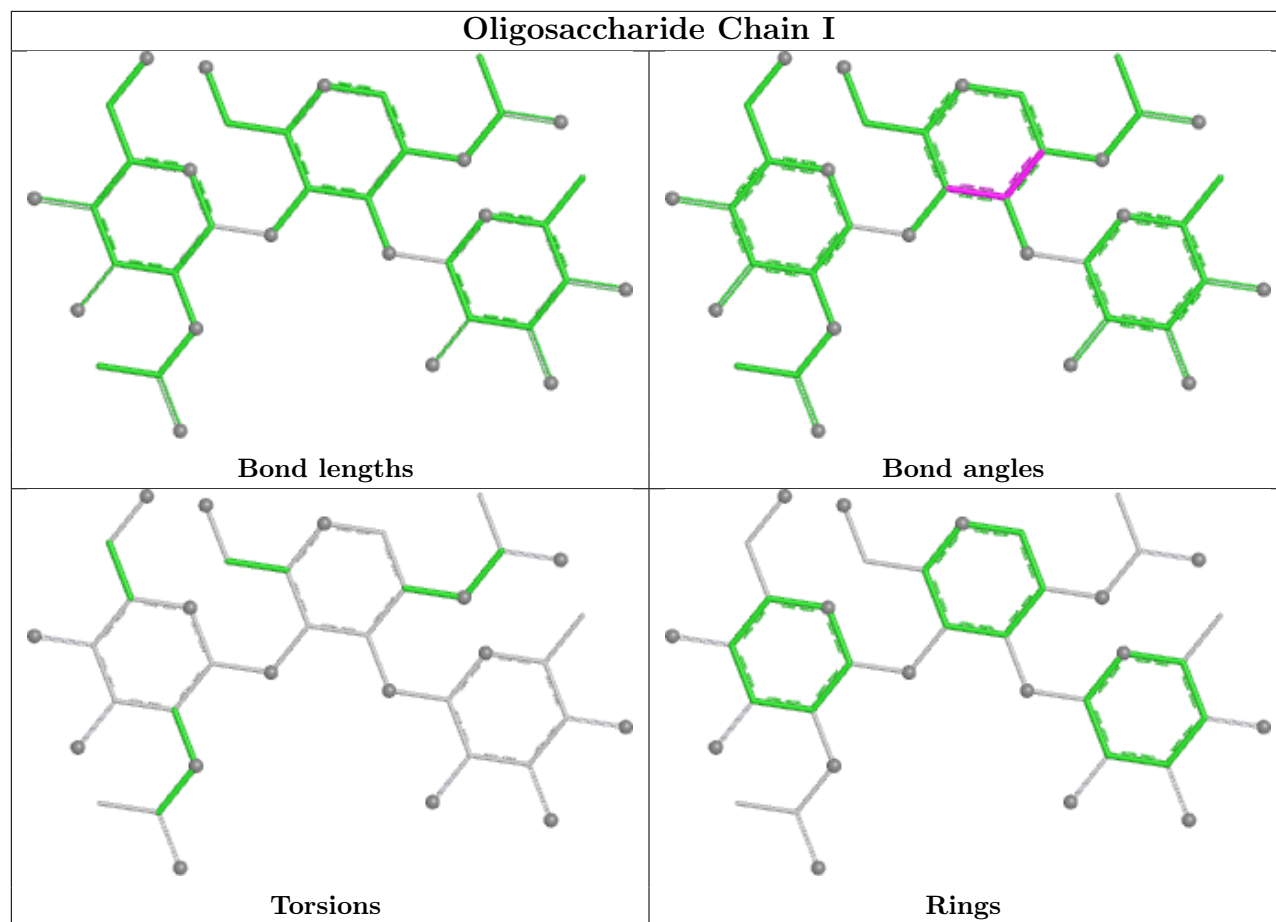
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	FUC	2	0
2	F	3	NAG	2	0
2	I	1	NAG	1	0
2	I	2	FUC	1	0

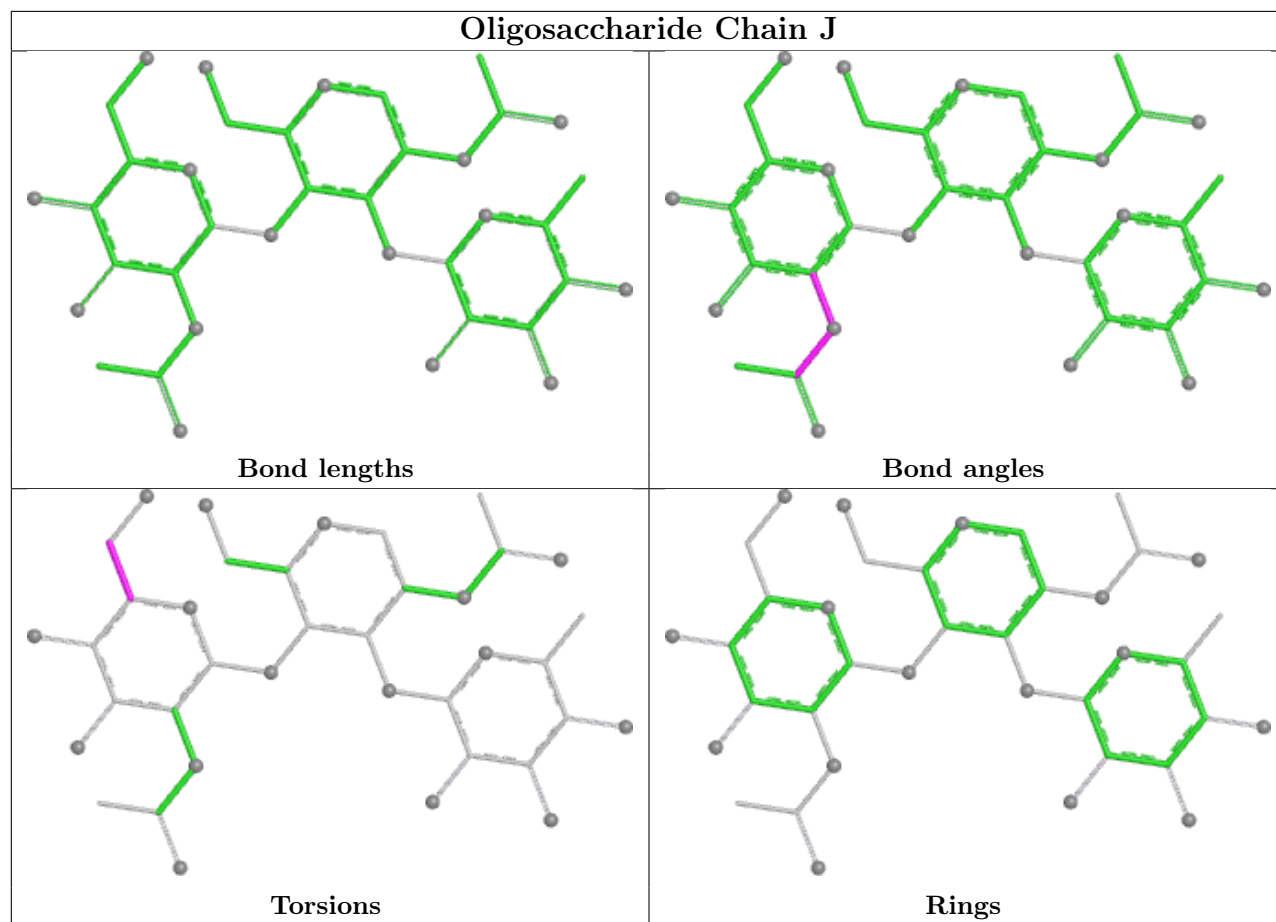
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

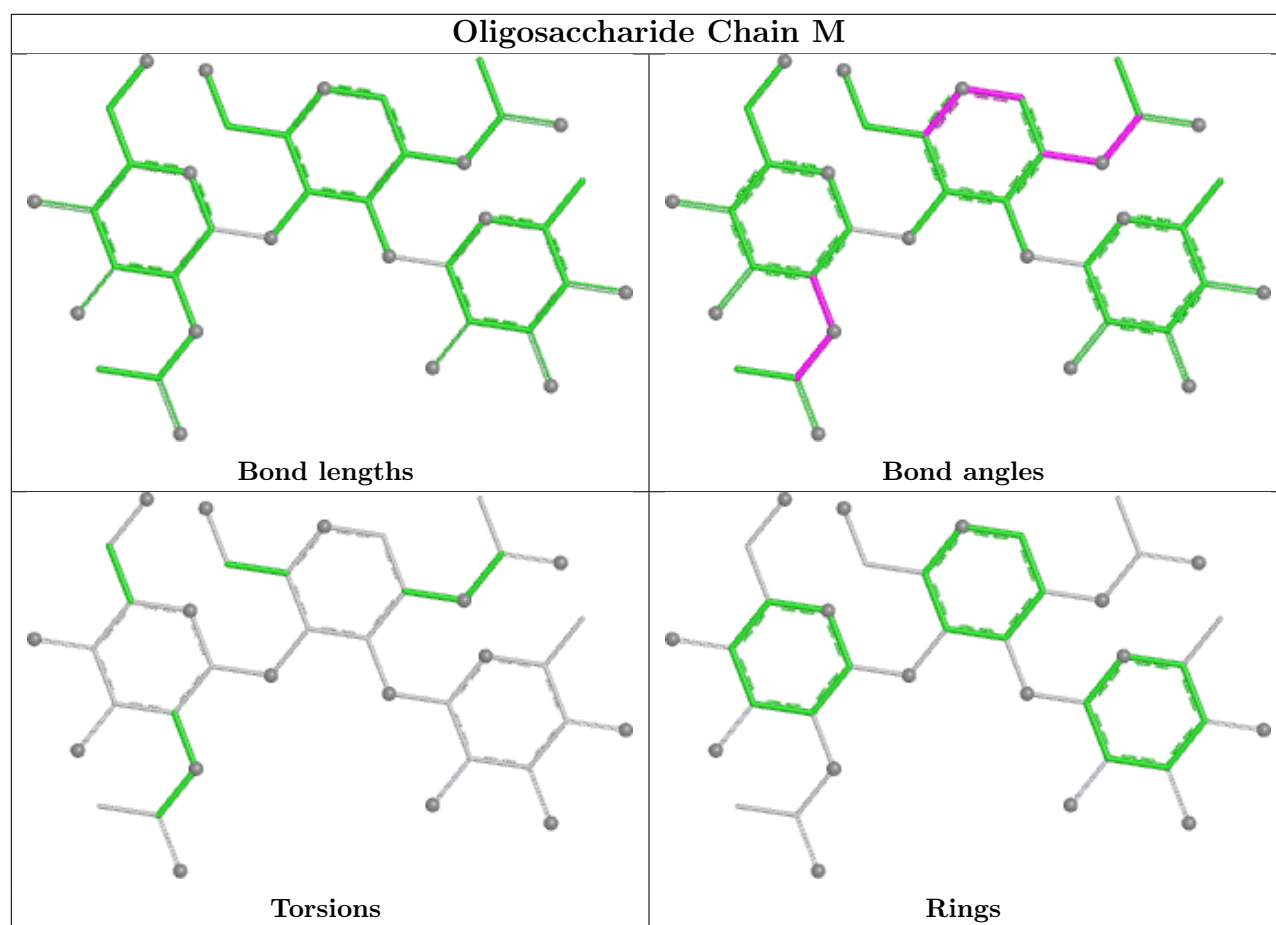




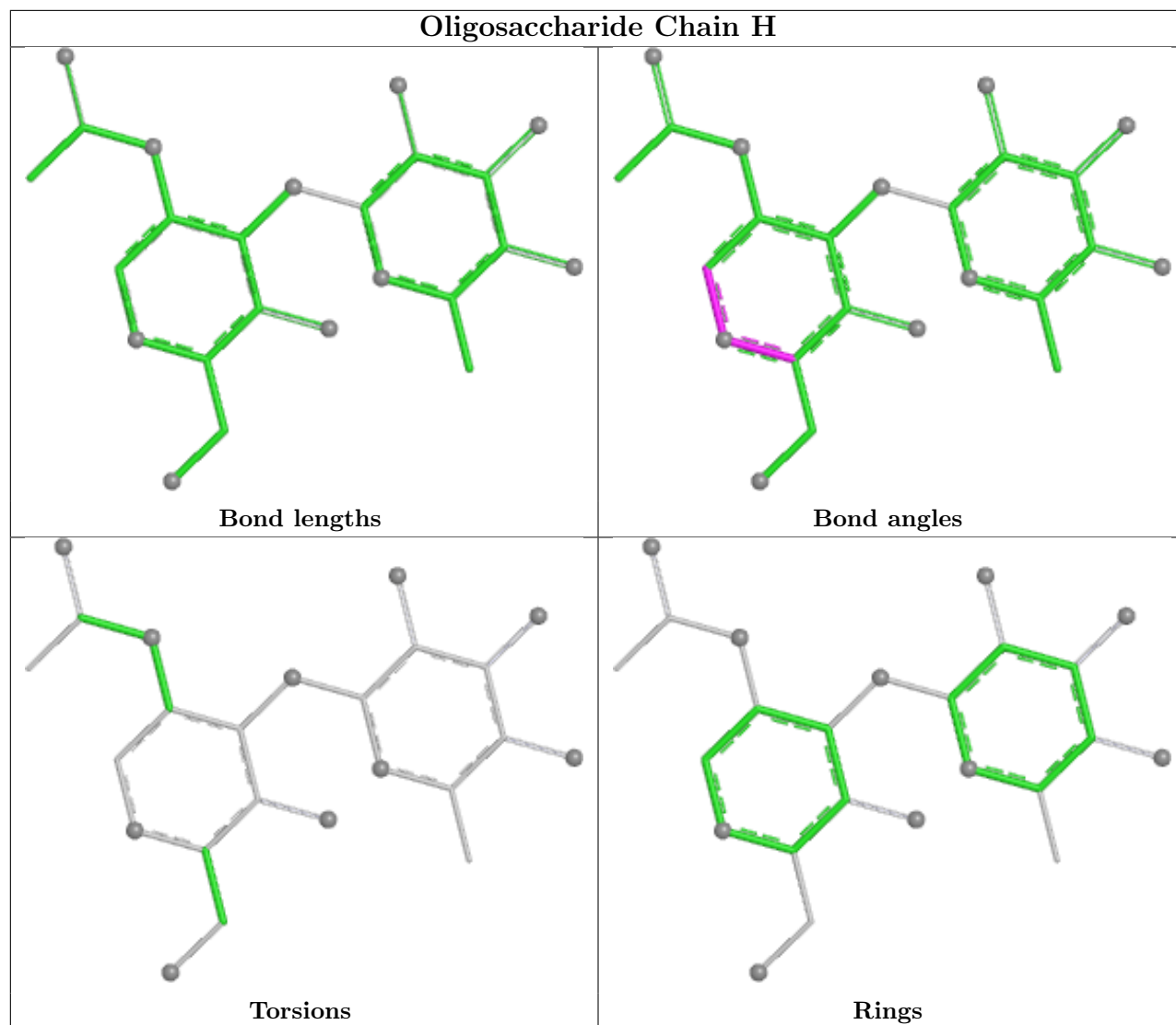


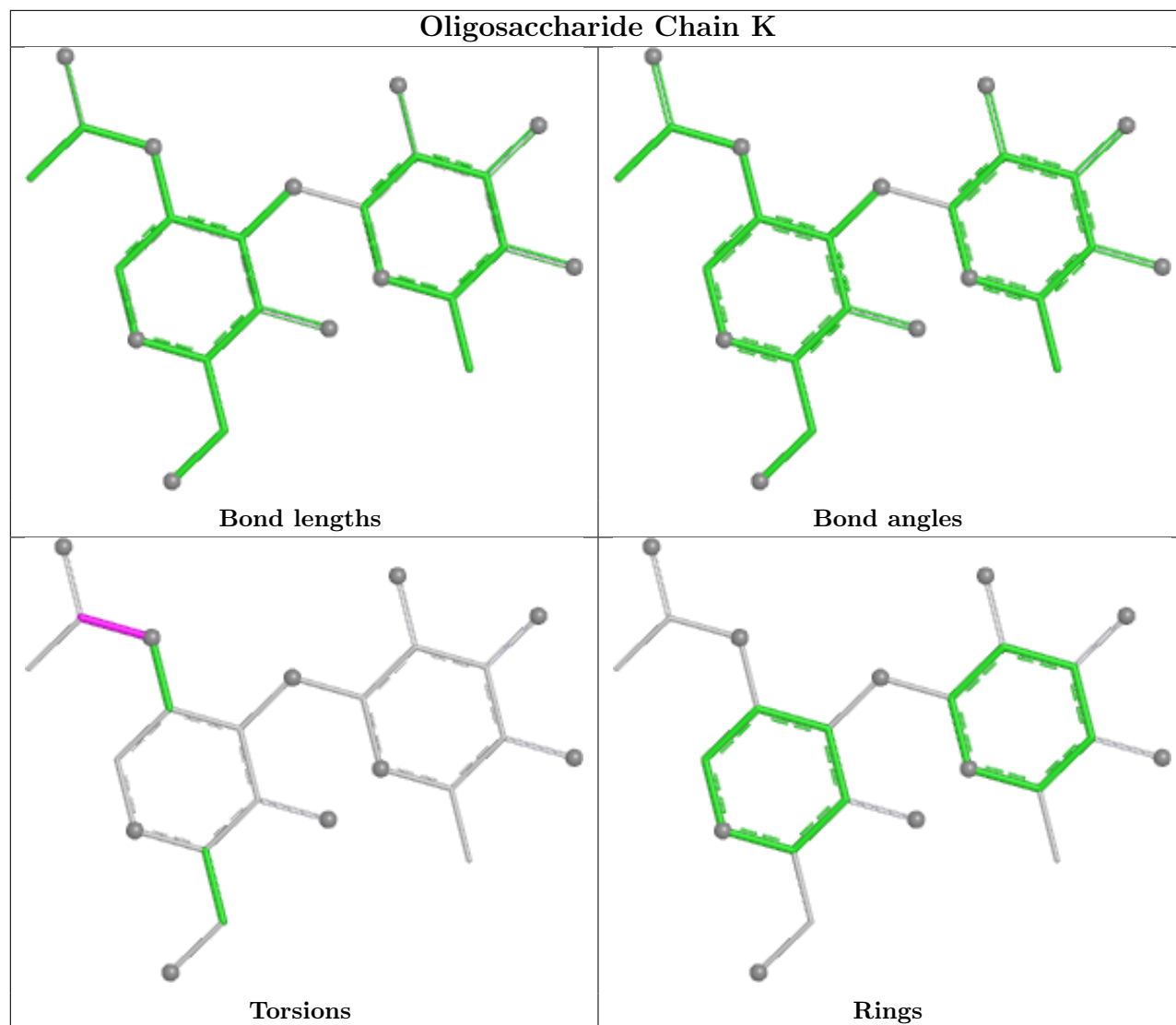


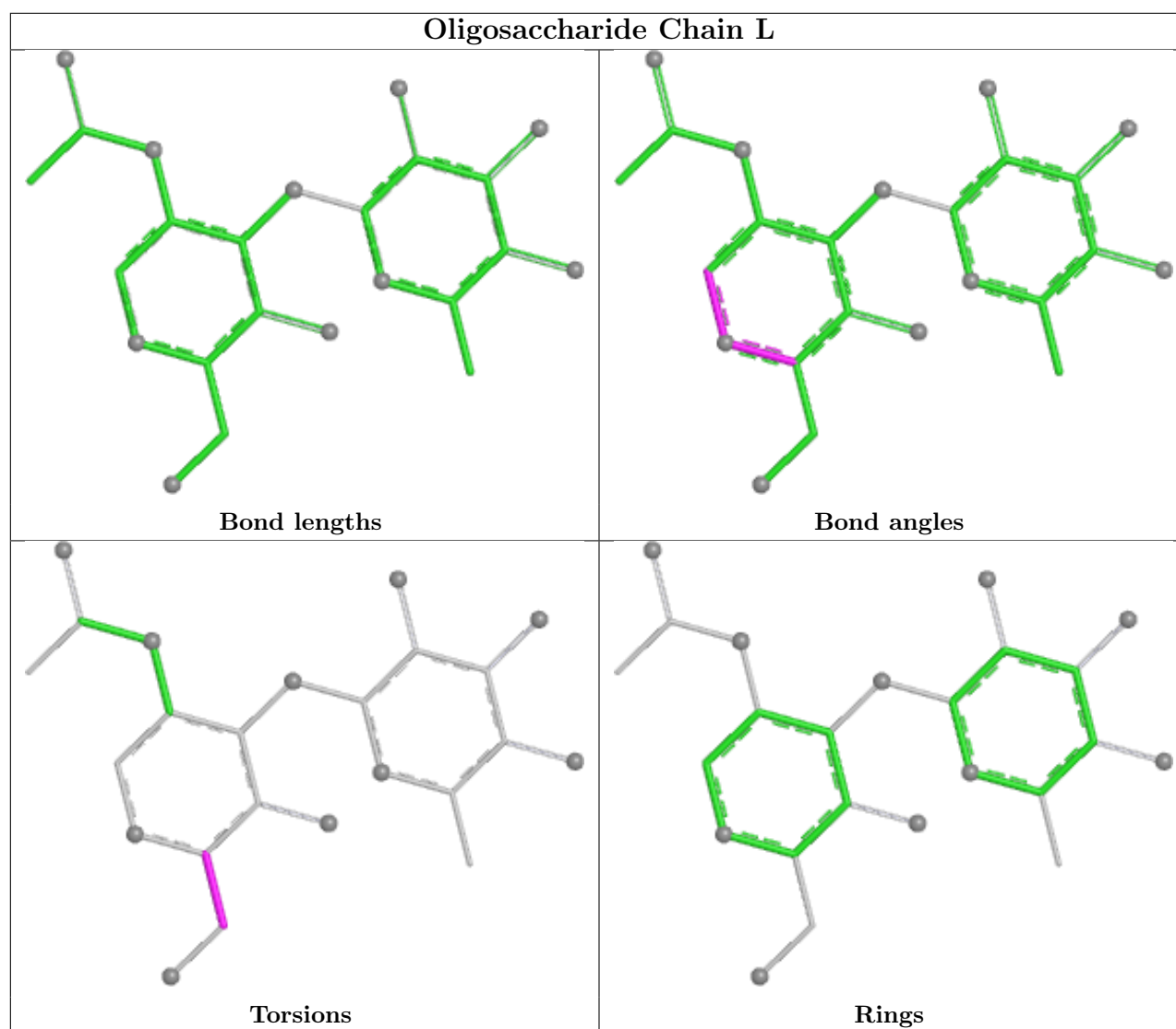




Oligosaccharide Chain H







5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 8 are monoatomic - leaving 25 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	OK7	C	503	5,4	16,16,16	1.10	1 (6%)	22,22,22	3.18	5 (22%)
7	GOL	A	504	-	5,5,5	0.38	0	5,5,5	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	A	508	1	14,14,15	0.50	0	17,19,21	0.78	1 (5%)
10	NAG	B	508	1	14,14,15	0.53	0	17,19,21	0.63	0
10	NAG	C	508	1	14,14,15	0.54	0	17,19,21	1.43	3 (17%)
10	NAG	D	509	1	14,14,15	0.49	0	17,19,21	0.68	0
9	EDO	D	507	-	3,3,3	0.46	0	2,2,2	0.36	0
9	EDO	A	507	-	3,3,3	0.48	0	2,2,2	0.44	0
6	OK7	D	503	5	8,8,16	1.53	2 (25%)	10,10,22	3.82	5 (50%)
8	SO4	B	506	-	4,4,4	0.29	0	6,6,6	0.29	0
9	EDO	D	506	-	3,3,3	0.51	0	2,2,2	0.43	0
10	NAG	D	517	1	14,14,15	0.43	0	17,19,21	1.31	2 (11%)
9	EDO	D	510	-	3,3,3	0.52	0	2,2,2	0.28	0
10	NAG	C	512	1	14,14,15	0.64	0	17,19,21	1.02	1 (5%)
8	SO4	D	505	-	4,4,4	0.29	0	6,6,6	0.22	0
7	GOL	C	504	-	5,5,5	0.39	0	5,5,5	0.37	0
8	SO4	A	505	-	4,4,4	0.26	0	6,6,6	0.20	0
9	EDO	D	508	-	3,3,3	0.55	0	2,2,2	0.16	0
7	GOL	D	504	-	5,5,5	0.30	0	5,5,5	0.47	0
8	SO4	A	506	-	4,4,4	0.32	0	6,6,6	0.15	0
8	SO4	C	505	-	4,4,4	0.29	0	6,6,6	0.10	0
10	NAG	B	507	1	14,14,15	0.47	0	17,19,21	1.41	2 (11%)
6	OK7	B	503	5,4	16,16,16	1.11	2 (12%)	22,22,22	3.48	7 (31%)
6	OK7	A	503	5,4	16,16,16	1.19	2 (12%)	22,22,22	3.58	7 (31%)
9	EDO	D	511	-	3,3,3	0.47	0	2,2,2	0.31	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	OK7	C	503	5,4	-	8/8/8/8	0/2/2/2
7	GOL	A	504	-	-	1/4/4/4	-
10	NAG	A	508	1	-	2/6/23/26	0/1/1/1
10	NAG	B	508	1	-	2/6/23/26	0/1/1/1
10	NAG	C	508	1	-	2/6/23/26	0/1/1/1
10	NAG	D	509	1	-	2/6/23/26	0/1/1/1
9	EDO	D	507	-	-	0/1/1/1	-
9	EDO	A	507	-	-	1/1/1/1	-
6	OK7	D	503	5	-	4/4/4/8	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	D	506	-	-	1/1/1/1	-
10	NAG	D	517	1	-	0/6/23/26	0/1/1/1
9	EDO	D	510	-	-	0/1/1/1	-
10	NAG	C	512	1	-	0/6/23/26	0/1/1/1
7	GOL	C	504	-	-	0/4/4/4	-
9	EDO	D	508	-	-	0/1/1/1	-
7	GOL	D	504	-	-	2/4/4/4	-
10	NAG	B	507	1	-	0/6/23/26	0/1/1/1
6	0K7	B	503	5,4	-	4/8/8/8	0/2/2/2
6	0K7	A	503	5,4	-	6/8/8/8	0/2/2/2
9	EDO	D	511	-	-	1/1/1/1	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	503	0K7	CAH-CAN	2.79	1.41	1.36
6	D	503	0K7	CAH-CAN	2.71	1.41	1.36
6	A	503	0K7	CAH-CAN	2.64	1.41	1.36
6	B	503	0K7	CAH-CAN	2.53	1.40	1.36
6	B	503	0K7	OAC-CAK	-2.33	1.24	1.30

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	503	0K7	CAH-SAJ-CAO	12.58	97.58	89.51
6	B	503	0K7	CAH-SAJ-CAO	11.54	96.91	89.51
6	C	503	0K7	CAH-SAJ-CAO	10.53	96.26	89.51
6	A	503	0K7	SAJ-CAO-NAI	-6.96	107.35	114.22
6	D	503	0K7	CAH-SAJ-CAO	6.56	97.57	89.47

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	503	0K7	OAC-CAK-CAN-NAI
6	A	503	0K7	OAB-CAK-CAN-NAI
6	A	503	0K7	OAC-CAK-CAN-CAH
6	A	503	0K7	OAB-CAK-CAN-CAH
6	B	503	0K7	OAC-CAK-CAN-NAI

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	503	0K7	2	0
10	B	508	NAG	1	0
9	D	507	EDO	1	0
6	D	503	0K7	1	0
9	D	510	EDO	2	0
8	A	505	SO4	1	0
9	D	508	EDO	1	0
7	D	504	GOL	1	0
6	B	503	0K7	4	0
6	A	503	0K7	3	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	424/426 (99%)	-0.94	1 (0%) 91 91	13, 21, 35, 52	1 (0%)
1	B	425/426 (99%)	-0.87	0 100 100	12, 24, 38, 69	3 (0%)
1	C	424/426 (99%)	-0.88	2 (0%) 87 87	12, 23, 38, 75	2 (0%)
1	D	422/426 (99%)	-0.88	0 100 100	16, 22, 36, 72	0
All	All	1695/1704 (99%)	-0.89	3 (0%) 91 91	12, 23, 37, 75	6 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	64	ASN	3.5
1	A	431	SER	2.8
1	C	65	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
3	FUC	K	2	10/11	0.72	0.17	68,79,84,85	0
3	NAG	K	1	14/15	0.75	0.16	42,68,74,84	0
2	FUC	E	2	10/11	0.80	0.14	55,63,69,69	0
2	NAG	F	3	14/15	0.81	0.12	45,55,61,66	0

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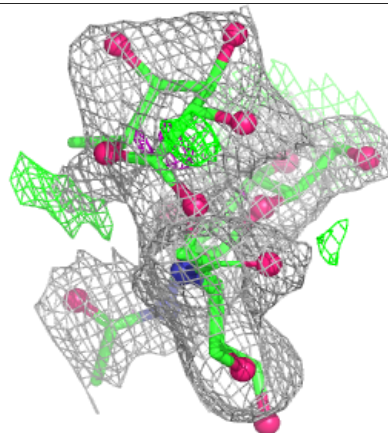
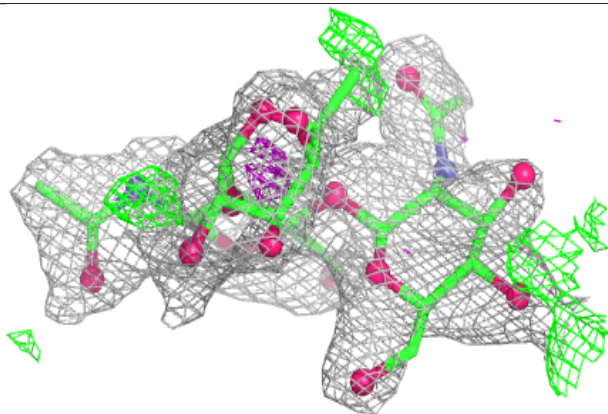
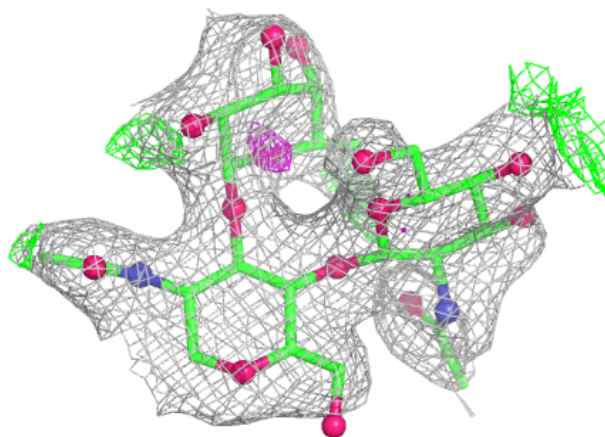
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	E	3	14/15	0.84	0.12	45,55,59,60	0
2	FUC	J	2	10/11	0.84	0.12	46,52,58,61	0
3	FUC	H	2	10/11	0.85	0.12	48,61,65,66	0
3	FUC	L	2	10/11	0.85	0.13	62,70,76,77	0
2	NAG	J	3	14/15	0.86	0.10	29,42,55,69	0
2	FUC	M	2	10/11	0.86	0.11	46,53,57,59	0
3	NAG	L	1	14/15	0.87	0.10	37,46,62,64	0
3	NAG	H	1	14/15	0.88	0.08	37,48,55,57	0
2	FUC	F	2	10/11	0.88	0.10	40,50,56,63	0
2	NAG	I	3	14/15	0.93	0.07	26,31,38,42	0
2	NAG	F	1	14/15	0.94	0.07	29,35,46,49	0
2	NAG	G	3	14/15	0.94	0.07	23,30,35,36	0
2	NAG	M	3	14/15	0.94	0.08	32,49,64,74	0
2	FUC	I	2	10/11	0.95	0.07	28,29,35,41	0
2	FUC	G	2	10/11	0.96	0.06	29,36,39,42	0
2	NAG	E	1	14/15	0.96	0.06	35,41,50,52	0
2	NAG	J	1	14/15	0.97	0.04	23,31,41,50	0
2	NAG	G	1	14/15	0.97	0.06	20,25,30,34	0
2	NAG	I	1	14/15	0.97	0.05	19,24,33,33	0
2	NAG	M	1	14/15	0.97	0.05	24,34,40,47	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.

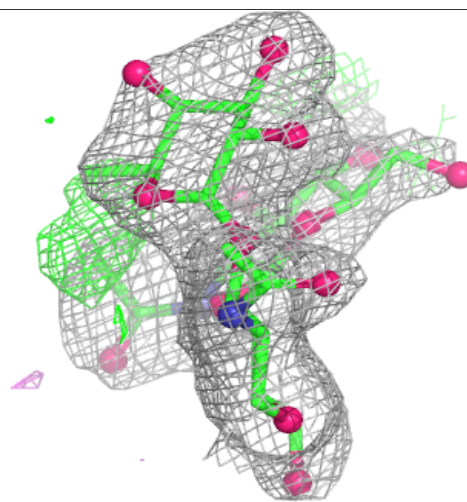
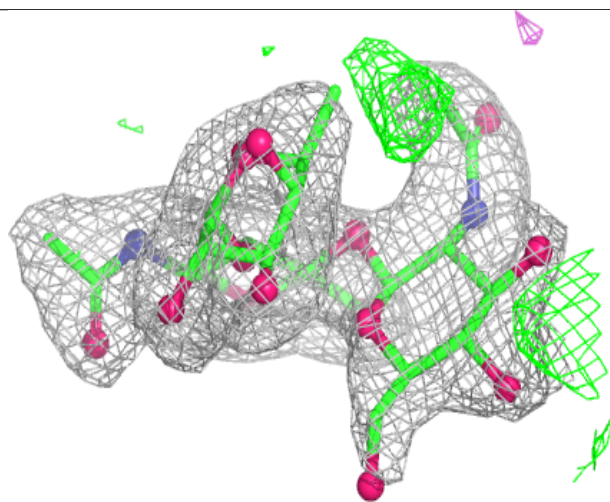
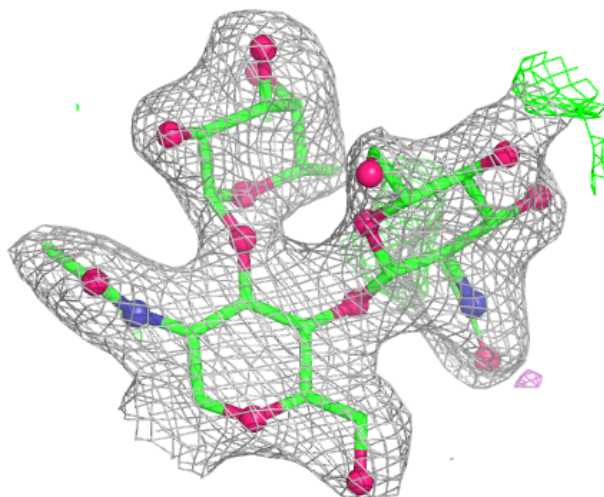
Electron density around Chain E:

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



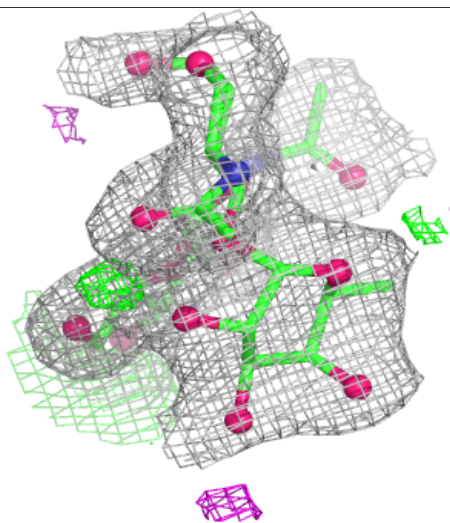
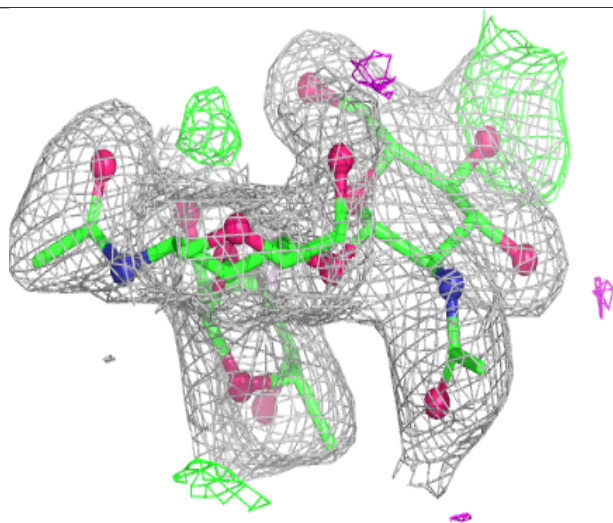
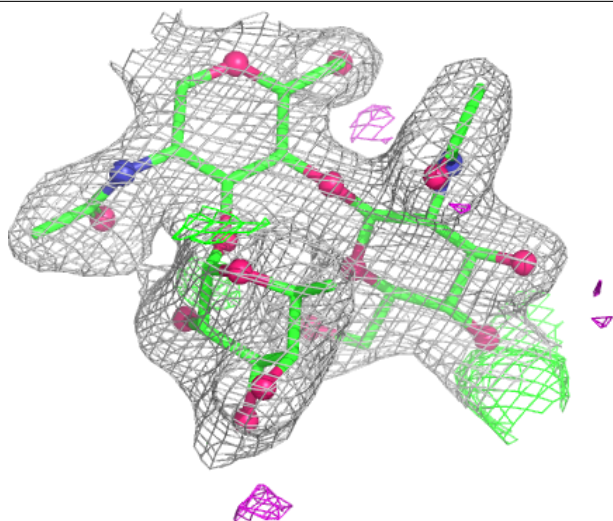
Electron density around Chain F:

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



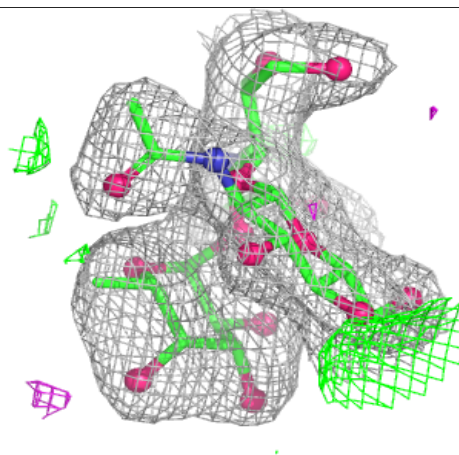
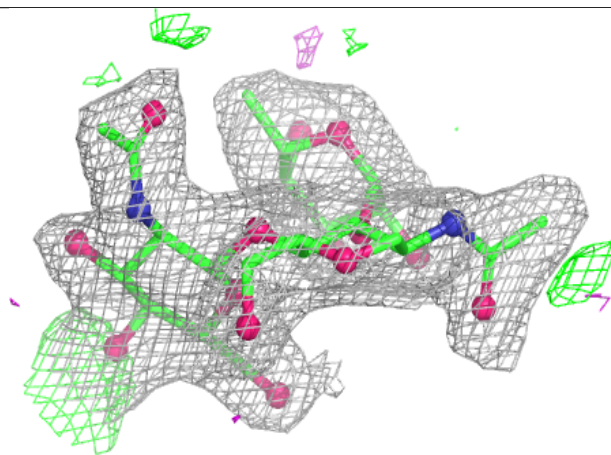
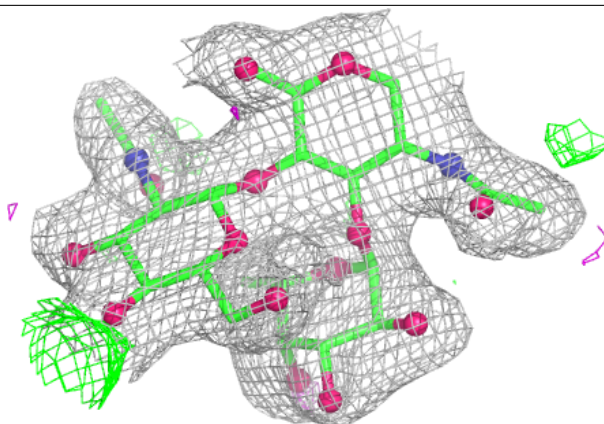
Electron density around Chain G:

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



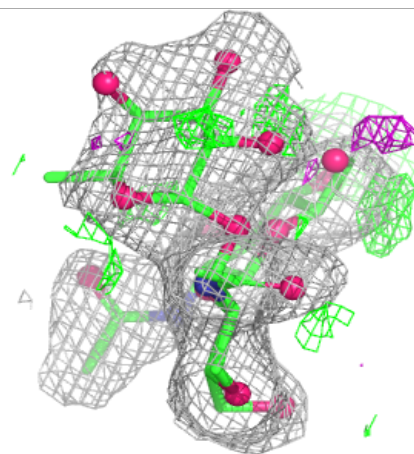
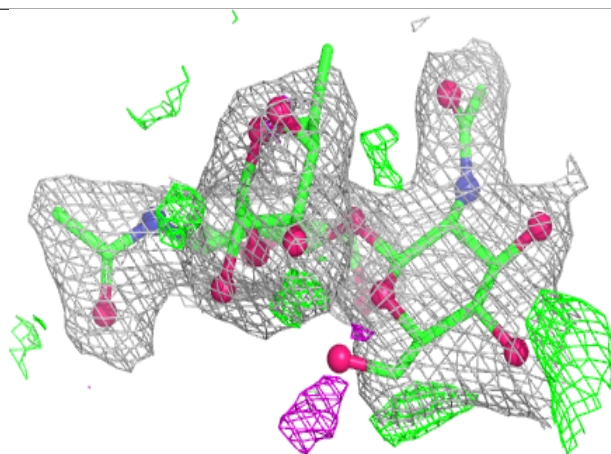
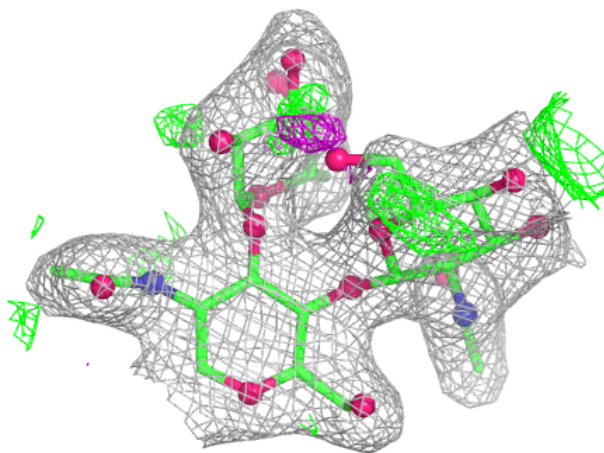
Electron density around Chain I:

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



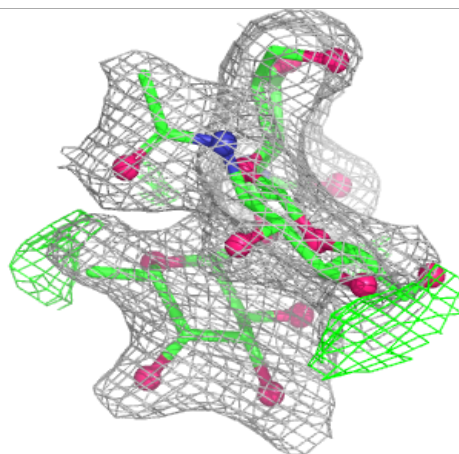
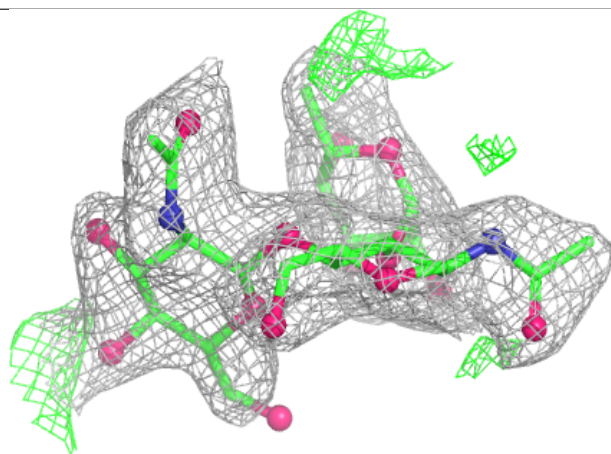
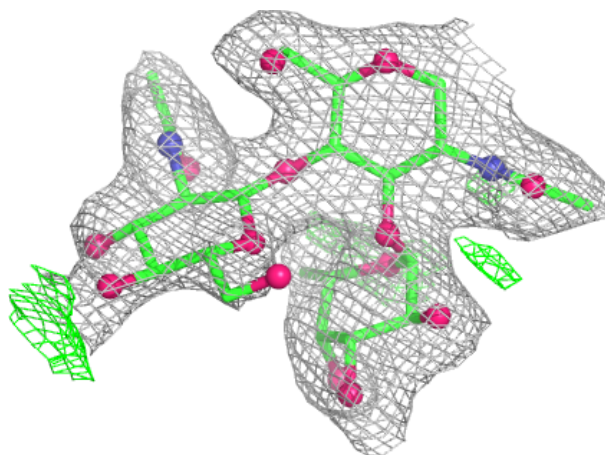
Electron density around Chain J:

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



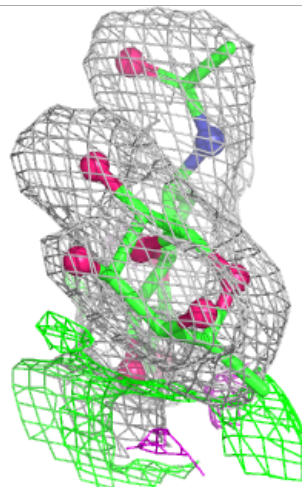
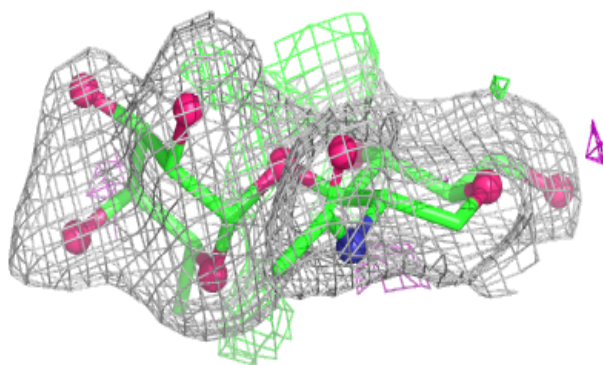
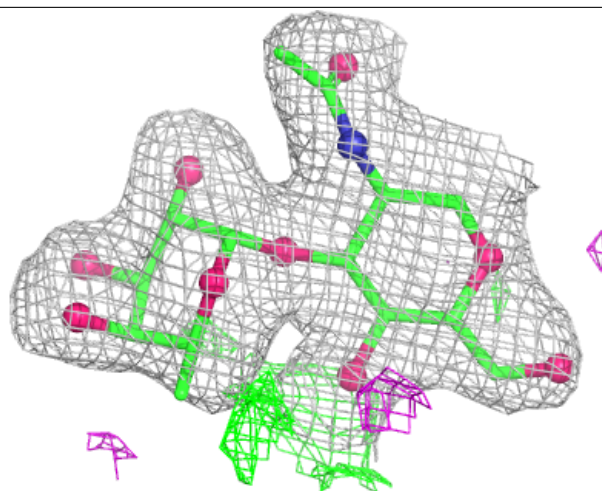
Electron density around Chain M:

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



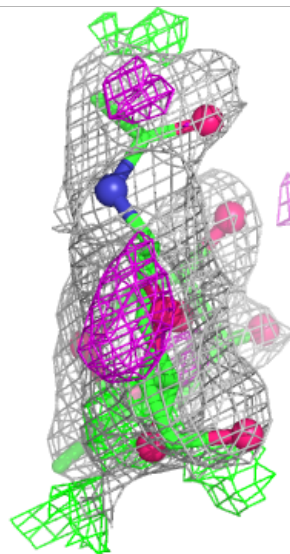
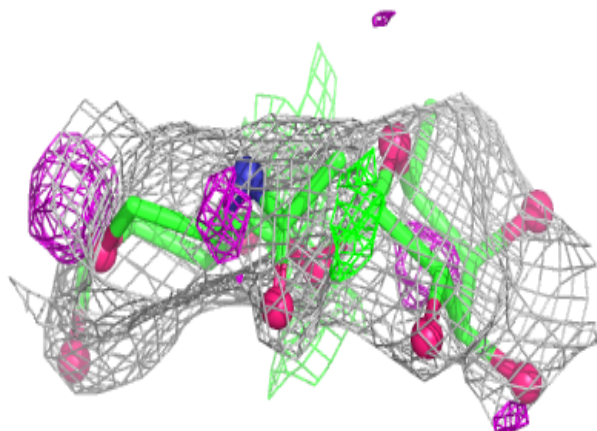
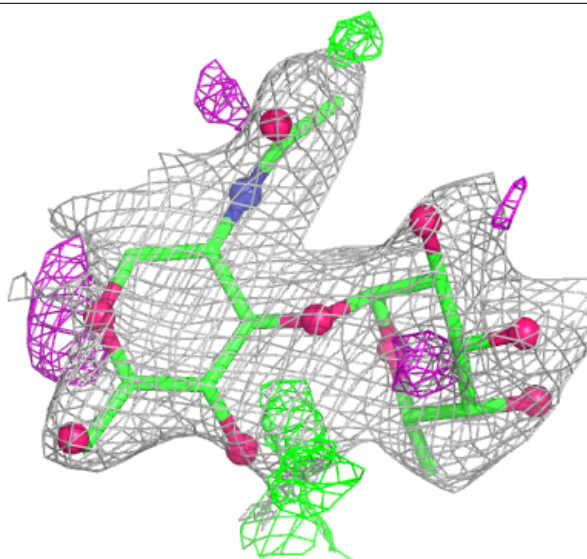
Electron density around Chain H:

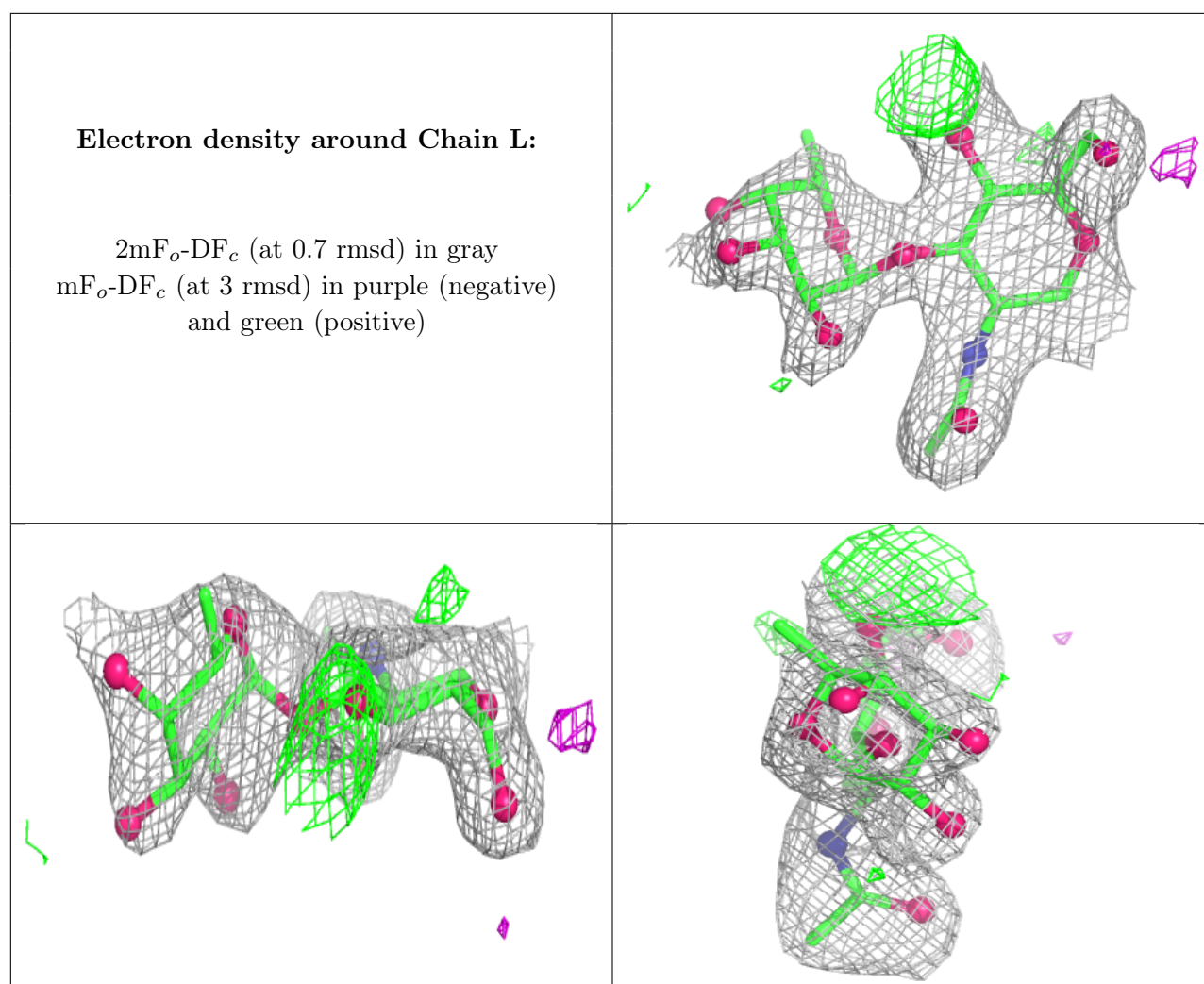
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
9	EDO	D	510	4/4	0.81	0.14	36,40,44,52	0
6	OK7	C	503	15/15	0.83	0.19	33,61,78,78	0
6	OK7	A	503	15/15	0.83	0.17	28,57,70,77	0
10	NAG	C	508	14/15	0.83	0.10	38,42,51,52	0
8	SO4	C	505	5/5	0.85	0.10	58,63,88,95	0
6	OK7	B	503	15/15	0.86	0.16	28,55,70,74	0
6	OK7	D	503	8/15	0.86	0.13	26,40,50,83	0
10	NAG	B	507	14/15	0.87	0.09	33,41,45,47	0
8	SO4	B	506	5/5	0.88	0.12	40,47,60,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	D	504	6/6	0.88	0.12	29,39,43,50	0
9	EDO	D	508	4/4	0.88	0.13	30,33,34,38	0
9	EDO	A	507	4/4	0.90	0.09	30,33,36,37	0
10	NAG	D	517	14/15	0.90	0.08	39,44,48,54	0
9	EDO	D	506	4/4	0.90	0.10	31,32,33,37	0
8	SO4	D	505	5/5	0.94	0.15	30,51,55,57	0
10	NAG	B	508	14/15	0.94	0.06	23,34,40,47	0
9	EDO	D	507	4/4	0.94	0.10	33,33,35,35	0
10	NAG	A	508	14/15	0.94	0.07	16,29,33,42	0
8	SO4	A	506	5/5	0.95	0.13	38,40,55,62	0
10	NAG	D	509	14/15	0.95	0.06	23,29,37,39	0
9	EDO	D	511	4/4	0.96	0.08	28,33,37,39	0
10	NAG	C	512	14/15	0.96	0.06	23,29,37,40	0
7	GOL	C	504	6/6	0.98	0.05	21,23,25,26	0
8	SO4	A	505	5/5	0.99	0.04	29,30,36,43	0
5	FE	A	502	1/1	0.99	0.04	27,27,27,27	0
7	GOL	A	504	6/6	0.99	0.03	17,20,23,23	0
5	FE	B	502	1/1	1.00	0.02	21,21,21,21	1
5	FE	D	502	1/1	1.00	0.02	29,29,29,29	1
5	FE	C	502	1/1	1.00	0.02	28,28,28,28	1
4	ZN	B	501	1/1	1.00	0.03	27,27,27,27	0
4	ZN	D	501	1/1	1.00	0.01	23,23,23,23	1
4	ZN	C	501	1/1	1.00	0.03	30,30,30,30	0
4	ZN	A	501	1/1	1.00	0.02	28,28,28,28	0

6.5 Other polymers

There are no such residues in this entry.