



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 29, 2024 – 08:13 PM EDT

PDB ID : 4DSY
Title : Crystal structure of red kidney bean purple acid phosphatase in complex with Maybridge fragment CC24201
Authors : Feder, D.; Hussein, W.M.; Clayton, D.J.; Kan, M.; Schenk, G.; McGeary, R.P.; Guddat, L.W.
Deposited on : 2012-02-20
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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

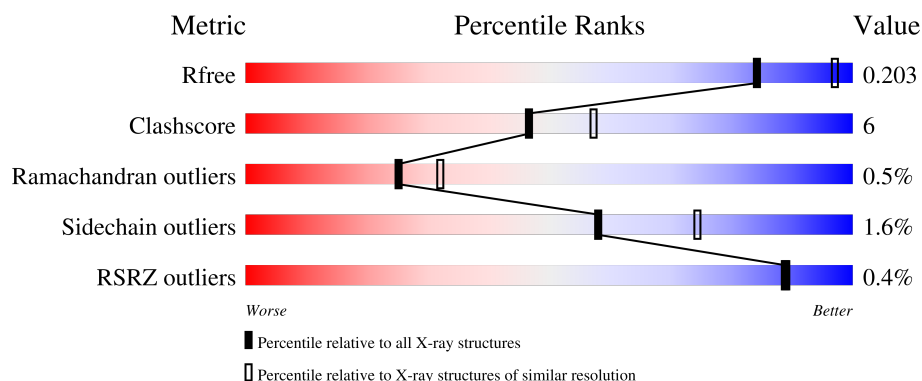
1 Overall quality at a glance

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}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (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	
1	B	426	
1	C	426	
1	D	426	
2	E	3	

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Mol	Chain	Length	Quality of chain
2	F	3	 100%
2	G	3	 67% 33%
2	I	3	 33% 67%
2	K	3	 33% 33% 33%
2	L	3	 33% 33% 33%
2	M	3	 67% 33%
3	H	2	 50% 50%
3	J	2	 50% 50%

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
10	EDO	A	521	-	-	X	-
7	GOL	C	512	-	-	X	-
7	GOL	D	512	-	-	X	-

2 Entry composition [i](#)

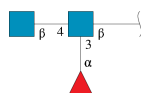
There are 12 unique types of molecules in this entry. The entry contains 16004 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	425	Total	C	N	O	S	0	2	0
			3524	2261	616	637	10			
1	B	426	Total	C	N	O	S	9	1	0
			3519	2258	612	639	10			
1	C	423	Total	C	N	O	S	1	1	0
			3496	2245	609	632	10			
1	D	426	Total	C	N	O	S	5	1	0
			3515	2257	610	637	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	K	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	L	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	J	2	Total	C	N	O	0	0	0
			24	14	1	9			

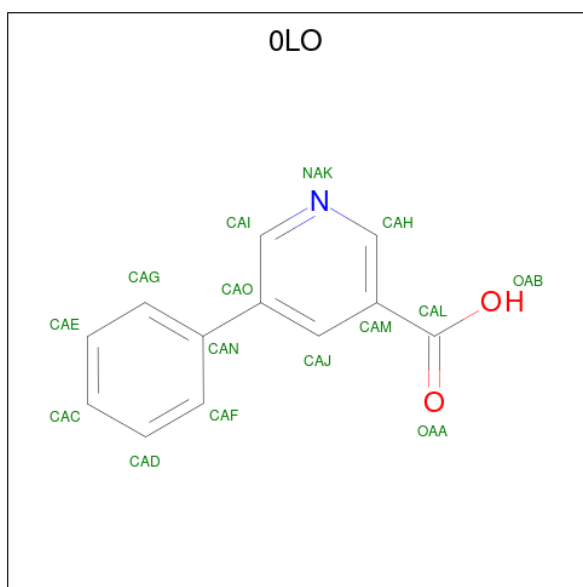
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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	C	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		

- Molecule 5 is FE (III) ION (three-letter code: 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	C	1	Total	Fe	0	0
			1	1		
5	D	1	Total	Fe	0	0
			1	1		

- Molecule 6 is 5-phenylpyridine-3-carboxylic acid (three-letter code: 0LO) (formula: C₁₂H₉NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			15	12	1	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



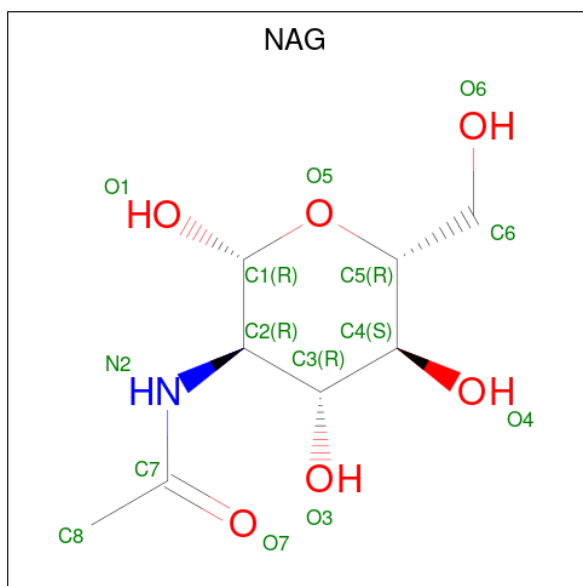
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		

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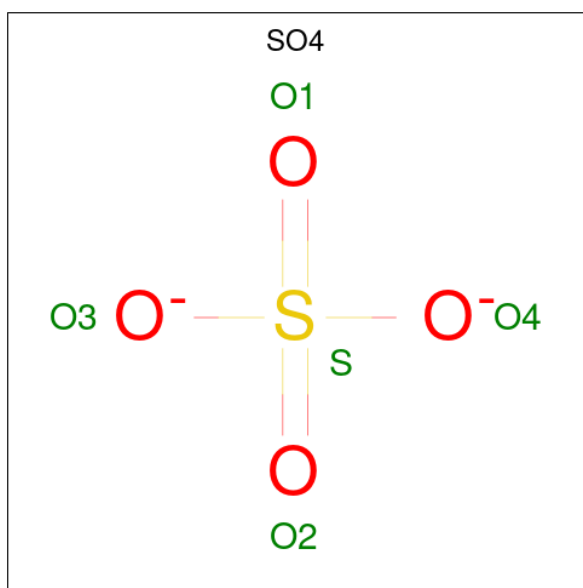
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



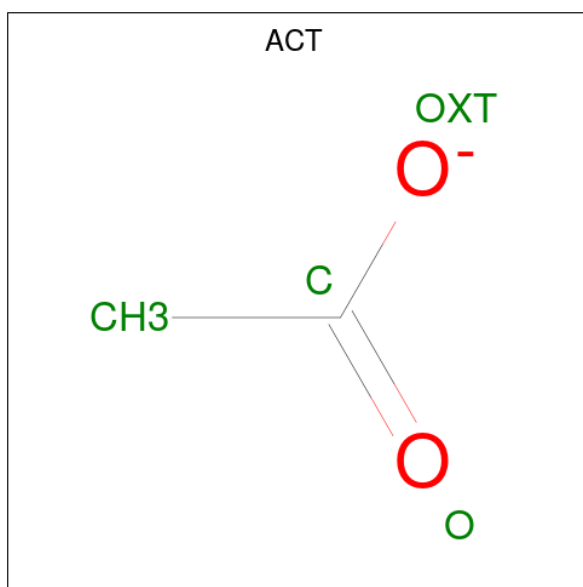
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total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

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 11 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

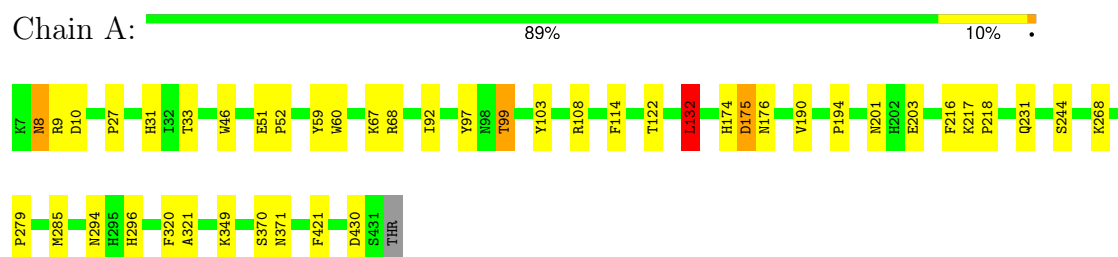
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	377	Total	O	0	0
			377	377		
12	B	322	Total	O	0	0
			322	322		
12	C	305	Total	O	0	0
			305	305		
12	D	354	Total	O	0	0
			354	354		

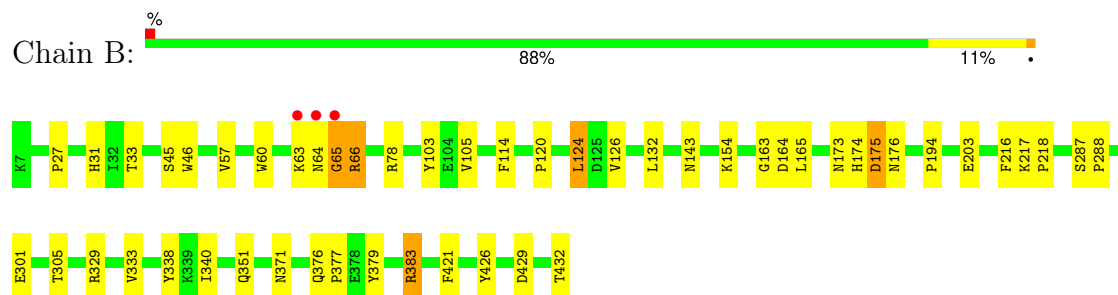
3 Residue-property plots [i](#)

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.

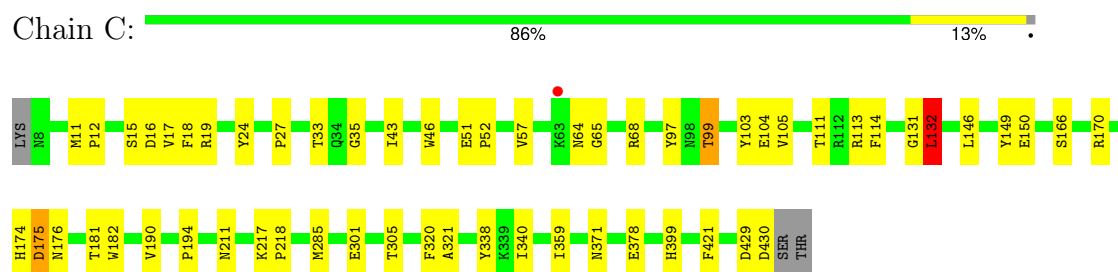
• Molecule 1: Purple acid phosphatase



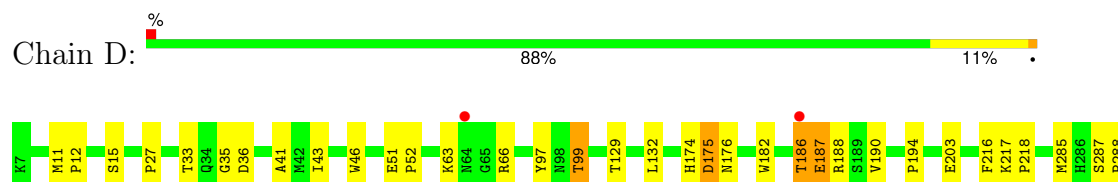
• Molecule 1: Purple acid phosphatase



• 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

Chain E: 100%



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

Chain F: 100%



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

Chain G: 67% 33%



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

Chain I: 33% 67%



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

Chain K: 33% 33% 33%



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

Chain L: 33% 33% 33%



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

Chain M:  67% 33%

MAG1
FUC2
MAG3

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

Chain H:  50% 50%

MAG1
FUC2

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

Chain J:  50% 50%

MAG1
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	127.70Å 127.70Å 299.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.86 – 2.30 19.86 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.86-2.30) 99.7 (19.86-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.30Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.161 , 0.207 0.158 , 0.203	Depositor DCC
R_{free} test set	6316 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16004	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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: ACT, FUC, SO4, ZN, FE, EDO, NAG, GOL, OLO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/3644	0.54	1/4953 (0.0%)
1	B	0.38	0/3638	0.53	1/4946 (0.0%)
1	C	0.38	0/3618	0.52	1/4919 (0.0%)
1	D	0.39	0/3637	0.54	0/4944
All	All	0.39	0/14537	0.53	3/19762 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	132	LEU	CA-CB-CG	-6.63	100.06	115.30
1	A	132	LEU	CA-CB-CG	-5.28	103.16	115.30
1	B	78	ARG	NE-CZ-NH2	-5.06	117.77	120.30

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	3524	0	3339	42	0
1	B	3519	0	3334	35	0
1	C	3496	0	3316	42	0
1	D	3515	0	3336	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	38	0	34	0	0
2	F	38	0	34	1	0
2	G	38	0	34	0	0
2	I	38	0	34	0	0
2	K	38	0	34	1	0
2	L	38	0	34	3	0
2	M	38	0	34	0	0
3	H	24	0	22	0	0
3	J	24	0	22	1	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	2	0
7	A	6	0	8	0	0
7	B	6	0	8	0	0
7	C	6	0	8	4	0
7	D	24	0	32	6	0
8	A	14	0	13	0	0
8	B	28	0	26	1	0
8	C	28	0	26	2	0
8	D	28	0	26	0	0
9	A	20	0	0	0	0
9	B	20	0	0	1	0
9	C	10	0	0	0	0
9	D	5	0	0	0	0
10	A	12	0	18	10	0
10	B	20	0	30	1	0
10	C	8	0	12	1	0
10	D	12	0	18	1	0
11	A	4	0	3	0	0
11	D	4	0	3	0	0
12	A	377	0	0	3	0
12	B	322	0	0	2	0
12	C	305	0	0	2	0
12	D	354	0	0	1	0
All	All	16004	0	13846	160	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 160 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:304:ARG:HH22	7:D:512:GOL:H12	1.17	1.04
1:A:370:SER:H	10:A:521:EDO:H22	1.26	1.00
1:D:304:ARG:NH2	7:D:512:GOL:H12	1.91	0.84
1:D:349:LYS:HD3	1:D:349:LYS:H	1.47	0.80
1:B:217:LYS:HB3	1:B:218:PRO:HD3	1.65	0.78

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	425/426 (100%)	403 (95%)	21 (5%)	1 (0%)	44	55
1	B	425/426 (100%)	400 (94%)	21 (5%)	4 (1%)	14	17
1	C	422/426 (99%)	400 (95%)	21 (5%)	1 (0%)	44	55
1	D	425/426 (100%)	405 (95%)	17 (4%)	3 (1%)	19	23
All	All	1697/1704 (100%)	1608 (95%)	80 (5%)	9 (0%)	25	32

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	63	LYS
1	D	187	GLU
1	B	64	ASN
1	B	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	376/375 (100%)	370 (98%)	6 (2%)	58	74
1	B	376/375 (100%)	370 (98%)	6 (2%)	58	74
1	C	373/375 (100%)	368 (99%)	5 (1%)	65	79
1	D	376/375 (100%)	369 (98%)	7 (2%)	52	69
All	All	1501/1500 (100%)	1477 (98%)	24 (2%)	58	74

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	176	ASN
1	D	66	ARG
1	C	378	GLU
1	D	99	THR
1	B	66	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	211	ASN
1	C	224	HIS
1	D	401	HIS
1	C	295	HIS
1	A	371	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 ⓘ

25 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	0.56	0	17,19,21	0.98	0
2	FUC	E	2	2	10,10,11	0.63	0	14,14,16	0.51	0
2	NAG	E	3	2	14,14,15	0.53	0	17,19,21	0.75	0
2	NAG	F	1	2,1	14,14,15	0.56	0	17,19,21	1.03	2 (11%)
2	FUC	F	2	2	10,10,11	0.65	0	14,14,16	0.60	0
2	NAG	F	3	2	14,14,15	0.55	0	17,19,21	0.79	0
2	NAG	G	1	2,1	14,14,15	0.77	0	17,19,21	1.23	2 (11%)
2	FUC	G	2	2	10,10,11	0.66	0	14,14,16	0.37	0
2	NAG	G	3	2	14,14,15	0.46	0	17,19,21	0.77	0
3	NAG	H	1	1,3	14,14,15	0.47	0	17,19,21	0.82	1 (5%)
3	FUC	H	2	3	10,10,11	0.64	0	14,14,16	0.56	0
2	NAG	I	1	2,1	14,14,15	0.56	0	17,19,21	0.97	1 (5%)
2	FUC	I	2	2	10,10,11	0.67	0	14,14,16	0.61	0
2	NAG	I	3	2	14,14,15	0.54	0	17,19,21	1.09	2 (11%)
3	NAG	J	1	1,3	14,14,15	0.58	0	17,19,21	0.84	0
3	FUC	J	2	3	10,10,11	0.62	0	14,14,16	0.51	0
2	NAG	K	1	2,1	14,14,15	0.66	0	17,19,21	1.08	1 (5%)
2	FUC	K	2	2	10,10,11	0.55	0	14,14,16	0.87	0
2	NAG	K	3	2	14,14,15	0.61	0	17,19,21	0.99	1 (5%)
2	NAG	L	1	2,1	14,14,15	0.55	0	17,19,21	0.81	0
2	FUC	L	2	2	10,10,11	0.67	0	14,14,16	0.83	0
2	NAG	L	3	2	14,14,15	0.47	0	17,19,21	1.11	2 (11%)
2	NAG	M	1	2,1	14,14,15	0.47	0	17,19,21	0.67	0
2	FUC	M	2	2	10,10,11	0.63	0	14,14,16	0.59	0
2	NAG	M	3	2	14,14,15	0.66	0	17,19,21	0.96	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	-	0/6/23/26	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	-	1/6/23/26	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	-	2/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	FUC	J	2	3	-	-	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	FUC	K	2	2	-	-	0/1/1/1
2	NAG	K	3	2	-	1/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	FUC	L	2	2	-	-	0/1/1/1
2	NAG	L	3	2	-	3/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	2/6/23/26	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 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	NAG	C2-N2-C7	-3.15	118.68	122.90
2	K	3	NAG	C2-N2-C7	-2.98	118.91	122.90
2	G	1	NAG	C3-C4-C5	-2.78	105.19	110.23
2	F	1	NAG	C2-N2-C7	-2.67	119.32	122.90
2	M	3	NAG	C2-N2-C7	-2.59	119.43	122.90

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

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

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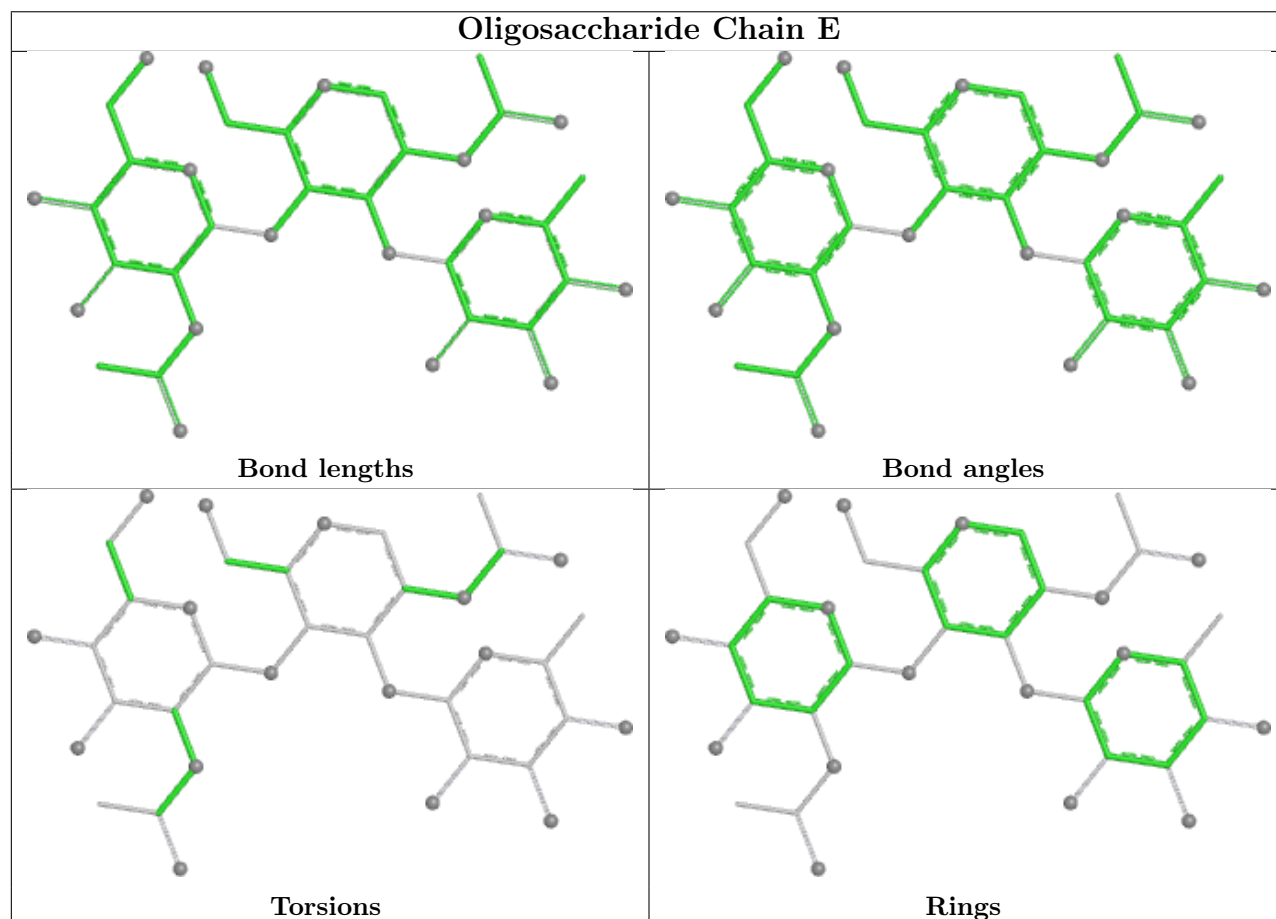
Mol	Chain	Res	Type	Atoms
2	F	3	NAG	C4-C5-C6-O6
2	F	3	NAG	C8-C7-N2-C2
2	F	3	NAG	O7-C7-N2-C2
2	I	3	NAG	O5-C5-C6-O6

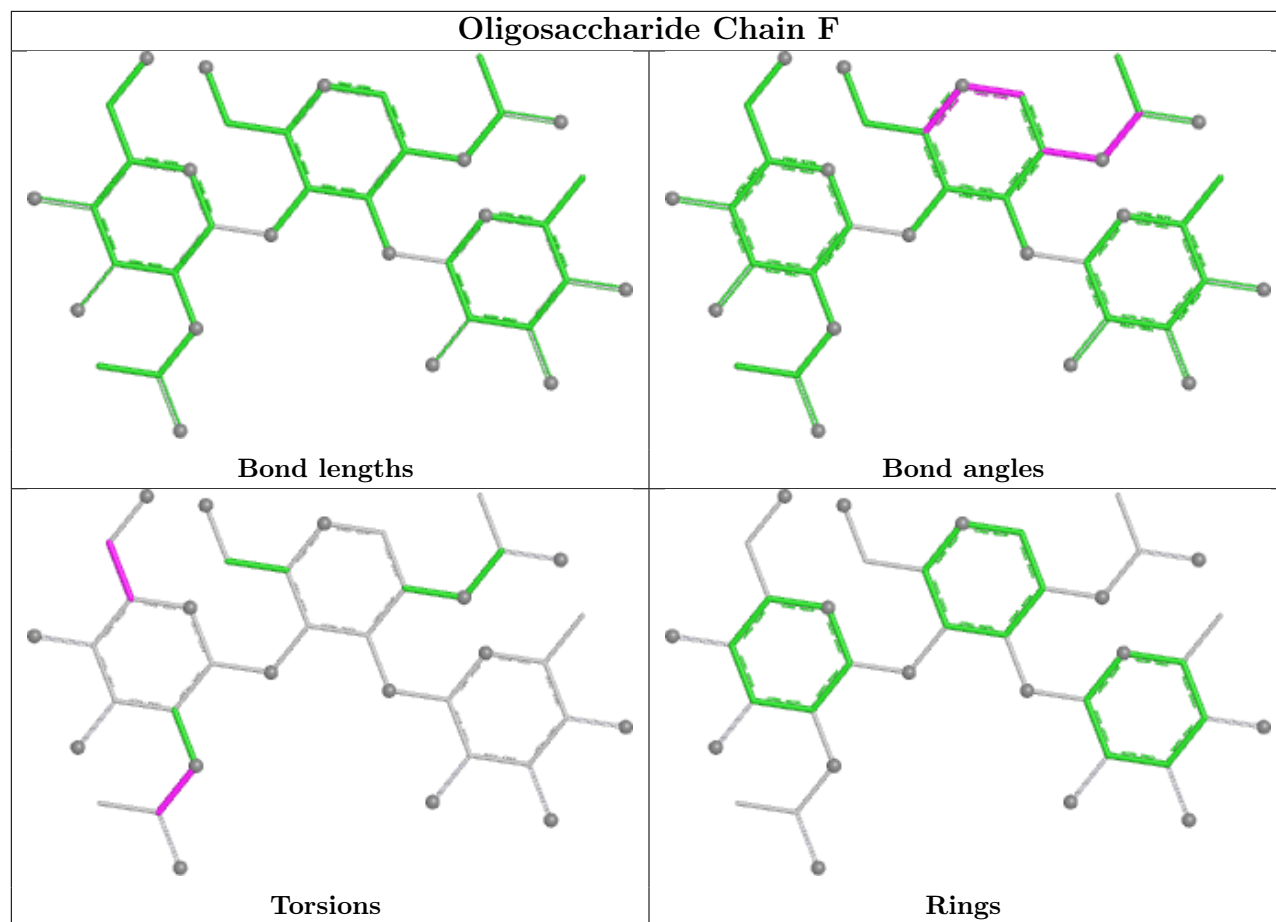
There are no ring outliers.

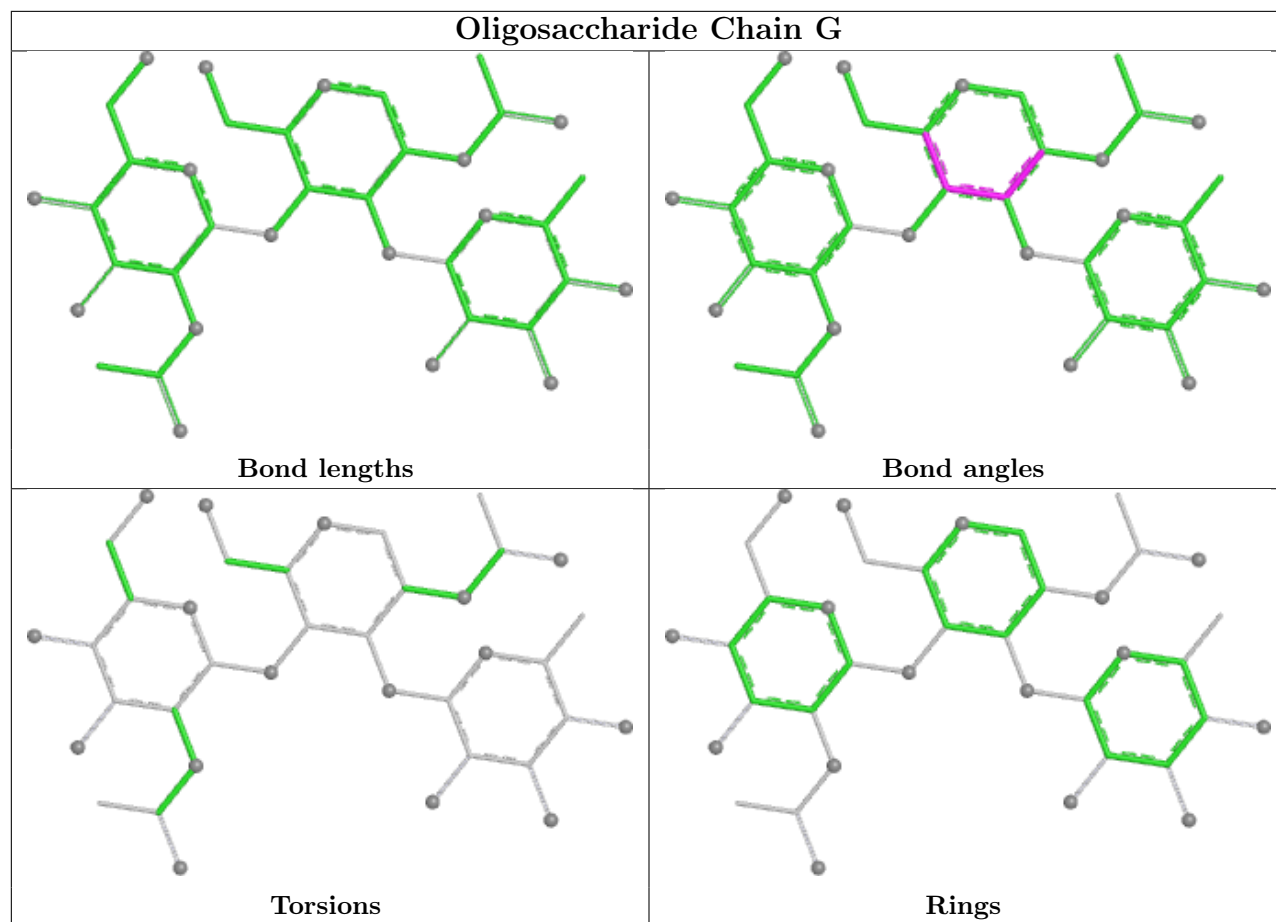
6 monomers are involved in 6 short contacts:

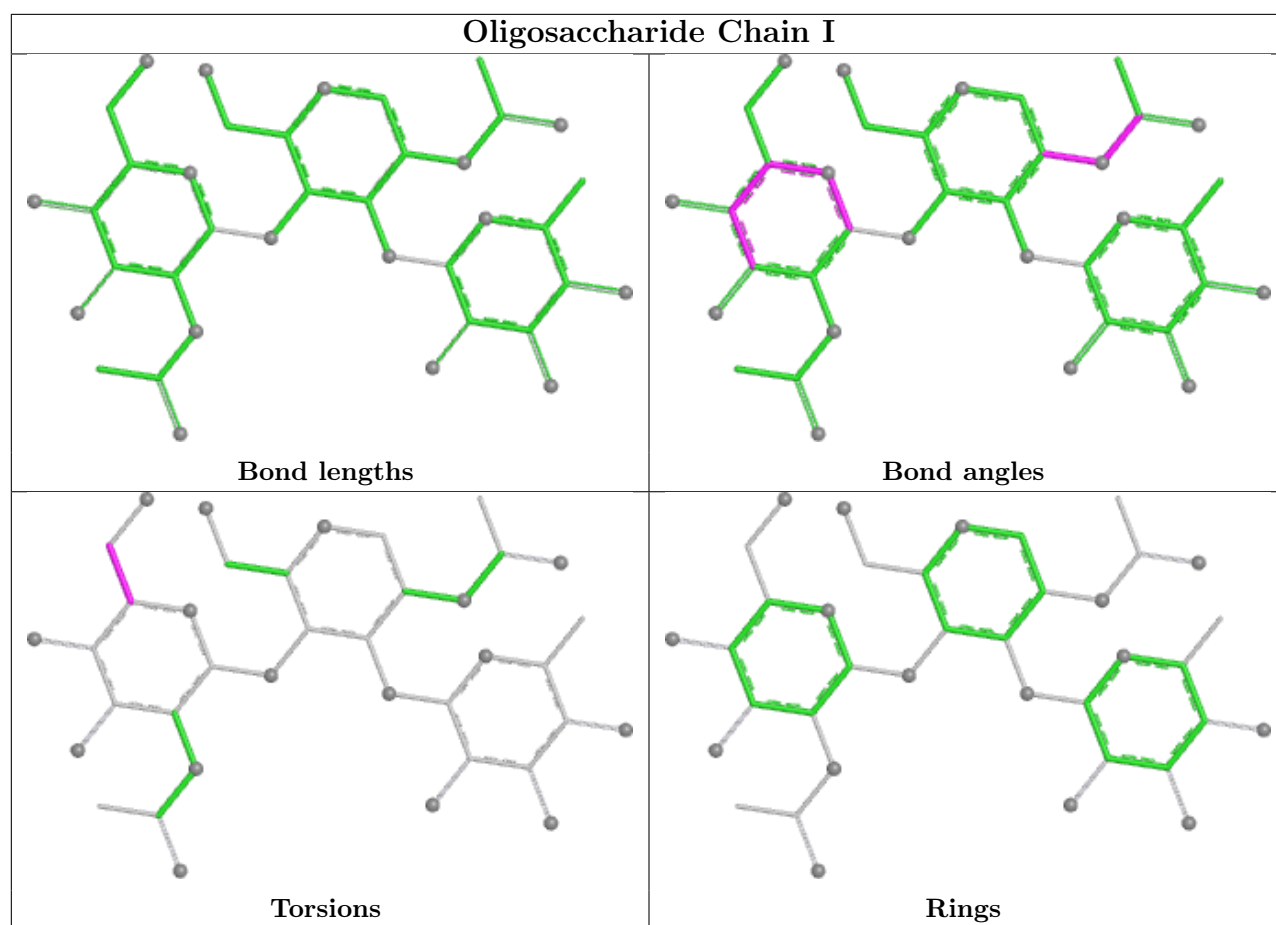
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	FUC	1	0
2	L	3	NAG	3	0
3	J	1	NAG	1	0
2	K	1	NAG	1	0
2	L	2	FUC	3	0
2	F	3	NAG	1	0

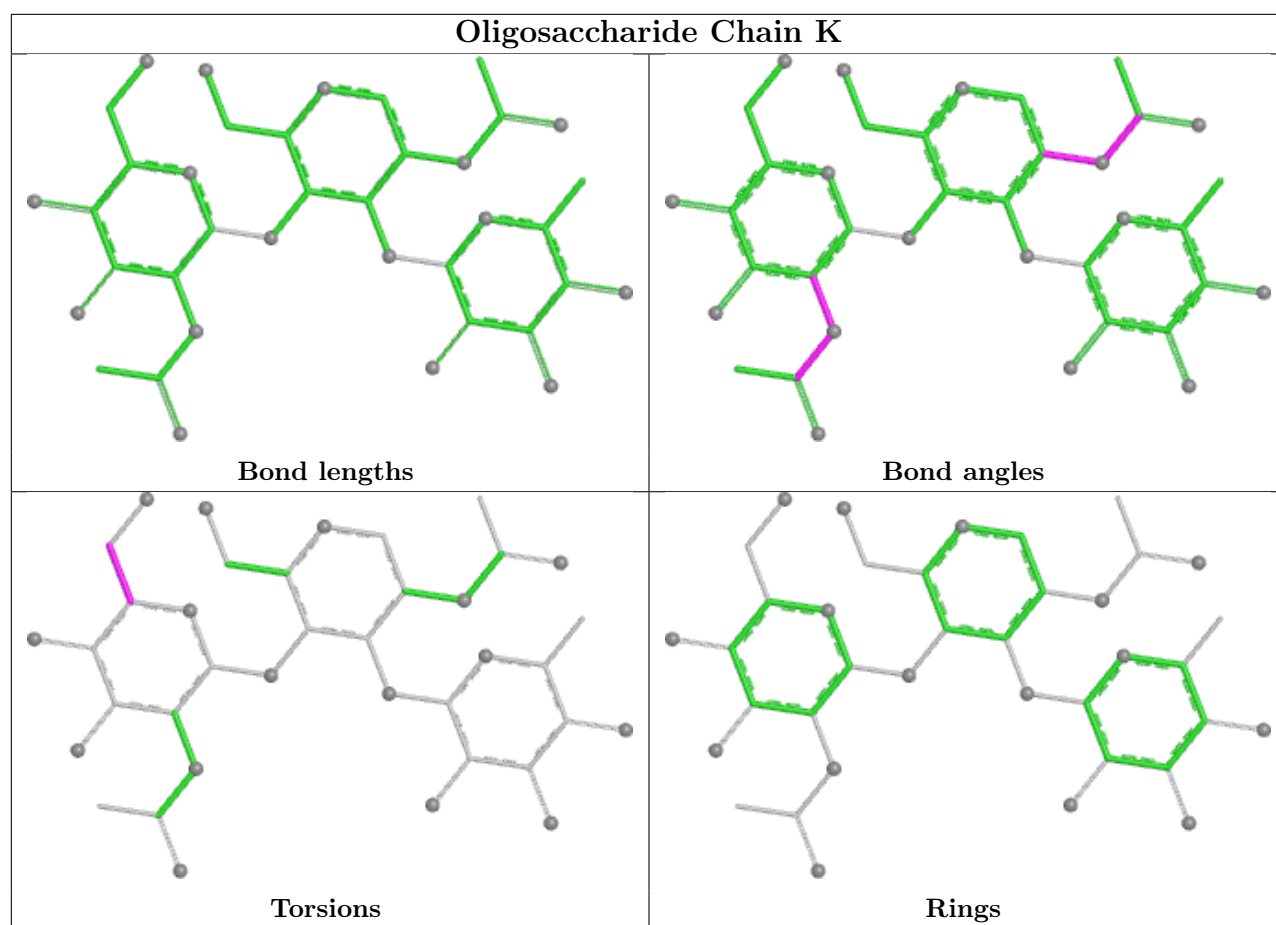
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

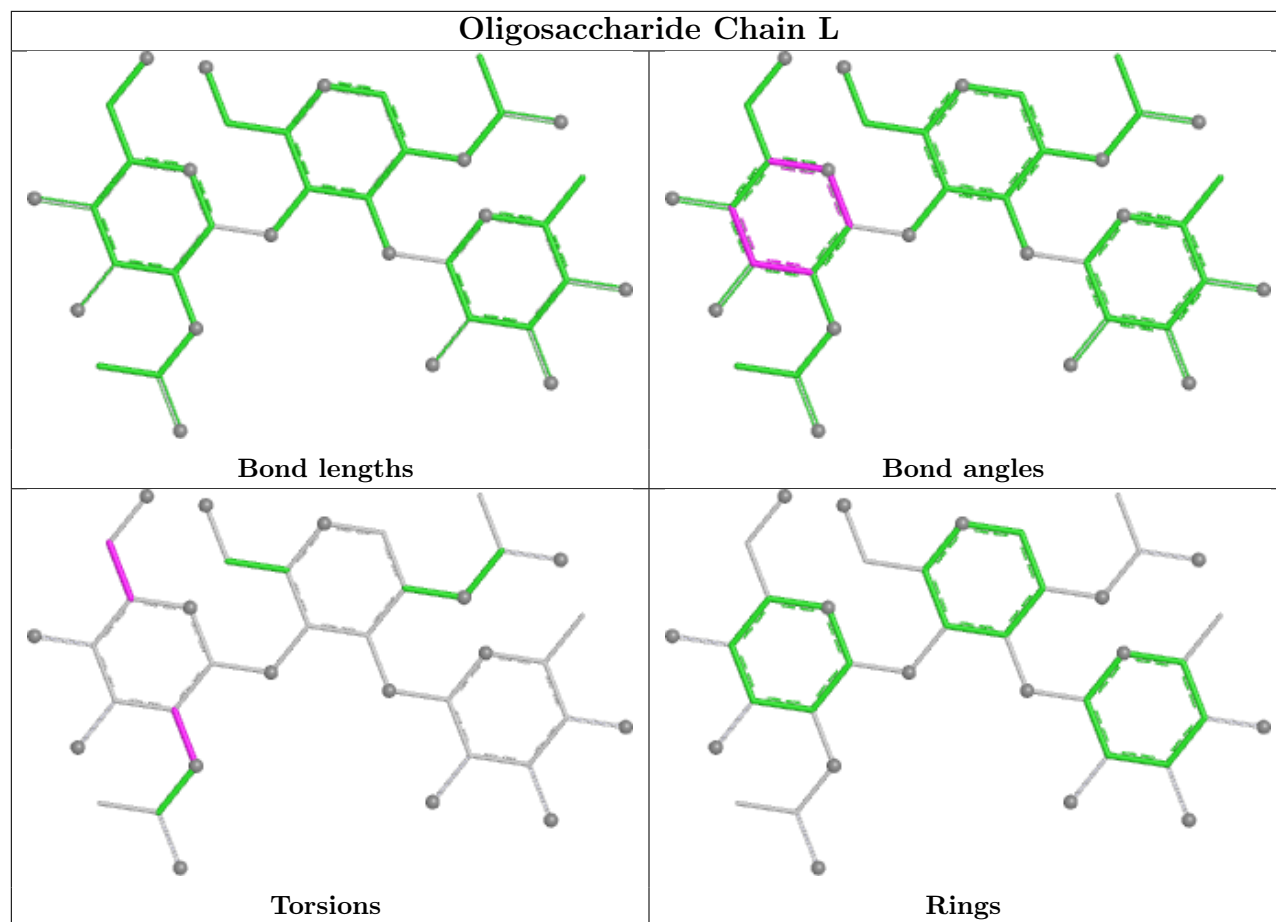


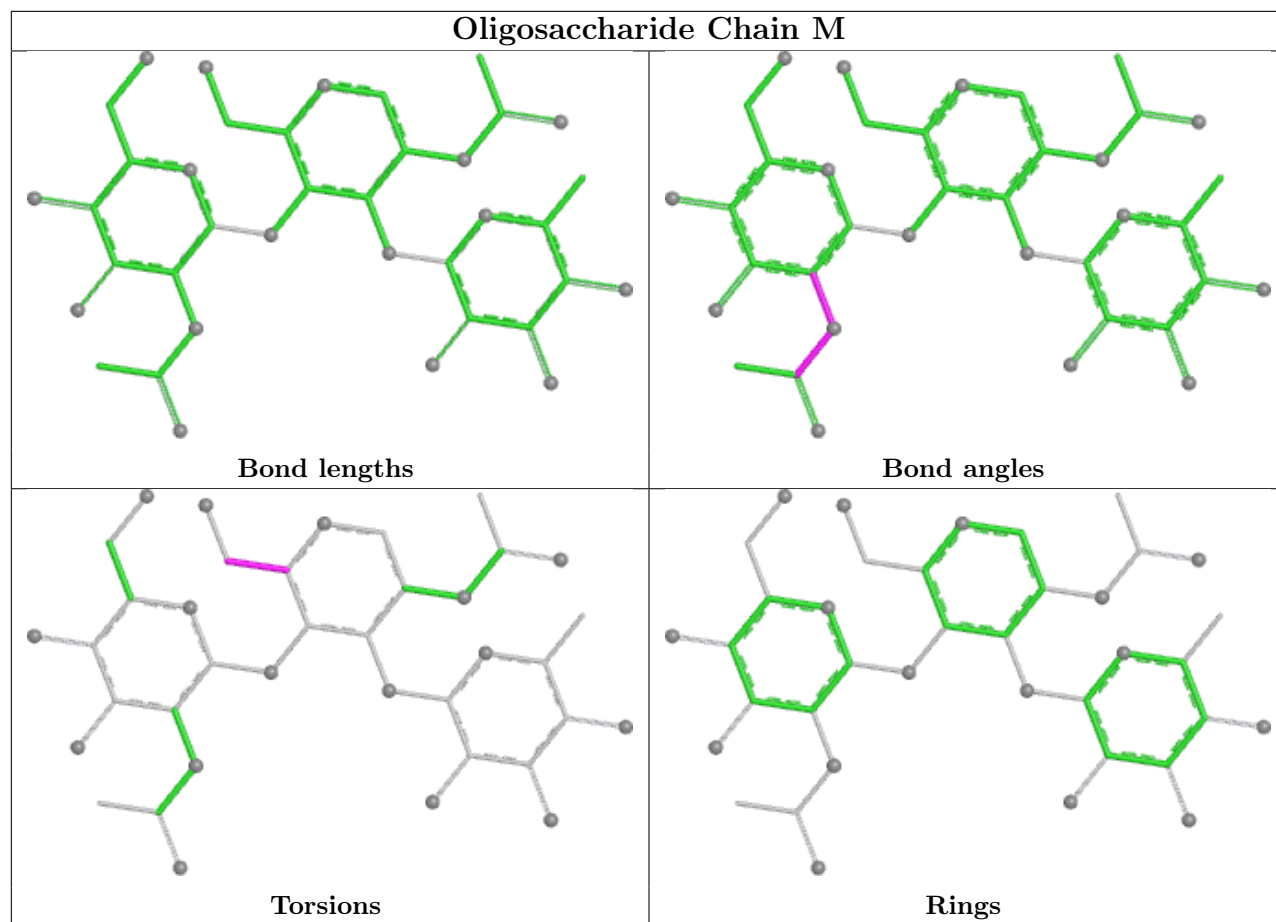


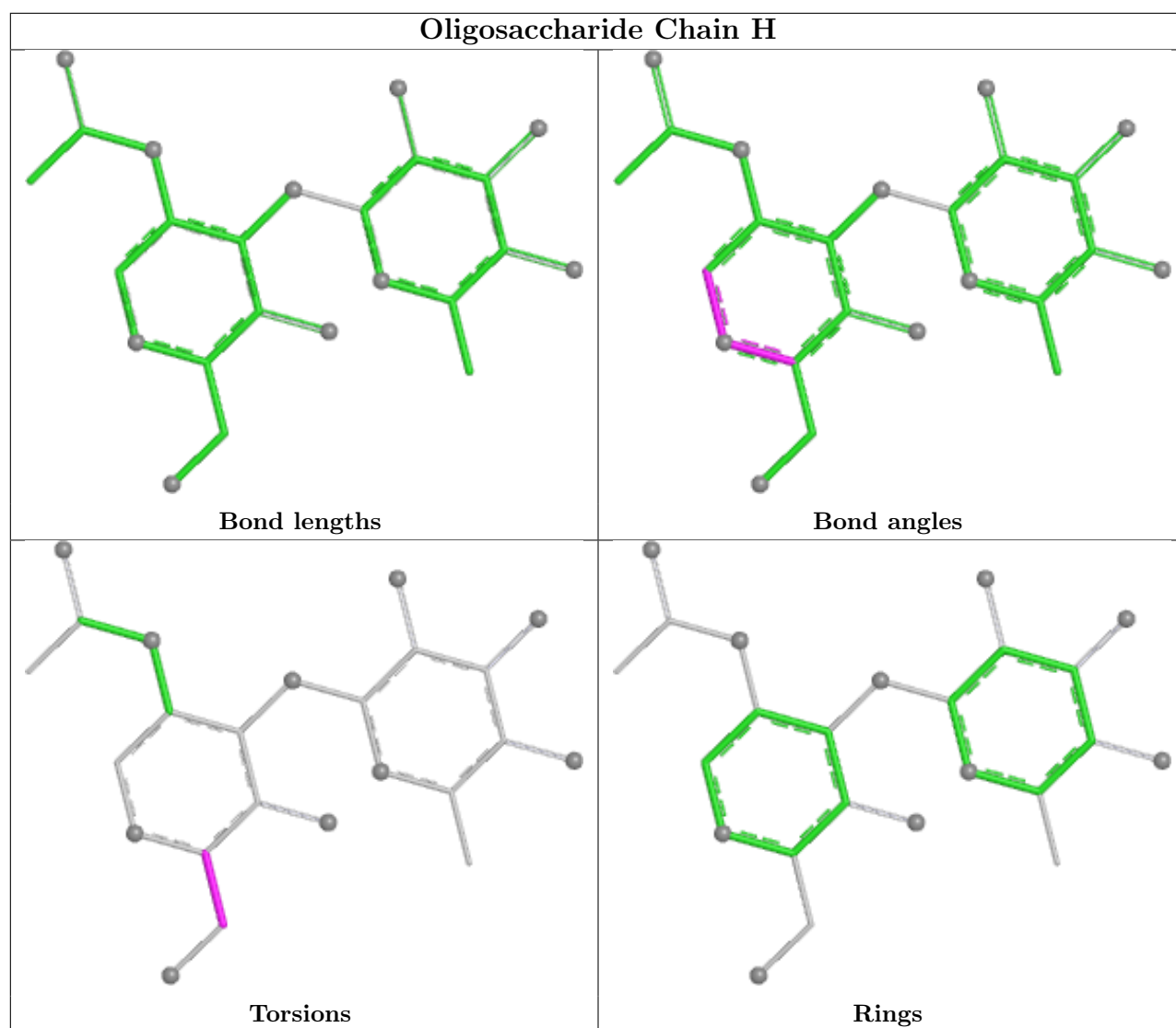


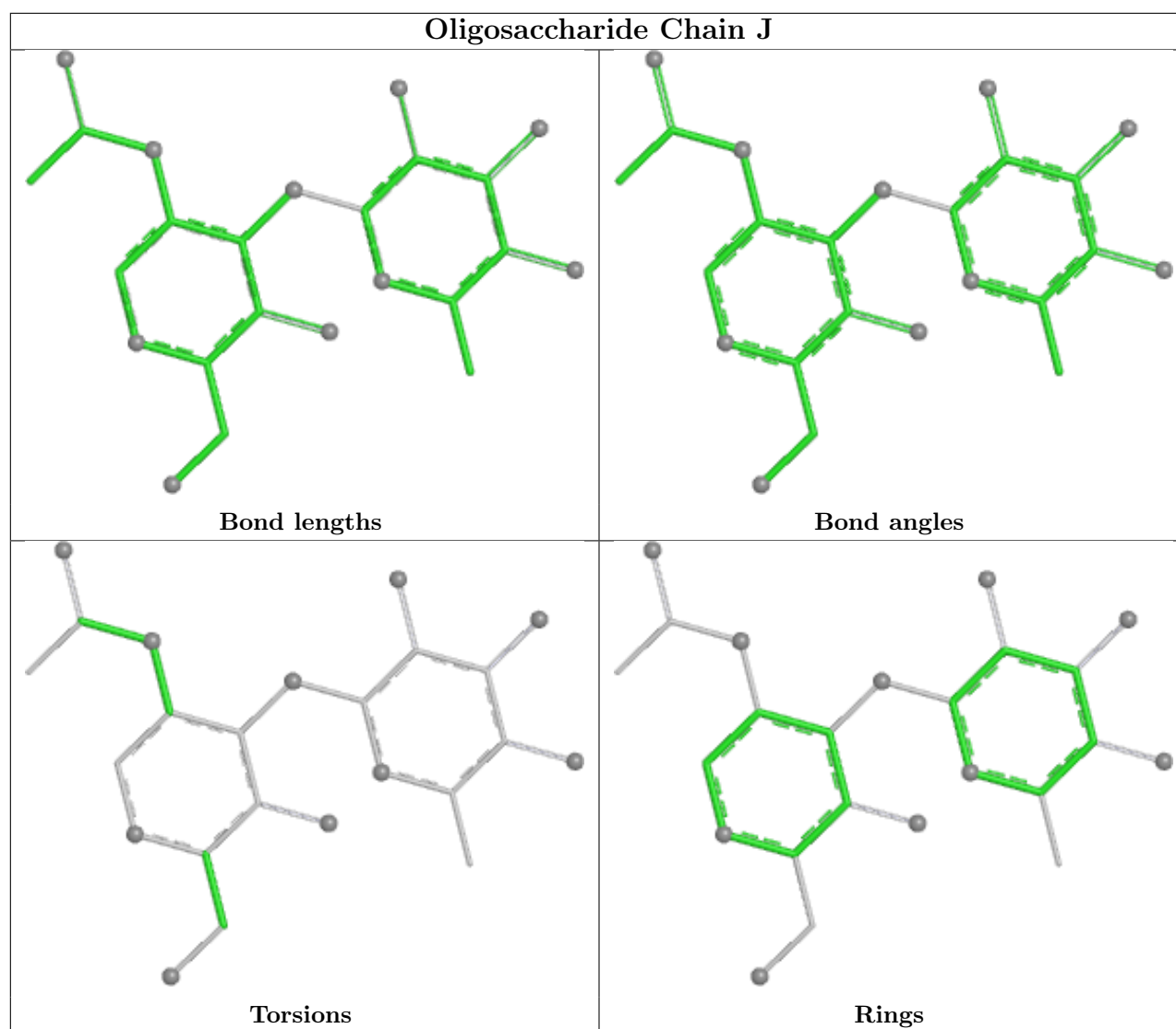












5.6 Ligand geometry [i](#)

Of 49 ligands modelled in this entry, 8 are monoatomic - leaving 41 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	$\# Z > 2$
10	EDO	D	518	-	3,3,3	0.56	0	2,2,2	0.28	0
8	NAG	D	504	1	14,14,15	0.58	0	17,19,21	0.98	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	B	510	-	5,5,5	0.32	0	5,5,5	0.84	0
9	SO4	C	513	-	4,4,4	0.25	0	6,6,6	0.18	0
10	EDO	C	501	-	3,3,3	0.44	0	2,2,2	0.48	0
8	NAG	B	506	1	14,14,15	0.49	0	17,19,21	0.67	0
9	SO4	A	517	-	4,4,4	0.31	0	6,6,6	0.08	0
7	GOL	D	514	-	5,5,5	0.40	0	5,5,5	0.64	0
8	NAG	A	505	1	14,14,15	0.60	0	17,19,21	0.62	0
10	EDO	A	520	-	3,3,3	0.45	0	2,2,2	0.41	0
10	EDO	A	519	-	3,3,3	0.49	0	2,2,2	0.45	0
9	SO4	C	502	-	4,4,4	0.24	0	6,6,6	0.14	0
10	EDO	B	517	-	3,3,3	0.38	0	2,2,2	0.58	0
10	EDO	D	516	-	3,3,3	0.48	0	2,2,2	0.26	0
9	SO4	B	512	-	4,4,4	0.25	0	6,6,6	0.08	0
8	NAG	B	505	1	14,14,15	0.52	0	17,19,21	1.52	4 (23%)
10	EDO	B	519	-	3,3,3	0.56	0	2,2,2	0.21	0
8	NAG	D	508	1	14,14,15	0.57	0	17,19,21	1.34	2 (11%)
9	SO4	A	509	-	4,4,4	0.25	0	6,6,6	0.23	0
7	GOL	A	504	-	5,5,5	0.34	0	5,5,5	0.38	0
10	EDO	B	515	-	3,3,3	0.45	0	2,2,2	0.31	0
10	EDO	B	516	-	3,3,3	0.47	0	2,2,2	0.34	0
6	OLO	A	503	4,5	16,16,16	0.52	0	21,21,21	1.48	4 (19%)
9	SO4	A	518	-	4,4,4	0.30	0	6,6,6	0.27	0
9	SO4	B	514	-	4,4,4	0.28	0	6,6,6	0.19	0
7	GOL	C	512	-	5,5,5	0.34	0	5,5,5	0.27	0
9	SO4	A	513	-	4,4,4	0.38	0	6,6,6	0.27	0
8	NAG	C	503	1	14,14,15	0.50	0	17,19,21	1.12	1 (5%)
10	EDO	D	517	-	3,3,3	0.49	0	2,2,2	0.22	0
9	SO4	D	515	-	4,4,4	0.32	0	6,6,6	0.20	0
7	GOL	D	513	-	5,5,5	0.55	0	5,5,5	0.30	0
9	SO4	B	513	-	4,4,4	0.27	0	6,6,6	0.11	0
9	SO4	B	511	-	4,4,4	0.23	0	6,6,6	0.18	0
11	ACT	D	519	-	3,3,3	0.79	0	3,3,3	1.38	0
8	NAG	C	506	1	14,14,15	0.50	0	17,19,21	1.60	2 (11%)
10	EDO	B	518	-	3,3,3	0.40	0	2,2,2	0.46	0
10	EDO	A	521	-	3,3,3	0.44	0	2,2,2	0.37	0
10	EDO	C	514	-	3,3,3	0.51	0	2,2,2	0.32	0
11	ACT	A	522	-	3,3,3	0.83	0	3,3,3	1.30	0
7	GOL	D	503	-	5,5,5	0.31	0	5,5,5	0.60	0
7	GOL	D	512	-	5,5,5	0.30	0	5,5,5	0.54	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
10	EDO	D	518	-	-	1/1/1/1	-
8	NAG	D	504	1	-	1/6/23/26	0/1/1/1
7	GOL	B	510	-	-	4/4/4/4	-
10	EDO	C	501	-	-	0/1/1/1	-
8	NAG	B	506	1	-	2/6/23/26	0/1/1/1
7	GOL	D	514	-	-	2/4/4/4	-
10	EDO	A	520	-	-	0/1/1/1	-
8	NAG	A	505	1	-	0/6/23/26	0/1/1/1
10	EDO	A	519	-	-	0/1/1/1	-
10	EDO	B	517	-	-	0/1/1/1	-
10	EDO	D	516	-	-	1/1/1/1	-
10	EDO	B	519	-	-	1/1/1/1	-
8	NAG	B	505	1	-	3/6/23/26	0/1/1/1
8	NAG	D	508	1	-	0/6/23/26	0/1/1/1
10	EDO	B	515	-	-	0/1/1/1	-
7	GOL	A	504	-	-	1/4/4/4	-
10	EDO	B	516	-	-	1/1/1/1	-
6	OLO	A	503	4,5	-	4/8/8/8	0/2/2/2
7	GOL	C	512	-	-	2/4/4/4	-
8	NAG	C	503	1	-	0/6/23/26	0/1/1/1
10	EDO	D	517	-	-	0/1/1/1	-
7	GOL	D	513	-	-	2/4/4/4	-
8	NAG	C	506	1	-	2/6/23/26	0/1/1/1
10	EDO	B	518	-	-	0/1/1/1	-
10	EDO	A	521	-	-	0/1/1/1	-
10	EDO	C	514	-	-	0/1/1/1	-
7	GOL	D	503	-	-	4/4/4/4	-
7	GOL	D	512	-	-	2/4/4/4	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	506	NAG	C1-O5-C5	4.07	117.63	112.19
6	A	503	OLO	CAH-NAK-CAI	3.45	122.20	117.51
8	C	506	NAG	C4-C3-C2	-3.33	106.14	111.02
8	B	505	NAG	C2-N2-C7	-3.23	118.57	122.90
6	A	503	OLO	OAB-CAL-CAM	3.22	123.09	114.84

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	503	0LO	OAB-CAL-CAM-CAH
6	A	503	0LO	OAA-CAL-CAM-CAH
7	D	503	GOL	O1-C1-C2-C3
7	D	503	GOL	C1-C2-C3-O3
7	D	512	GOL	O1-C1-C2-C3

There are no ring outliers.

12 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	501	EDO	1	0
8	B	506	NAG	1	0
10	A	520	EDO	2	0
10	D	516	EDO	1	0
10	B	519	EDO	1	0
6	A	503	0LO	2	0
9	B	514	SO4	1	0
7	C	512	GOL	4	0
8	C	503	NAG	2	0
10	A	521	EDO	8	0
7	D	503	GOL	2	0
7	D	512	GOL	4	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	425/426 (99%)	-0.97	0	100 100	12, 22, 38, 63	2 (0%)
1	B	425/426 (99%)	-0.80	3 (0%)	84 84	16, 27, 45, 83	0
1	C	423/426 (99%)	-0.83	1 (0%)	92 92	16, 27, 43, 75	2 (0%)
1	D	426/426 (100%)	-0.87	3 (0%)	84 84	15, 25, 42, 76	2 (0%)
All	All	1699/1704 (99%)	-0.86	7 (0%)	89 89	12, 25, 42, 83	6 (0%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	186	THR	3.6
1	D	64	ASN	2.4
1	C	63	LYS	2.4
1	B	64	ASN	2.2
1	D	432	THR	2.2

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	H	2	10/11	0.46	0.19	67,73,80,80	0
2	NAG	L	3	14/15	0.69	0.16	73,82,90,90	0

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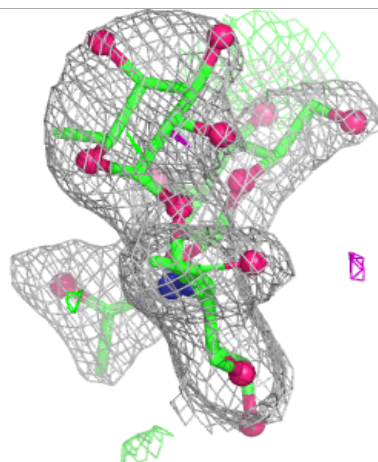
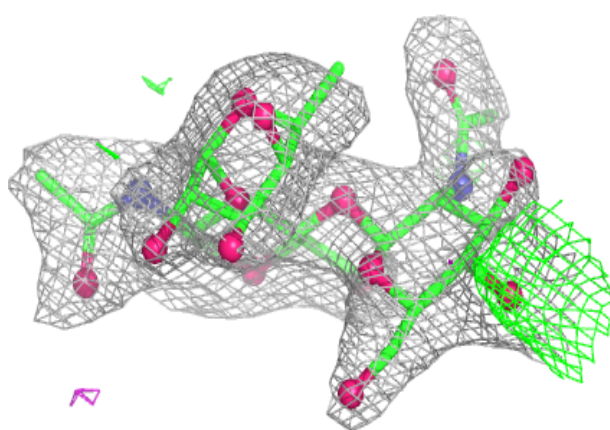
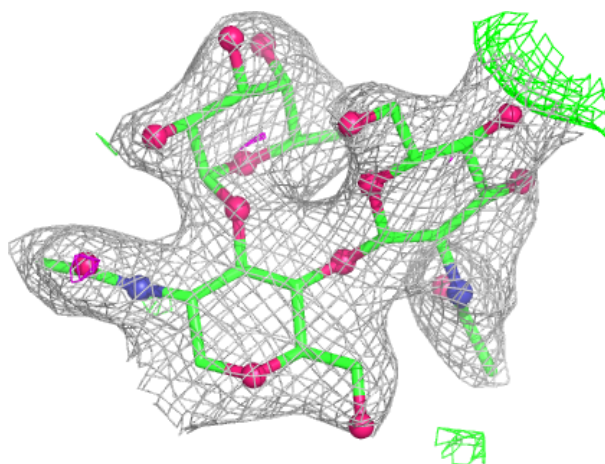
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	E	3	14/15	0.78	0.12	47,60,65,70	0
2	FUC	L	2	10/11	0.78	0.15	63,74,80,81	0
3	NAG	J	1	14/15	0.78	0.12	41,57,68,70	0
2	FUC	K	2	10/11	0.79	0.13	49,57,62,63	0
2	FUC	M	2	10/11	0.81	0.12	38,53,60,60	0
2	FUC	E	2	10/11	0.82	0.11	61,63,67,68	0
2	NAG	F	3	14/15	0.82	0.11	60,66,74,76	0
2	NAG	K	3	14/15	0.84	0.11	37,55,71,74	0
2	FUC	F	2	10/11	0.84	0.11	54,59,64,64	0
3	FUC	J	2	10/11	0.84	0.14	64,72,78,78	0
2	NAG	M	3	14/15	0.85	0.10	37,52,62,66	0
3	NAG	H	1	14/15	0.87	0.10	37,53,63,72	0
2	NAG	L	1	14/15	0.88	0.10	44,57,70,75	0
2	NAG	F	1	14/15	0.89	0.09	36,46,57,62	0
2	NAG	G	3	14/15	0.91	0.07	29,34,38,38	0
2	NAG	I	3	14/15	0.92	0.08	31,41,47,48	0
2	FUC	G	2	10/11	0.93	0.07	33,37,39,40	0
2	NAG	E	1	14/15	0.93	0.08	35,44,53,53	0
2	FUC	I	2	10/11	0.93	0.08	30,37,42,51	0
2	NAG	M	1	14/15	0.94	0.06	28,37,42,44	0
2	NAG	K	1	14/15	0.95	0.06	29,36,43,47	0
2	NAG	I	1	14/15	0.96	0.06	24,31,36,39	0
2	NAG	G	1	14/15	0.97	0.06	24,29,35,37	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.

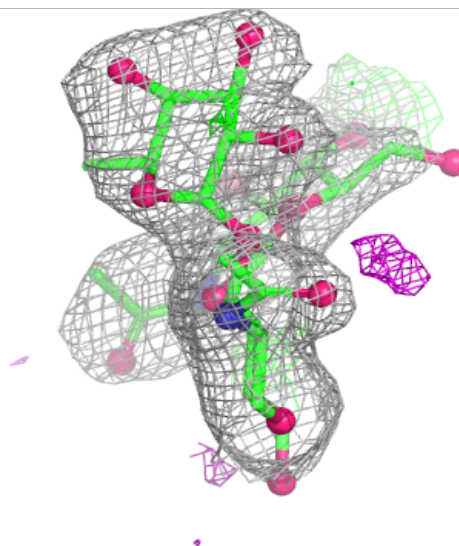
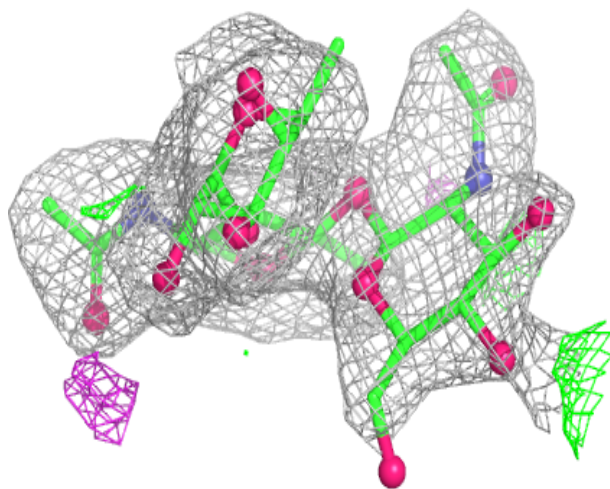
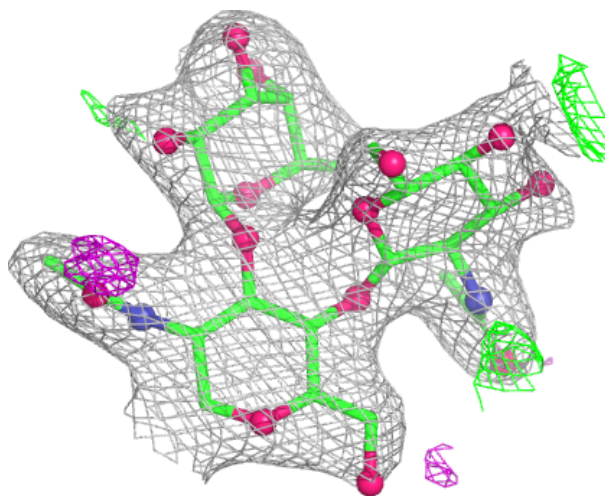
Electron density around Chain E:

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



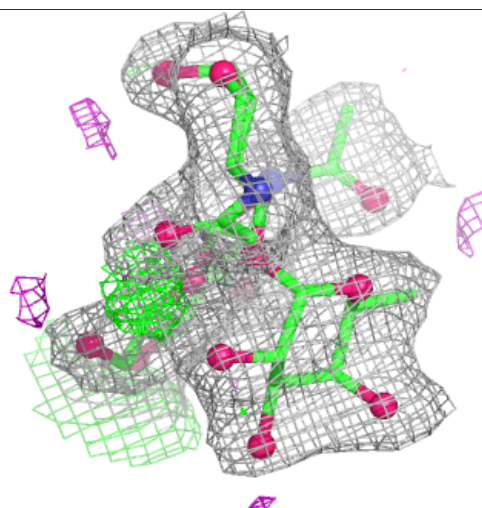
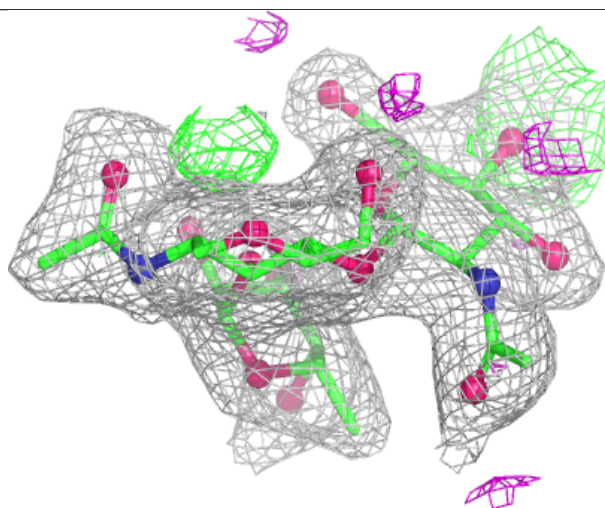
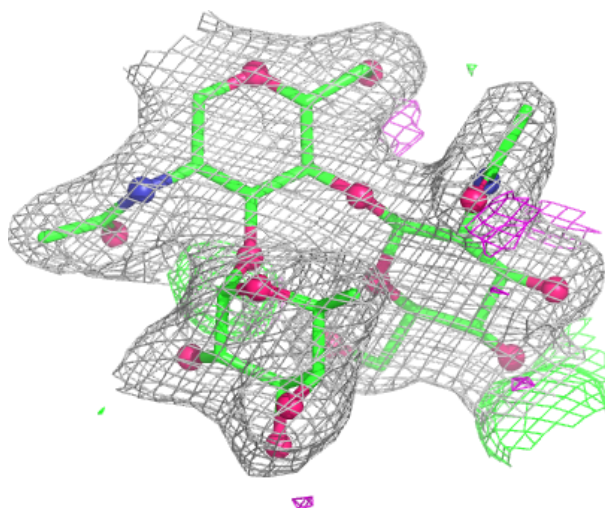
Electron density around Chain F:

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



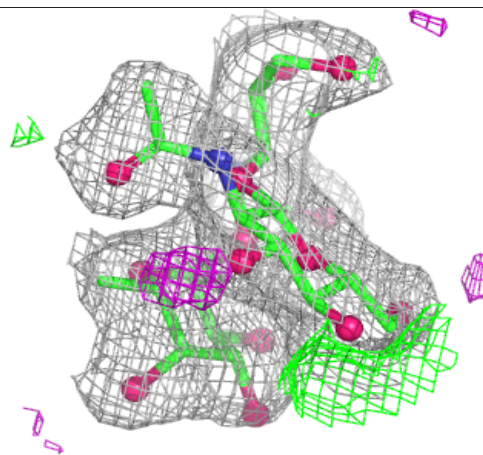
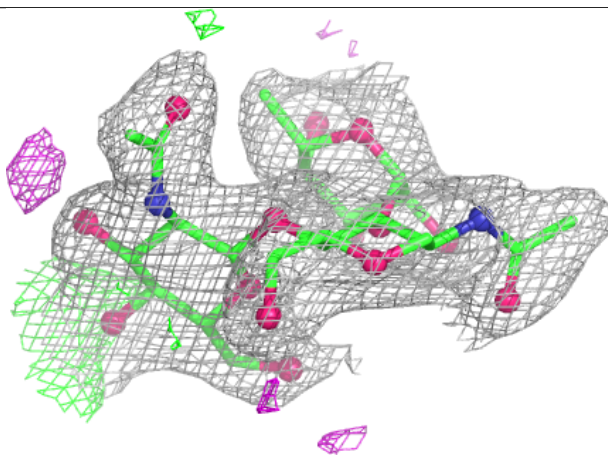
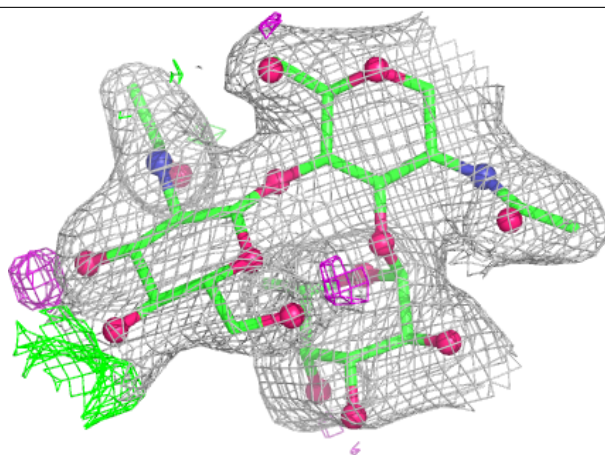
Electron density around Chain G:

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



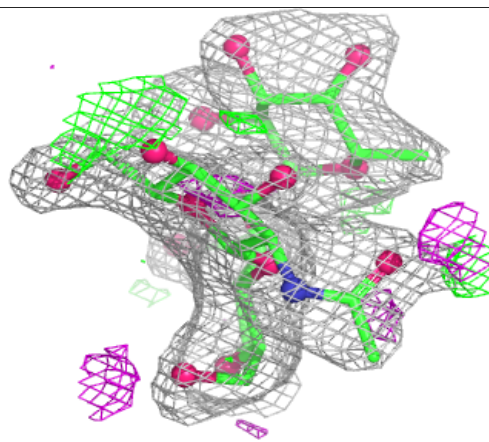
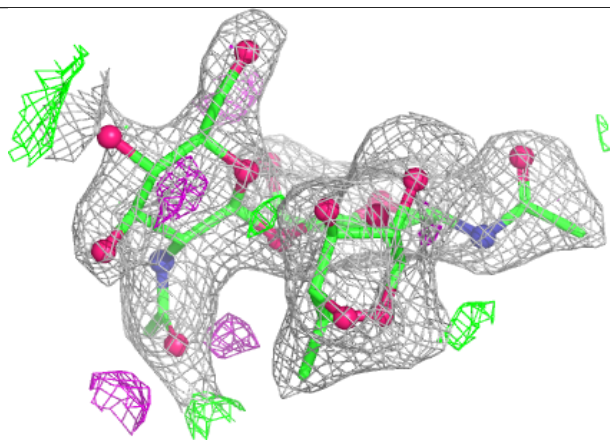
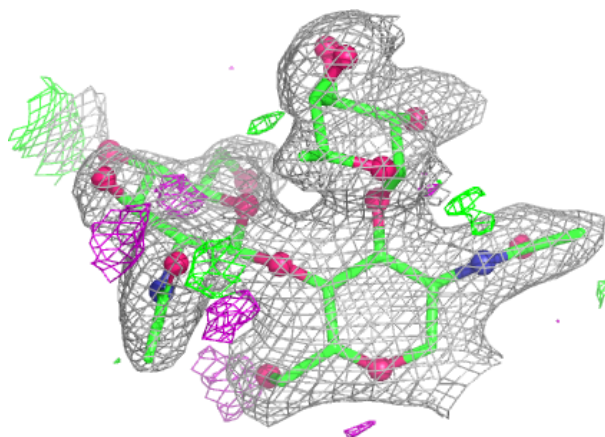
Electron density around Chain I:

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



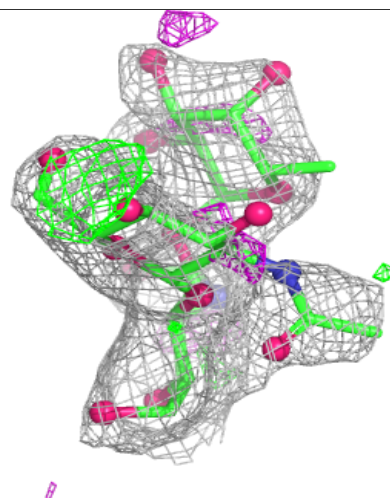
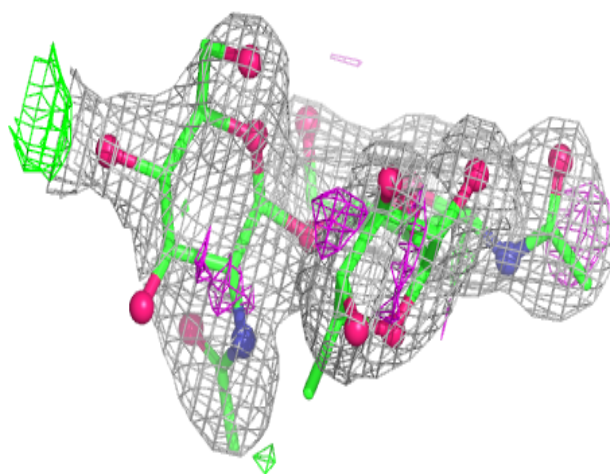
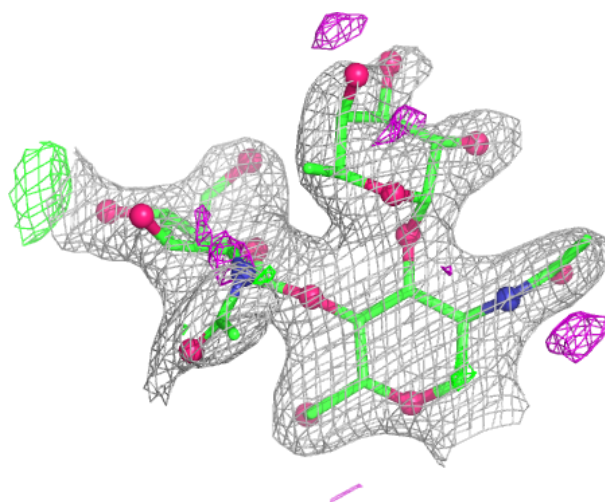
Electron density around Chain K:

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



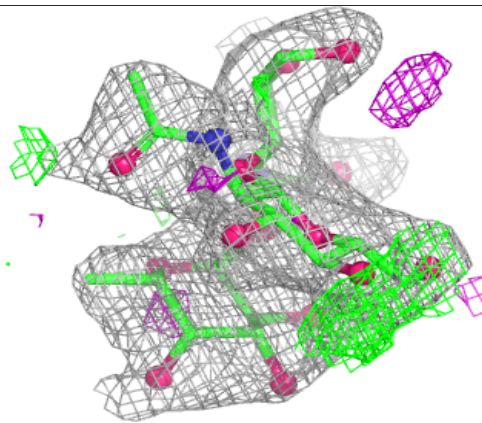
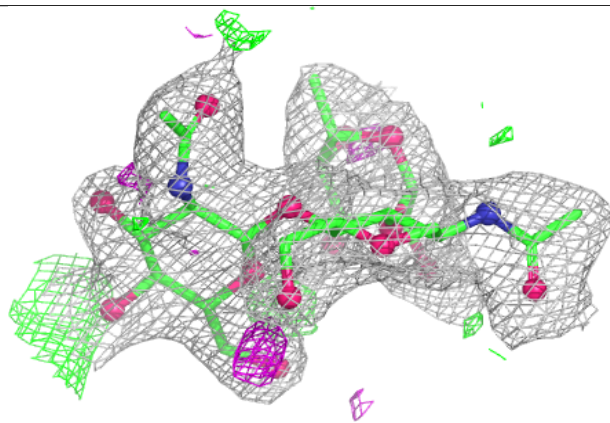
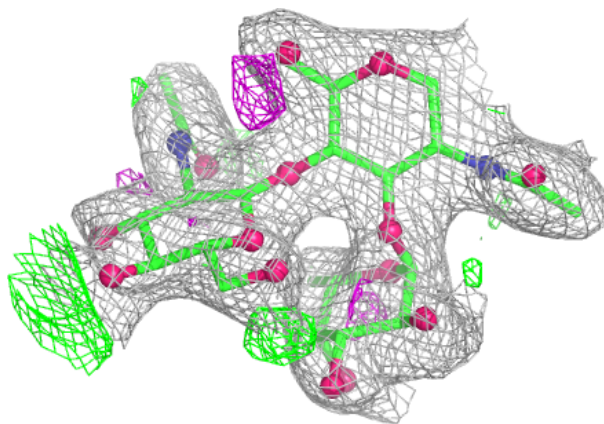
Electron density around Chain L:

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



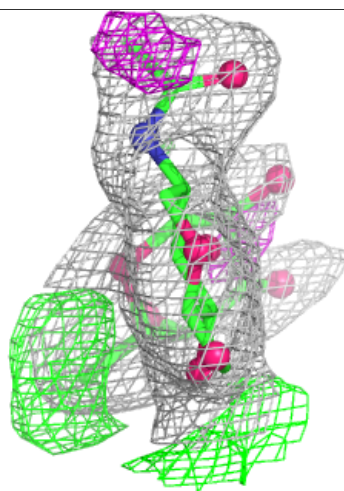
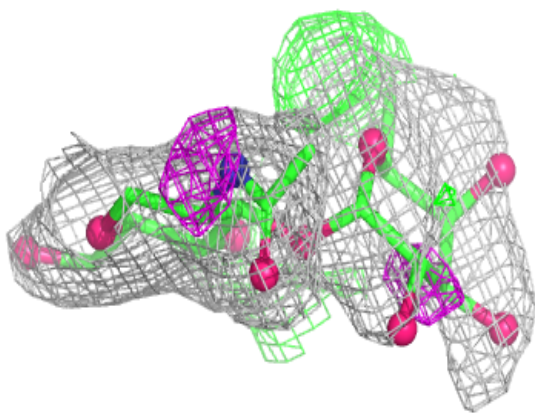
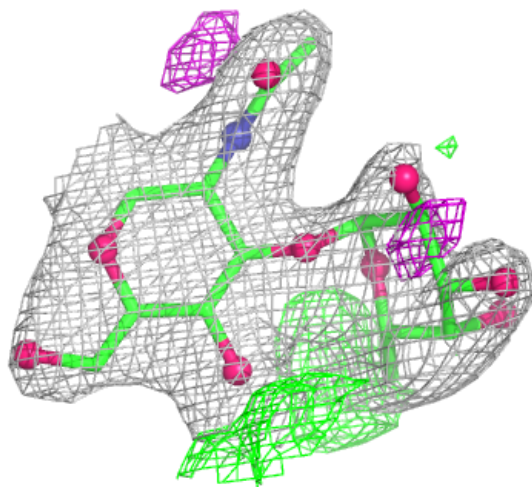
Electron density around Chain M:

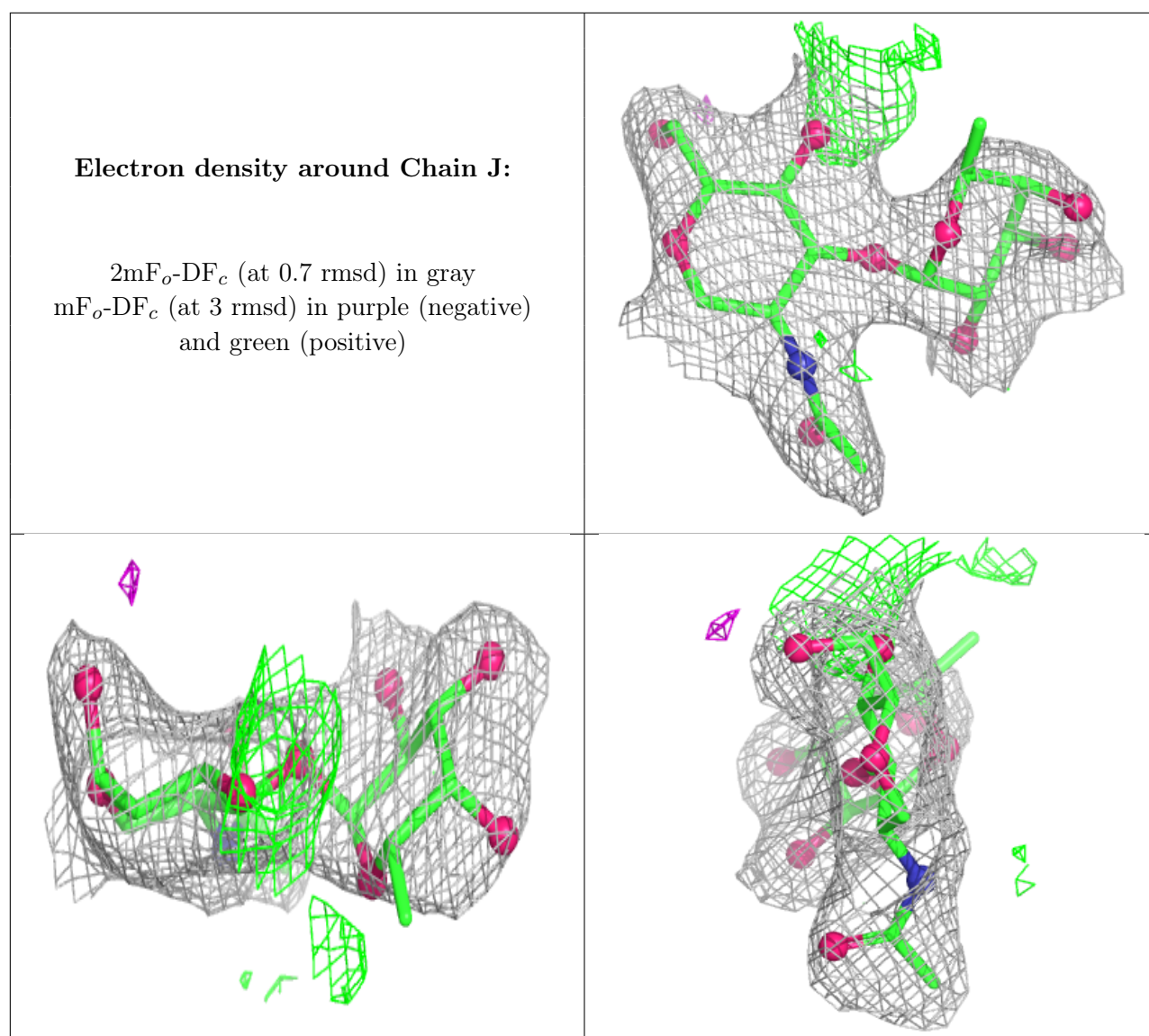
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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(Å ²)	Q<0.9
10	EDO	B	518	4/4	0.67	0.21	58,66,67,73	0
11	ACT	A	522	4/4	0.73	0.15	51,56,63,64	0
9	SO4	C	502	5/5	0.78	0.13	81,86,91,99	0
10	EDO	B	519	4/4	0.78	0.16	45,46,52,53	0
10	EDO	B	517	4/4	0.78	0.15	54,55,57,68	0
10	EDO	C	501	4/4	0.79	0.14	44,45,47,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	EDO	B	515	4/4	0.80	0.16	52,56,59,61	0
9	SO4	A	518	5/5	0.80	0.14	35,47,64,74	0
7	GOL	C	512	6/6	0.80	0.13	56,56,61,64	0
6	OLO	A	503	15/15	0.81	0.17	30,43,64,65	0
7	GOL	B	510	6/6	0.82	0.13	37,43,48,50	0
10	EDO	D	517	4/4	0.82	0.14	49,51,52,54	0
7	GOL	D	514	6/6	0.82	0.13	36,46,49,52	0
8	NAG	B	505	14/15	0.83	0.11	45,50,60,64	0
9	SO4	D	515	5/5	0.84	0.26	34,49,62,67	0
10	EDO	A	519	4/4	0.84	0.14	29,32,32,42	0
8	NAG	C	506	14/15	0.84	0.09	39,43,49,54	0
7	GOL	D	503	6/6	0.85	0.12	36,39,41,44	0
7	GOL	D	513	6/6	0.86	0.13	29,37,50,54	0
11	ACT	D	519	4/4	0.86	0.10	34,50,51,52	0
8	NAG	D	508	14/15	0.87	0.12	43,52,60,66	0
10	EDO	A	520	4/4	0.87	0.12	36,48,51,55	0
9	SO4	A	513	5/5	0.88	0.13	29,37,55,74	0
7	GOL	D	512	6/6	0.88	0.16	33,38,39,41	0
9	SO4	B	511	5/5	0.89	0.17	55,58,71,75	0
10	EDO	A	521	4/4	0.90	0.12	30,30,39,49	0
9	SO4	C	513	5/5	0.90	0.12	48,58,71,79	0
9	SO4	B	514	5/5	0.90	0.19	51,52,62,71	0
10	EDO	C	514	4/4	0.91	0.13	41,43,48,49	0
8	NAG	B	506	14/15	0.91	0.08	31,39,49,51	0
8	NAG	D	504	14/15	0.91	0.08	31,37,46,47	0
9	SO4	B	512	5/5	0.91	0.16	62,68,82,86	0
10	EDO	D	516	4/4	0.92	0.08	34,40,43,44	0
10	EDO	B	516	4/4	0.92	0.09	28,39,40,41	0
10	EDO	D	518	4/4	0.92	0.10	31,35,36,38	0
9	SO4	A	517	5/5	0.92	0.22	54,57,59,78	0
8	NAG	C	503	14/15	0.92	0.07	33,38,46,46	0
9	SO4	B	513	5/5	0.93	0.16	43,70,79,86	0
8	NAG	A	505	14/15	0.94	0.06	23,29,37,42	0
7	GOL	A	504	6/6	0.97	0.05	22,25,27,28	0
5	FE	C	511	1/1	0.98	0.03	32,32,32,32	1
5	FE	D	502	1/1	0.98	0.03	28,28,28,28	1
4	ZN	C	510	1/1	0.99	0.01	25,25,25,25	1
4	ZN	D	501	1/1	0.99	0.02	24,24,24,24	1
5	FE	B	502	1/1	0.99	0.03	29,29,29,29	1
4	ZN	A	501	1/1	0.99	0.02	28,28,28,28	0
9	SO4	A	509	5/5	0.99	0.04	30,35,36,40	0
4	ZN	B	501	1/1	1.00	0.02	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	FE	A	502	1/1	1.00	0.01	23,23,23,23	1

6.5 Other polymers [i](#)

There are no such residues in this entry.