



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 09:16 PM BST

PDB ID : 5M8R
Title : Crystal structure of human tyrosinase related protein 1 (T391V-R374S-Y362F)
in complex with mimosine
Authors : Lai, X.; Soler-Lopez, M.; Wichers, H.J.; Dijkstra, B.W.
Deposited on : 2016-10-29
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

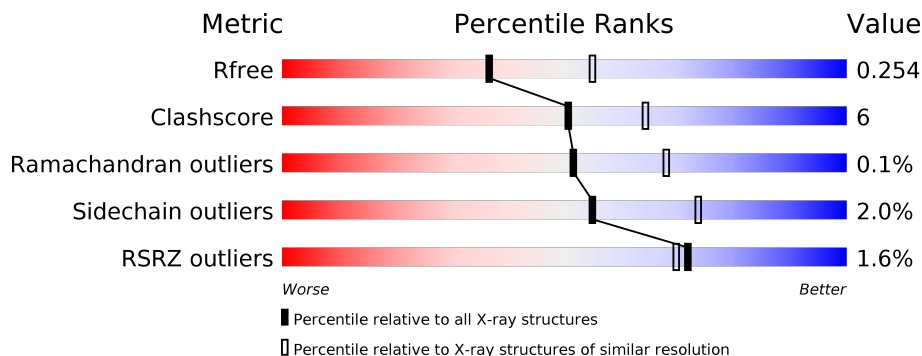
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.



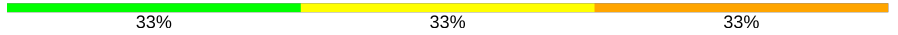



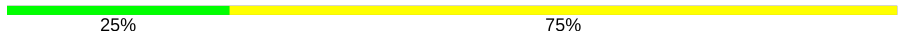
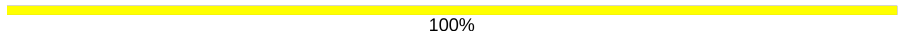
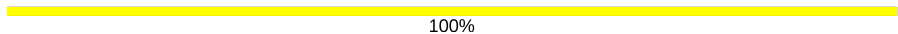
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on 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	446	
1	B	446	
1	C	446	
1	D	446	
2	E	3	
2	F	3	

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Mol	Chain	Length	Quality of chain
2	I	3	 33% 33% 33%
2	J	3	 67% 33%
3	G	2	 100%
3	K	2	 50% 50%
4	H	4	 25% 75%
4	L	4	 100%
5	M	2	 100%

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 14806 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.

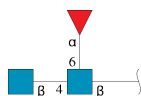
- Molecule 1 is a protein called 5,6-dihydroxyindole-2-carboxylic acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	446	3554	2231	629	671	23	0	0	0
1	B	446	3554	2231	629	671	23	0	0	0
1	C	446	3554	2231	629	671	23	0	0	0
1	D	446	3554	2231	629	671	23	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	362	PHE	TYR	engineered mutation	UNP P17643
A	374	SER	ARG	engineered mutation	UNP P17643
A	391	VAL	THR	engineered mutation	UNP P17643
B	362	PHE	TYR	engineered mutation	UNP P17643
B	374	SER	ARG	engineered mutation	UNP P17643
B	391	VAL	THR	engineered mutation	UNP P17643
C	362	PHE	TYR	engineered mutation	UNP P17643
C	374	SER	ARG	engineered mutation	UNP P17643
C	391	VAL	THR	engineered mutation	UNP P17643
D	362	PHE	TYR	engineered mutation	UNP P17643
D	374	SER	ARG	engineered mutation	UNP P17643
D	391	VAL	THR	engineered mutation	UNP P17643

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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



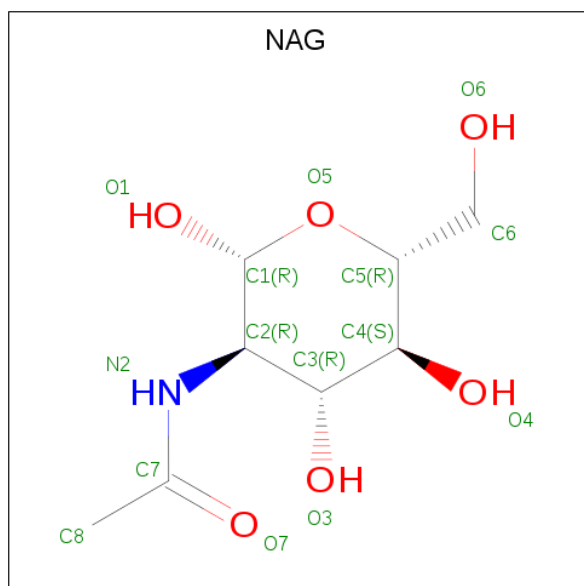
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	L	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	M	2	24	14	1	9	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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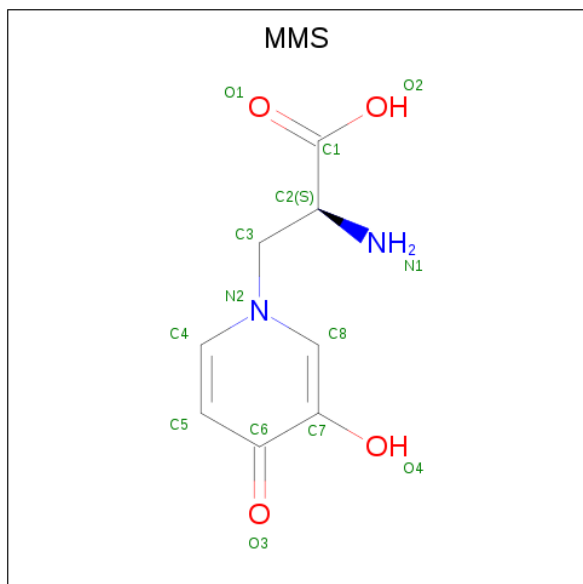
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Zn	0	0
			2	2		
7	A	3	Total	Zn	0	0
			3	3		
7	D	2	Total	Zn	0	0
			2	2		
7	C	2	Total	Zn	0	0
			2	2		

- Molecule 8 is MIMOSINE (three-letter code: MMS) (formula: C₈H₁₀N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	2	4		
8	B	1	Total	C	N	O	0	0
			14	8	2	4		
8	C	1	Total	C	N	O	0	0
			14	8	2	4		
8	D	1	Total	C	N	O	0	0
			14	8	2	4		

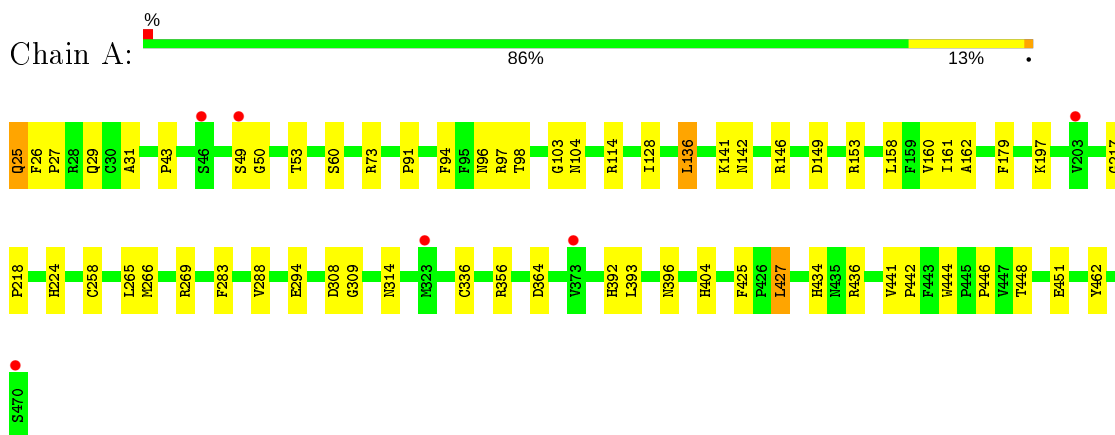
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	6	Total O 6 6	0	0
9	B	11	Total O 11 11	0	0
9	C	9	Total O 9 9	0	0
9	D	13	Total O 13 13	0	0

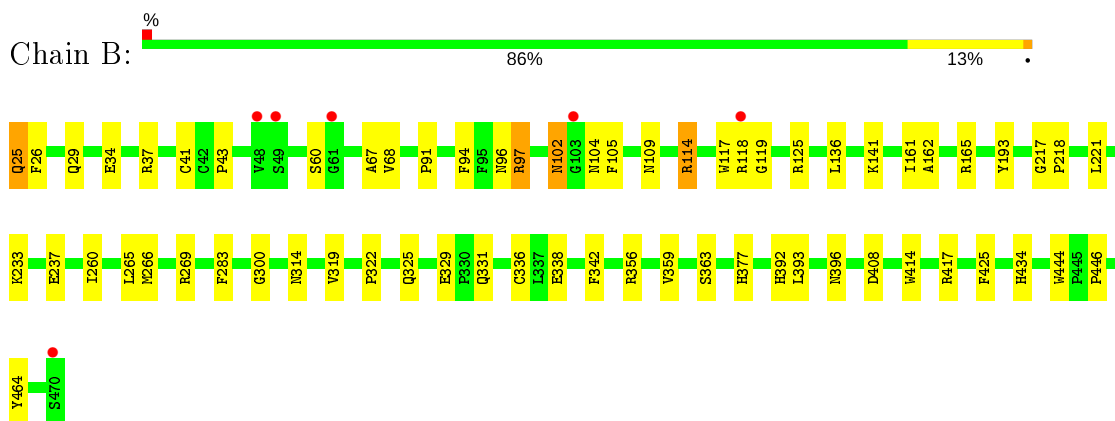
3 Residue-property plots [i](#)

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.

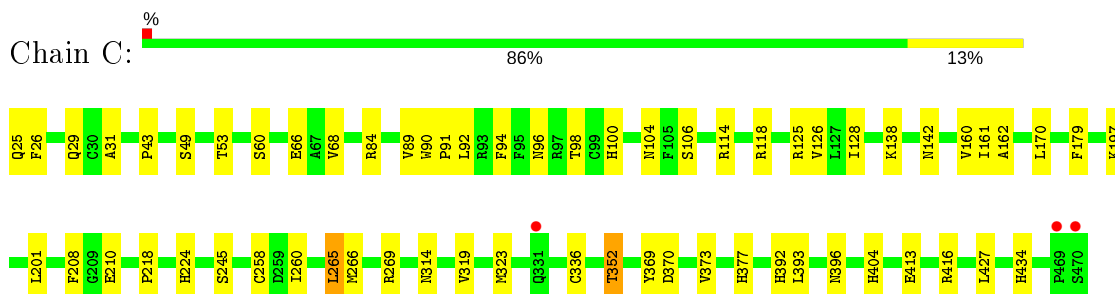
- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase



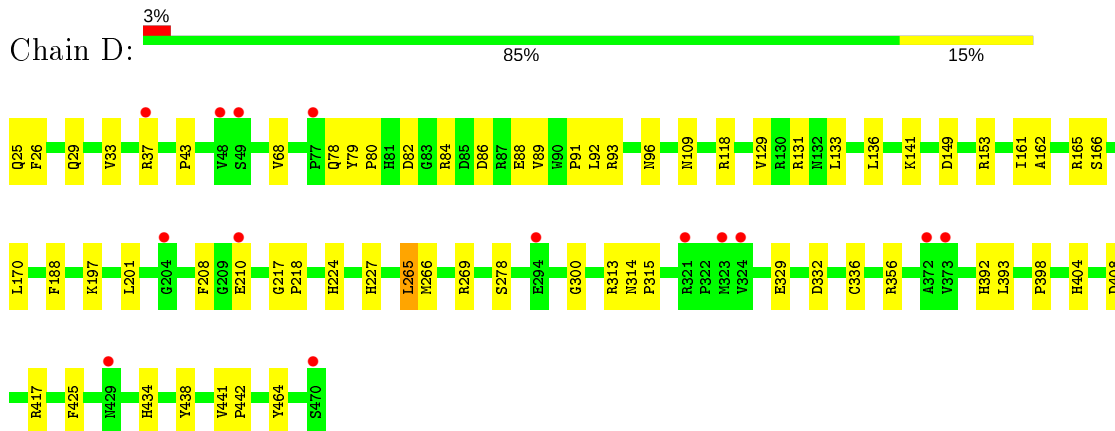
- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase



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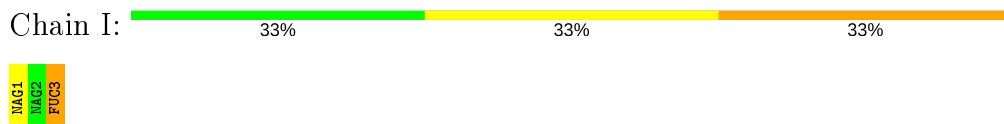
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



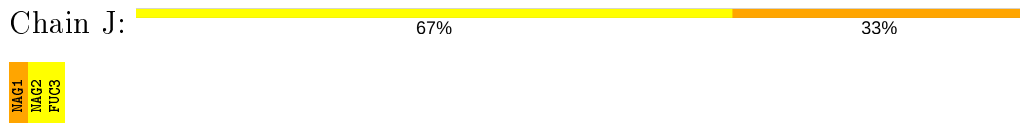
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



MAG1
MAG2

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

Chain K:  50% 50%MAG1
MAG2

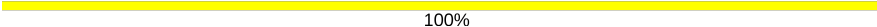
- Molecule 4: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  25% 75%MAG1
MAG2
MAN3
MAN4

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

Chain L:  100%MAG1
MAG2
MAN3
MAN4

- Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%MAG1
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.35Å 139.73Å 190.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.74 – 2.40 47.74 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.74-2.40) 94.6 (47.74-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.39Å)	Xtrriage
Refinement program	REFMAC, PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.200 , 0.249 0.210 , 0.254	Depositor DCC
R_{free} test set	4651 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtrriage
Anisotropy	0.406	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14806	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MAN, NAG, MMS, 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	0.46	0/3661	0.65	2/4990 (0.0%)
1	B	0.49	0/3661	0.67	4/4990 (0.1%)
1	C	0.46	0/3661	0.64	0/4990
1	D	0.44	0/3661	0.60	1/4990 (0.0%)
All	All	0.46	0/14644	0.64	7/19960 (0.0%)

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(°)
1	B	114	ARG	NE-CZ-NH2	-11.65	114.48	120.30
1	D	265	LEU	CA-CB-CG	7.31	132.11	115.30
1	A	427	LEU	CB-CG-CD1	-6.71	99.59	111.00
1	B	25	GLN	C-N-CA	-5.86	107.04	121.70
1	A	25	GLN	C-N-CA	-5.69	107.48	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3554	0	3320	37	0
1	B	3554	0	3320	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3554	0	3320	41	0
1	D	3554	0	3320	38	0
2	E	38	0	34	2	0
2	F	38	0	34	2	0
2	I	38	0	34	2	0
2	J	38	0	34	1	0
3	G	28	0	25	0	0
3	K	28	0	25	0	0
4	H	50	0	43	0	0
4	L	50	0	43	0	0
5	M	24	0	22	2	0
6	A	56	0	52	0	0
6	B	28	0	26	2	0
6	C	14	0	13	2	0
6	D	56	0	52	0	0
7	A	3	0	0	0	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
7	D	2	0	0	0	0
8	A	14	0	0	0	0
8	B	14	0	0	0	0
8	C	14	0	0	0	0
8	D	14	0	0	0	0
9	A	6	0	0	0	0
9	B	11	0	0	1	0
9	C	9	0	0	1	0
9	D	13	0	0	2	0
All	All	14806	0	13717	162	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 162 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:C:25:GLN:HG3	1:C:26:PHE:H	1.36	0.90
1:B:392:HIS:NE2	1:B:393:LEU:HD23	1.92	0.85
1:C:269:ARG:NH1	1:C:314:ASN:OD1	2.11	0.83
1:B:25:GLN:HG3	1:B:26:PHE:H	1.46	0.78
1:D:25:GLN:HG3	1:D:26:PHE:H	1.48	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	444/446 (100%)	420 (95%)	24 (5%)	0	100	100
1	B	444/446 (100%)	425 (96%)	19 (4%)	0	100	100
1	C	444/446 (100%)	424 (96%)	19 (4%)	1 (0%)	47	62
1	D	444/446 (100%)	422 (95%)	22 (5%)	0	100	100
All	All	1776/1784 (100%)	1691 (95%)	84 (5%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	266	MET

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	395/395 (100%)	387 (98%)	8 (2%)	55	74
1	B	395/395 (100%)	387 (98%)	8 (2%)	55	74
1	C	395/395 (100%)	387 (98%)	8 (2%)	55	74
1	D	395/395 (100%)	387 (98%)	8 (2%)	55	74
All	All	1580/1580 (100%)	1548 (98%)	32 (2%)	55	74

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	377	HIS
1	C	197	LYS
1	D	417	ARG
1	C	60	SER
1	C	258	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	429	ASN
1	D	467	GLN

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 [i](#)

26 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	1,2	14,14,15	0.32	0	17,19,21	0.79	1 (5%)
2	NAG	E	2	2	14,14,15	0.50	0	17,19,21	0.52	0
2	FUC	E	3	2	10,10,11	1.13	0	14,14,16	1.44	2 (14%)
2	NAG	F	1	1,2	14,14,15	0.26	0	17,19,21	0.99	1 (5%)
2	NAG	F	2	2	14,14,15	0.82	1 (7%)	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FUC	F	3	2	10,10,11	1.15	1 (10%)	14,14,16	1.26	2 (14%)
3	NAG	G	1	1,3	14,14,15	0.37	0	17,19,21	0.51	0
3	NAG	G	2	3	14,14,15	0.32	0	17,19,21	0.38	0
4	NAG	H	1	1,4	14,14,15	0.30	0	17,19,21	0.74	0
4	NAG	H	2	4	14,14,15	0.73	1 (7%)	17,19,21	0.69	0
4	MAN	H	3	4	11,11,12	1.22	1 (9%)	15,15,17	1.40	3 (20%)
4	MAN	H	4	4	11,11,12	1.09	0	15,15,17	1.25	2 (13%)
2	NAG	I	1	1,2	14,14,15	0.44	0	17,19,21	0.61	0
2	NAG	I	2	2	14,14,15	0.51	0	17,19,21	0.48	0
2	FUC	I	3	2	10,10,11	1.23	1 (10%)	14,14,16	1.51	2 (14%)
2	NAG	J	1	1,2	14,14,15	0.89	1 (7%)	17,19,21	0.85	0
2	NAG	J	2	2	14,14,15	0.89	1 (7%)	17,19,21	0.92	1 (5%)
2	FUC	J	3	2	10,10,11	1.69	4 (40%)	14,14,16	1.30	3 (21%)
3	NAG	K	1	1,3	14,14,15	0.51	0	17,19,21	0.48	0
3	NAG	K	2	3	14,14,15	0.57	1 (7%)	17,19,21	0.57	0
4	NAG	L	1	1,4	14,14,15	0.39	0	17,19,21	0.92	1 (5%)
4	NAG	L	2	4	14,14,15	0.69	1 (7%)	17,19,21	1.09	1 (5%)
4	MAN	L	3	4	11,11,12	2.08	4 (36%)	15,15,17	2.09	4 (26%)
4	MAN	L	4	4	11,11,12	1.39	3 (27%)	15,15,17	1.61	3 (20%)
5	NAG	M	1	1,5	14,14,15	0.40	0	17,19,21	0.70	0
5	FUC	M	2	5	10,10,11	0.89	0	14,14,16	1.40	3 (21%)

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	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	FUC	E	3	2	-	-	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	FUC	F	3	2	-	-	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	H	3	4	-	0/2/19/22	1/1/1/1
4	MAN	H	4	4	-	2/2/19/22	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	FUC	I	3	2	-	-	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	FUC	J	3	2	-	-	0/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
4	NAG	L	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1
4	MAN	L	3	4	-	1/2/19/22	1/1/1/1
4	MAN	L	4	4	-	2/2/19/22	1/1/1/1
5	NAG	M	1	1,5	-	2/6/23/26	0/1/1/1
5	FUC	M	2	5	-	-	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	3	MAN	O5-C5	3.91	1.51	1.43
2	J	3	FUC	O5-C5	3.26	1.50	1.43
2	J	2	NAG	C1-C2	3.11	1.57	1.52
4	L	3	MAN	O3-C3	3.10	1.50	1.43
4	L	4	MAN	C1-C2	2.85	1.58	1.52

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	3	MAN	O3-C3-C2	4.57	118.74	109.99
4	L	3	MAN	C1-O5-C5	4.20	117.88	112.19
2	I	3	FUC	O5-C5-C4	3.47	115.75	109.52
4	L	2	NAG	C1-O5-C5	3.28	116.64	112.19
2	J	2	NAG	C1-O5-C5	3.13	116.44	112.19

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	4	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	K	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
4	L	4	MAN	O5-C5-C6-O6
4	H	4	MAN	C4-C5-C6-O6

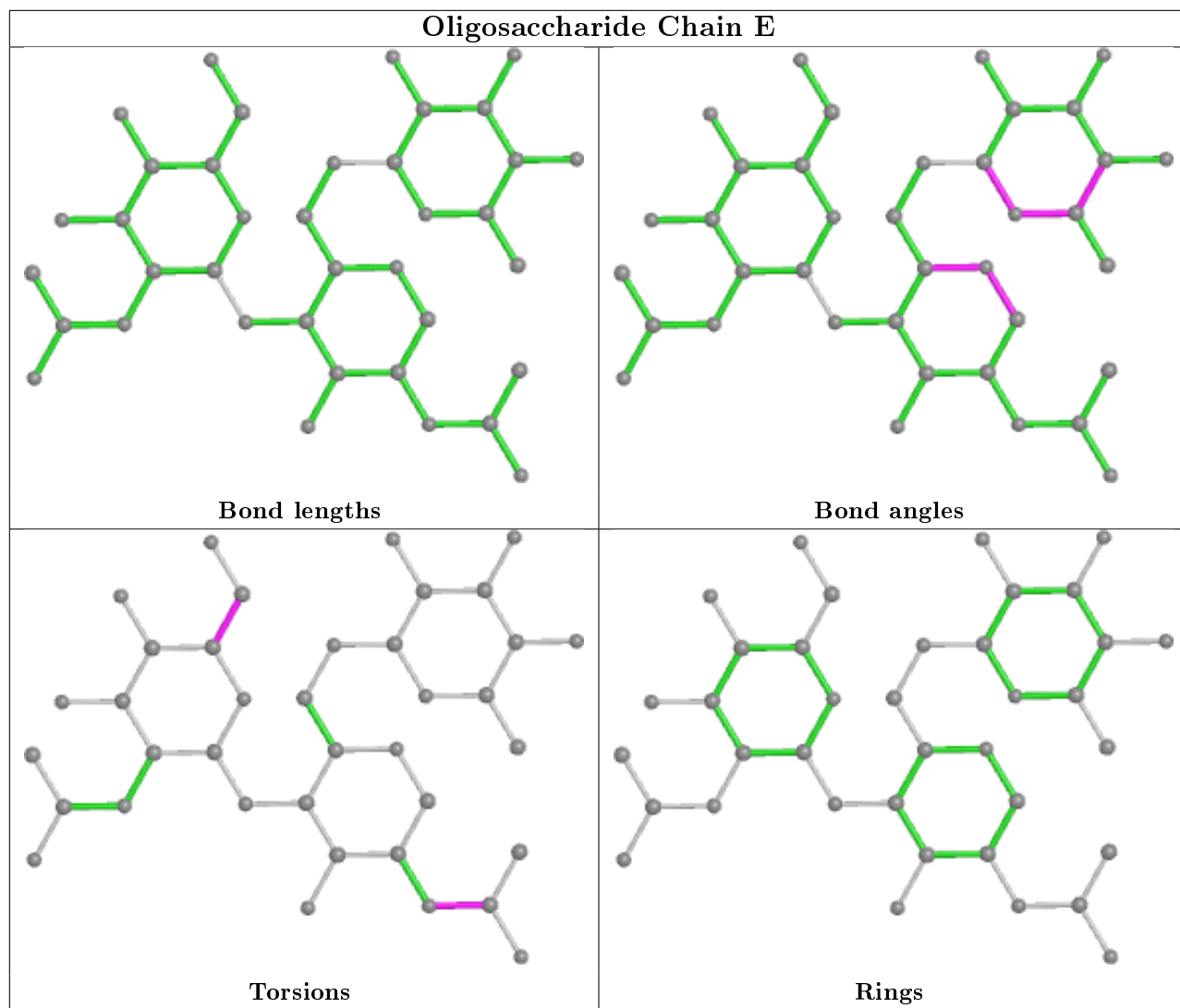
All (3) ring outliers are listed below:

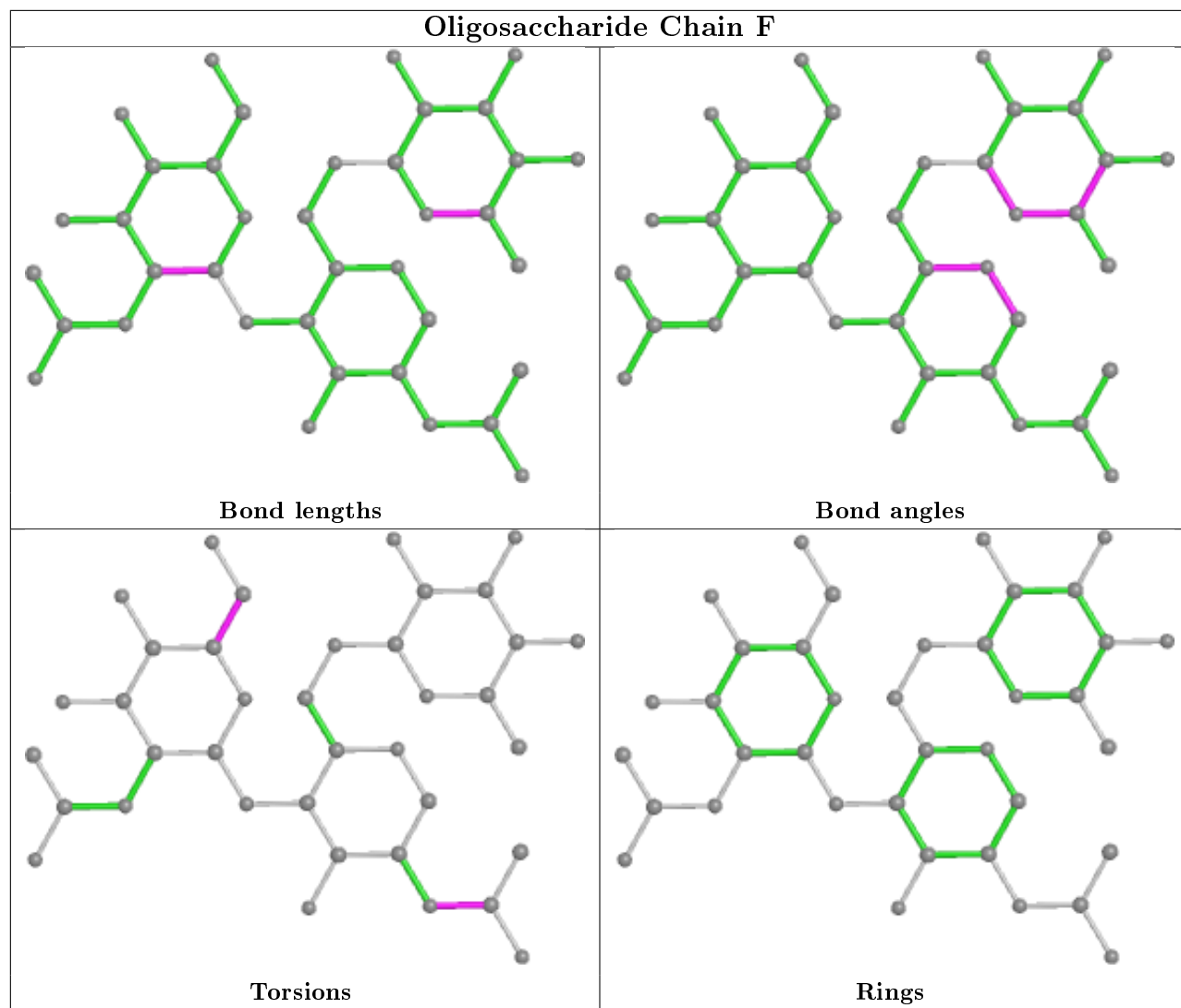
Mol	Chain	Res	Type	Atoms
4	H	3	MAN	C1-C2-C3-C4-C5-O5
4	L	3	MAN	C1-C2-C3-C4-C5-O5
4	L	4	MAN	C1-C2-C3-C4-C5-O5

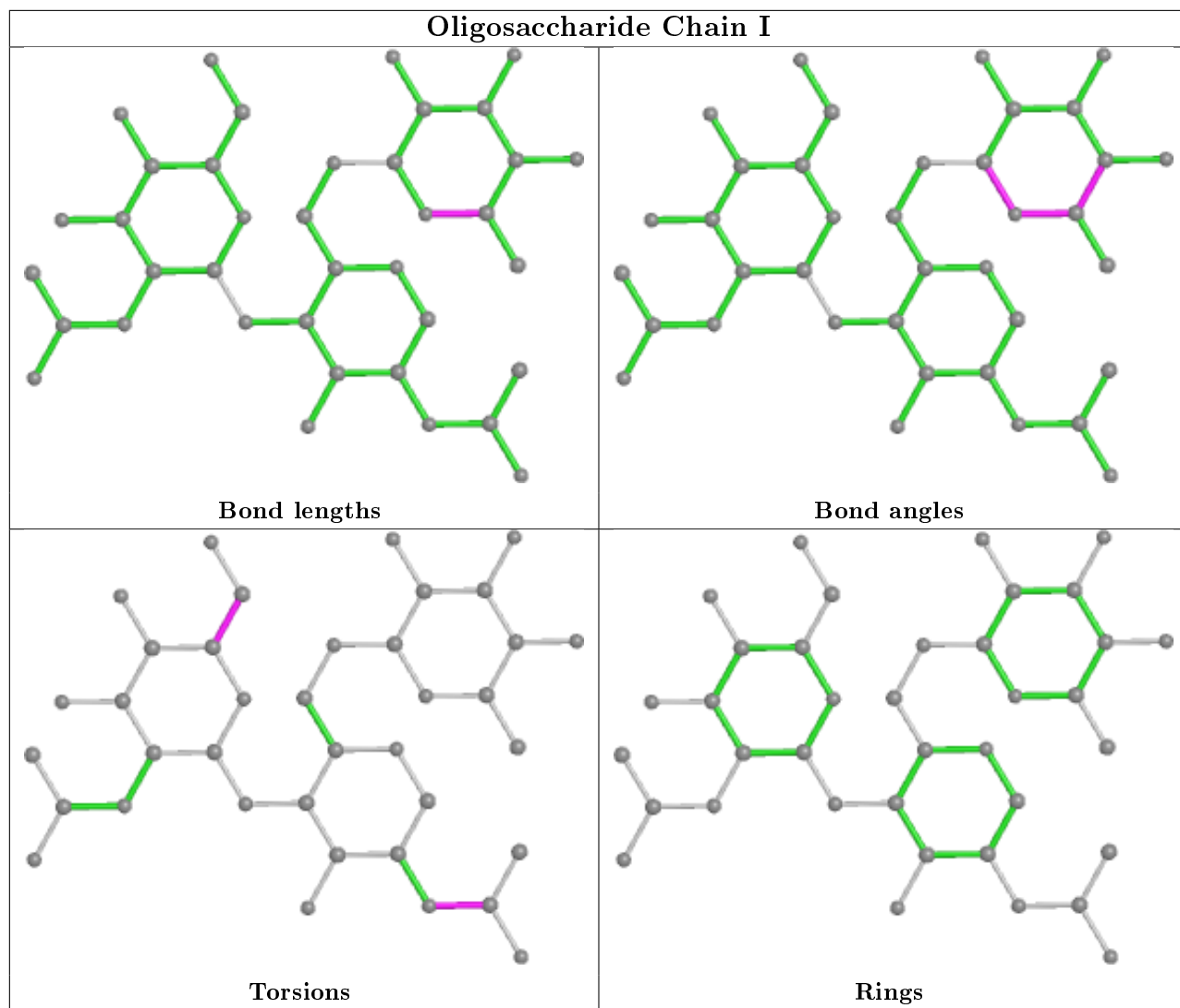
8 monomers are involved in 9 short contacts:

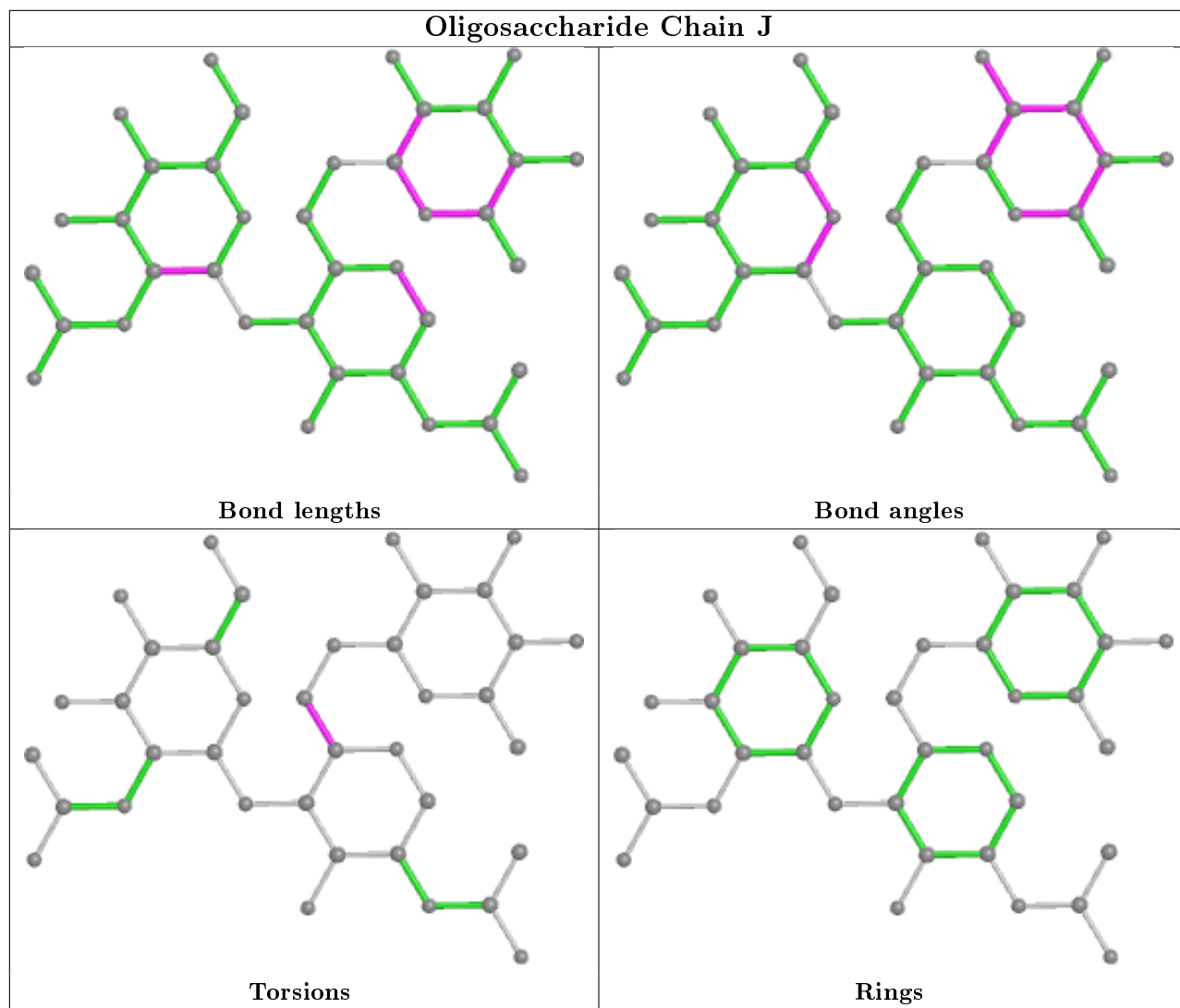
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	3	FUC	1	0
2	J	1	NAG	1	0
2	I	1	NAG	1	0
2	E	3	FUC	1	0
2	F	1	NAG	1	0
5	M	1	NAG	2	0
2	F	3	FUC	1	0
2	E	1	NAG	1	0

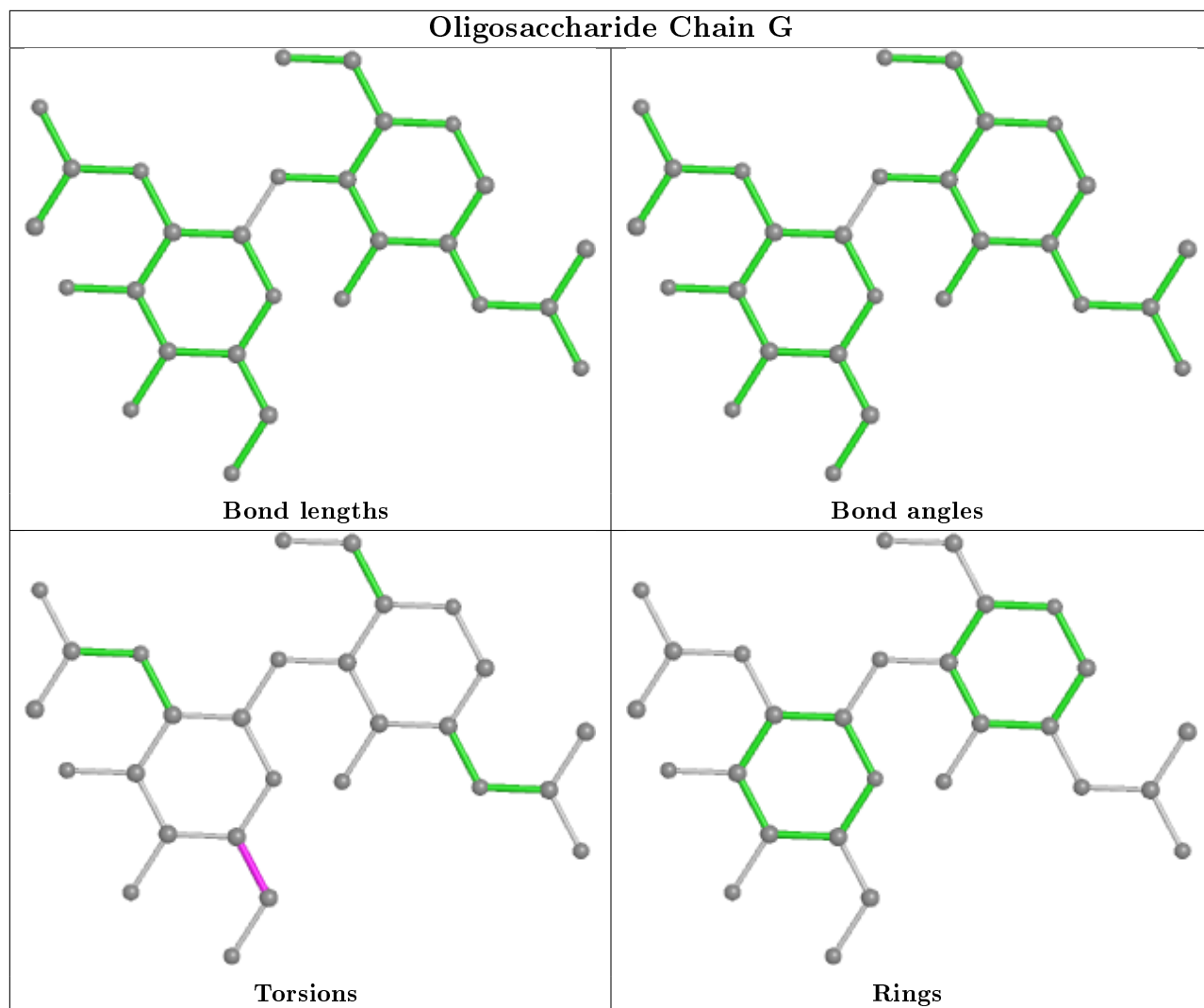
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

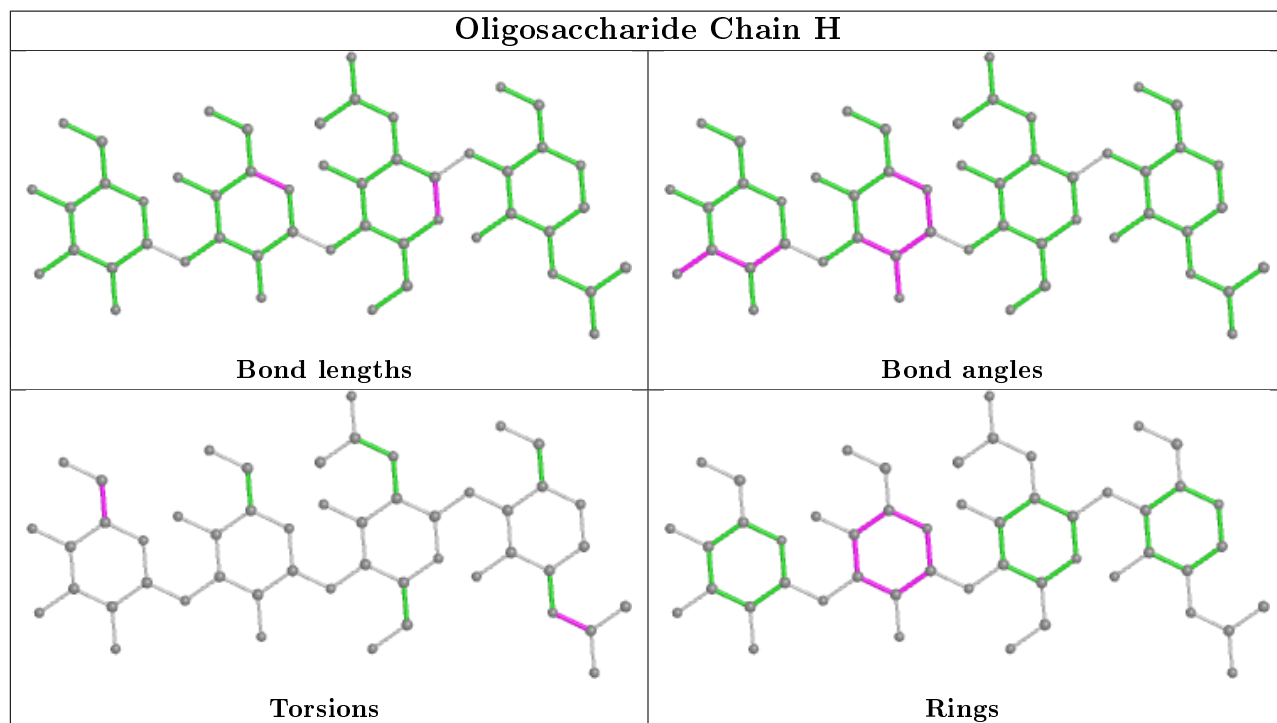
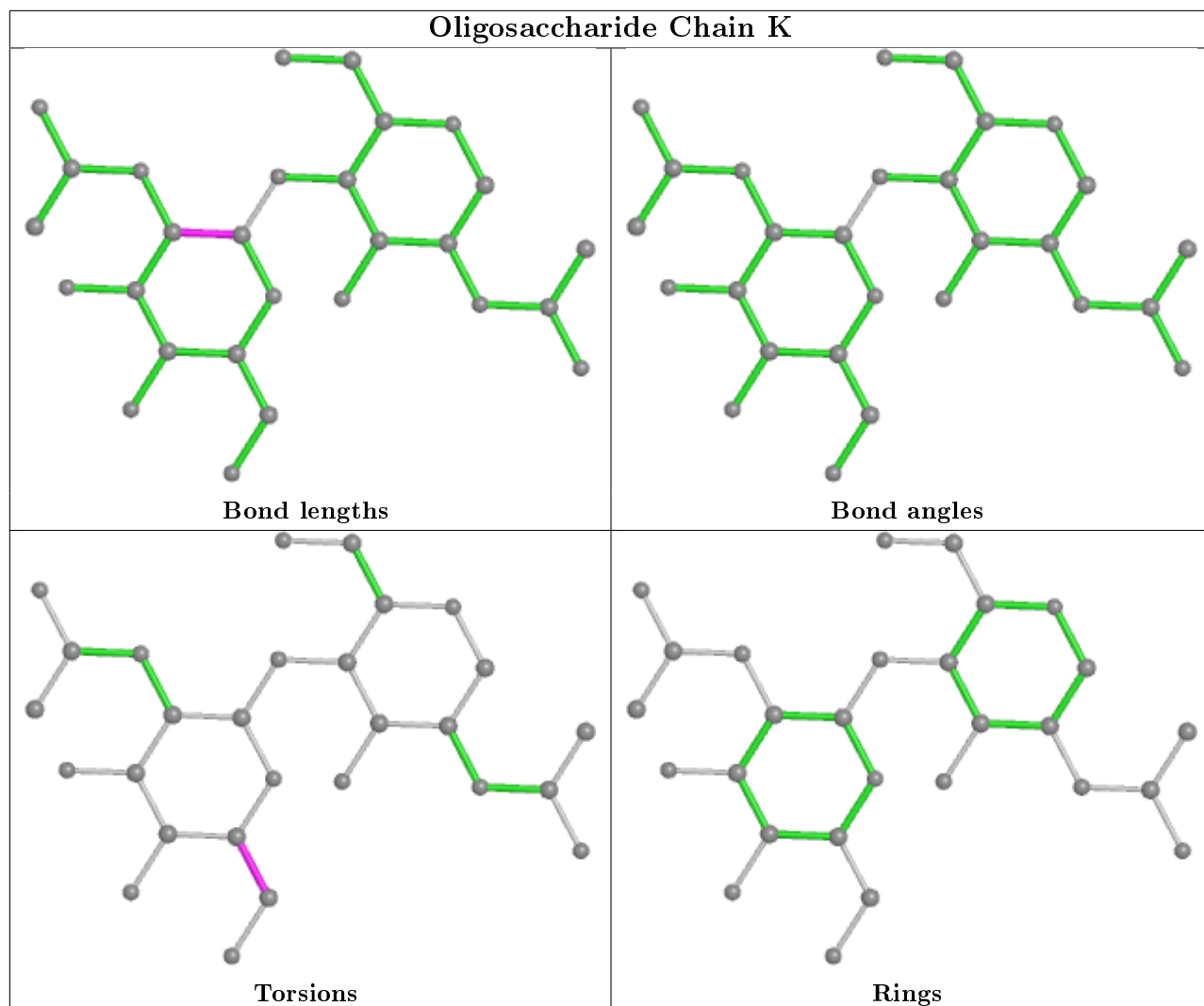


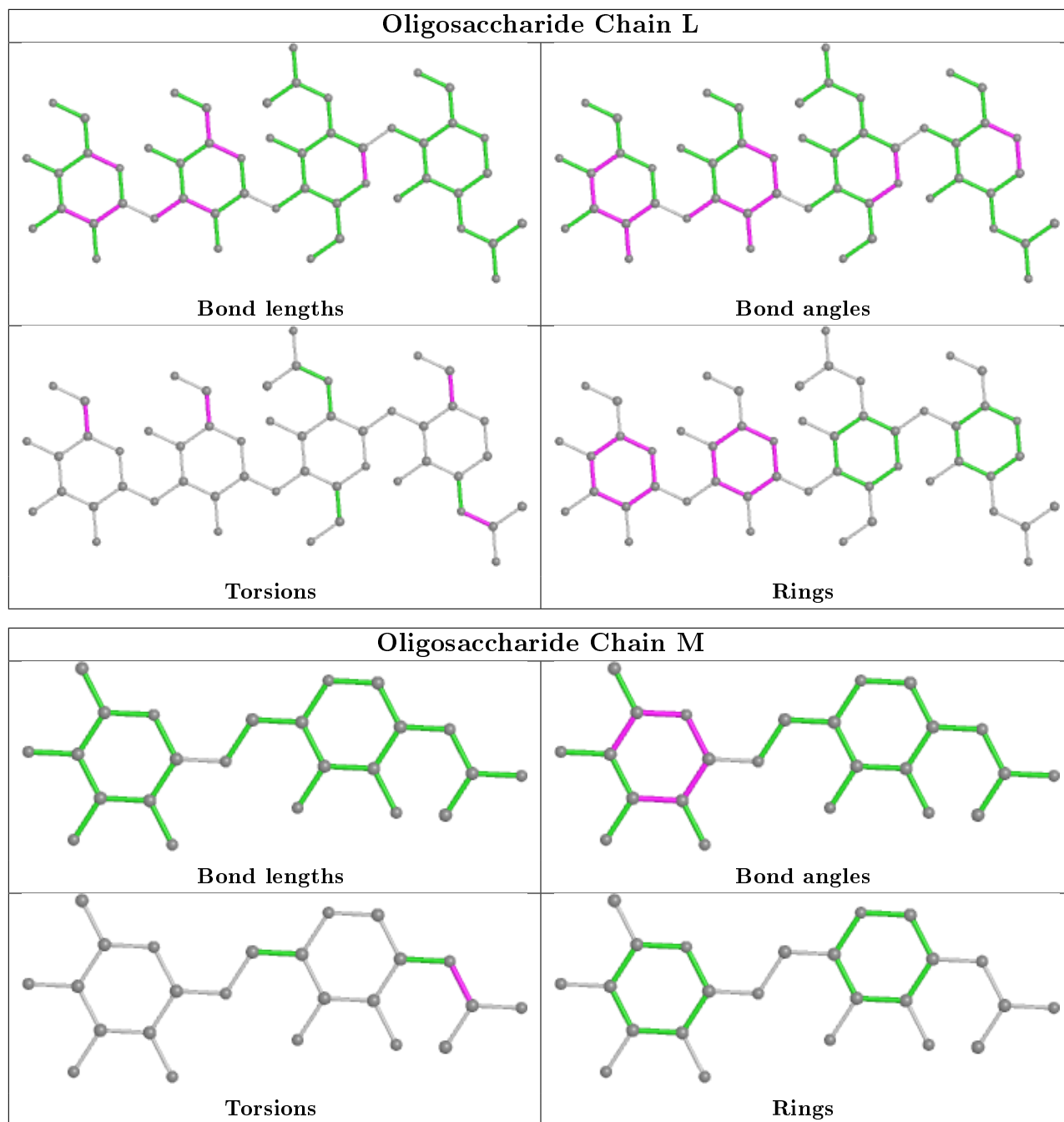












5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 9 are monoatomic - leaving 15 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	511	1	14,14,15	0.51	0	17,19,21	0.65	1 (5%)
6	NAG	C	513	1	14,14,15	1.10	1 (7%)	17,19,21	0.74	1 (5%)
6	NAG	D	506	1	14,14,15	0.32	0	17,19,21	0.82	1 (5%)
6	NAG	A	507	1	14,14,15	0.69	0	17,19,21	0.76	0
6	NAG	D	503	1	14,14,15	1.25	2 (14%)	17,19,21	1.12	2 (11%)
6	NAG	A	505	1	14,14,15	0.60	1 (7%)	17,19,21	0.76	1 (5%)
6	NAG	A	504	1	14,14,15	1.35	2 (14%)	17,19,21	1.42	2 (11%)
8	MMS	C	516	-	10,14,14	4.64	8 (80%)	8,19,19	0.77	0
6	NAG	B	504	1	14,14,15	1.67	3 (21%)	17,19,21	1.30	2 (11%)
6	NAG	A	506	1	14,14,15	0.57	0	17,19,21	0.56	0
6	NAG	D	504	1	14,14,15	0.30	0	17,19,21	0.65	0
8	MMS	A	511	-	10,14,14	4.69	8 (80%)	8,19,19	0.92	0
6	NAG	D	505	1	14,14,15	0.62	0	17,19,21	0.61	0
8	MMS	B	514	-	10,14,14	4.74	7 (70%)	8,19,19	1.05	0
8	MMS	D	509	-	10,14,14	4.75	8 (80%)	8,19,19	0.84	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	511	1	-	1/6/23/26	0/1/1/1
6	NAG	C	513	1	-	2/6/23/26	0/1/1/1
6	NAG	D	506	1	-	0/6/23/26	0/1/1/1
6	NAG	A	507	1	-	0/6/23/26	0/1/1/1
6	NAG	D	503	1	-	0/6/23/26	0/1/1/1
6	NAG	A	505	1	-	0/6/23/26	0/1/1/1
6	NAG	A	504	1	-	0/6/23/26	0/1/1/1
8	MMS	C	516	-	-	2/4/8/8	0/1/1/1
6	NAG	B	504	1	-	0/6/23/26	0/1/1/1
6	NAG	A	506	1	-	2/6/23/26	0/1/1/1
6	NAG	D	504	1	-	0/6/23/26	0/1/1/1
8	MMS	A	511	-	-	2/4/8/8	0/1/1/1
6	NAG	D	505	1	-	2/6/23/26	0/1/1/1
8	MMS	B	514	-	-	2/4/8/8	0/1/1/1
8	MMS	D	509	-	-	2/4/8/8	0/1/1/1

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	514	MMS	C8-N2	10.07	1.50	1.35
8	A	511	MMS	C8-N2	9.07	1.48	1.35
8	C	516	MMS	C8-N2	8.93	1.48	1.35
8	D	509	MMS	C8-N2	8.92	1.48	1.35
8	D	509	MMS	C4-N2	6.77	1.50	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	504	NAG	C4-C3-C2	4.78	118.03	111.02
6	B	504	NAG	C4-C3-C2	4.06	116.96	111.02
6	D	506	NAG	C1-O5-C5	2.93	116.16	112.19
6	D	503	NAG	O5-C5-C4	-2.52	104.70	110.83
6	A	504	NAG	O5-C5-C4	-2.48	104.80	110.83

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	514	MMS	C2-C3-N2-C8
8	B	514	MMS	C2-C3-N2-C4
8	A	511	MMS	C2-C3-N2-C8
8	A	511	MMS	C2-C3-N2-C4
8	C	516	MMS	C2-C3-N2-C8

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	511	NAG	2	0
6	C	513	NAG	2	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	446/446 (100%)	-0.25	6 (1%) 77 75	21, 36, 54, 78	0
1	B	446/446 (100%)	-0.25	6 (1%) 77 75	23, 36, 60, 96	0
1	C	446/446 (100%)	-0.23	3 (0%) 87 86	21, 36, 53, 81	0
1	D	446/446 (100%)	-0.12	14 (3%) 49 47	24, 41, 63, 82	0
All	All	1784/1784 (100%)	-0.21	29 (1%) 72 70	21, 37, 58, 96	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	48	VAL	7.3
1	A	470	SER	5.4
1	D	48	VAL	4.5
1	B	49	SER	3.6
1	A	373	VAL	3.2

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
5	NAG	M	1	14/15	0.78	0.20	56,64,69,71	0
4	MAN	L	4	11/12	0.81	0.17	48,56,62,66	0

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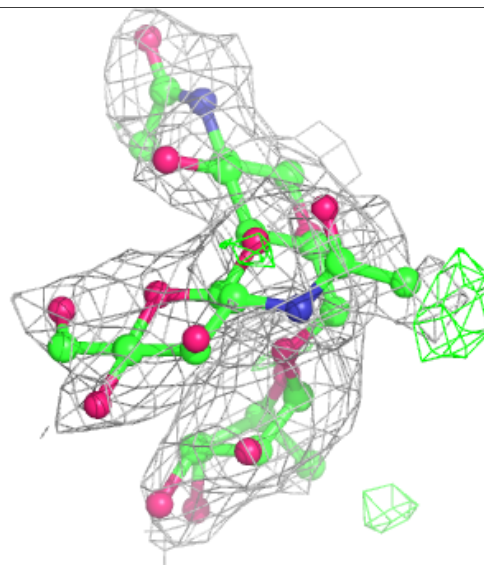
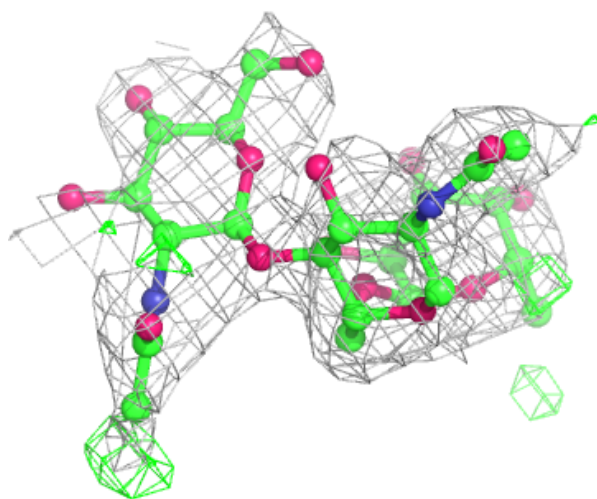
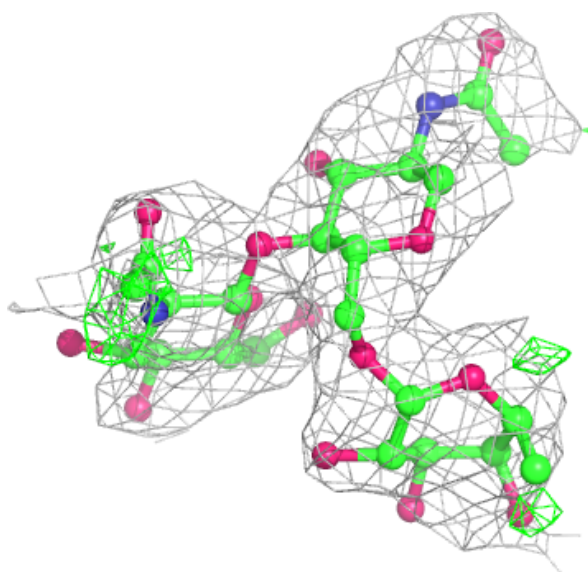
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	J	2	14/15	0.84	0.20	46,52,60,65	0
2	NAG	E	2	14/15	0.84	0.18	60,68,75,77	0
2	NAG	F	2	14/15	0.84	0.19	49,67,76,78	0
2	NAG	I	2	14/15	0.85	0.30	58,73,81,82	0
2	FUC	J	3	10/11	0.86	0.21	51,59,64,64	0
5	FUC	M	2	10/11	0.87	0.23	63,68,75,78	0
2	NAG	E	1	14/15	0.87	0.16	48,54,66,67	0
4	MAN	L	3	11/12	0.87	0.14	36,40,48,52	0
4	NAG	L	1	14/15	0.88	0.15	35,38,40,41	0
3	NAG	G	2	14/15	0.88	0.16	47,53,60,68	0
4	MAN	H	4	11/12	0.88	0.23	55,63,71,71	0
4	MAN	H	3	11/12	0.89	0.13	46,52,56,56	0
2	NAG	J	1	14/15	0.89	0.19	28,44,49,62	0
2	FUC	E	3	10/11	0.90	0.17	50,59,64,67	0
3	NAG	K	2	14/15	0.90	0.21	43,49,65,66	0
2	FUC	F	3	10/11	0.90	0.17	48,53,62,65	0
2	FUC	I	3	10/11	0.91	0.21	47,54,64,67	0
2	NAG	I	1	14/15	0.91	0.17	41,54,61,65	0
2	NAG	F	1	14/15	0.91	0.15	45,56,61,65	0
3	NAG	G	1	14/15	0.96	0.11	35,39,45,46	0
4	NAG	H	1	14/15	0.96	0.12	37,41,46,47	0
4	NAG	L	2	14/15	0.96	0.14	35,39,46,47	0
3	NAG	K	1	14/15	0.96	0.12	35,40,41,43	0
4	NAG	H	2	14/15	0.97	0.11	38,44,47,55	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.

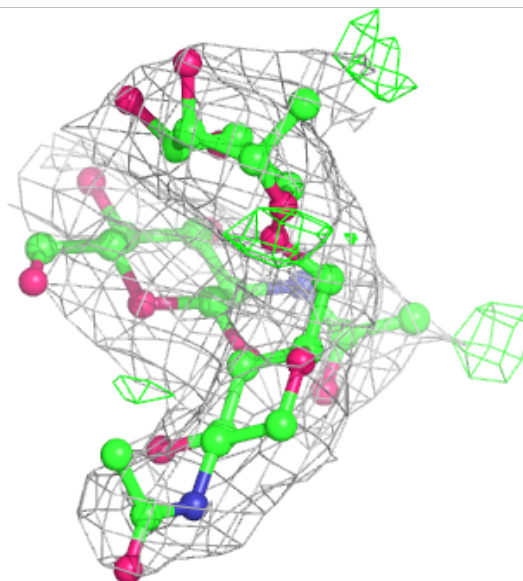
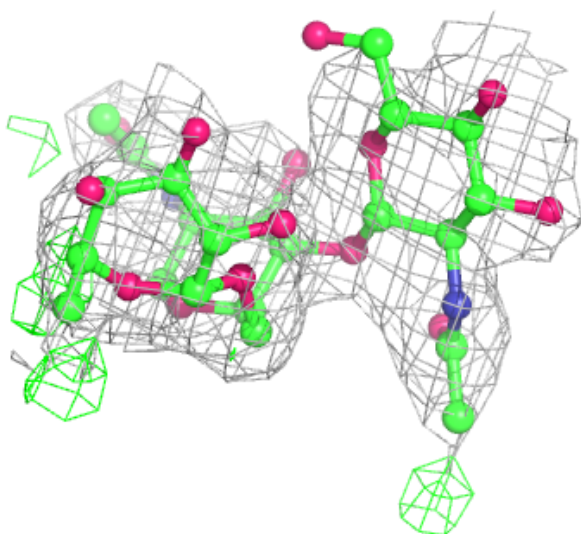
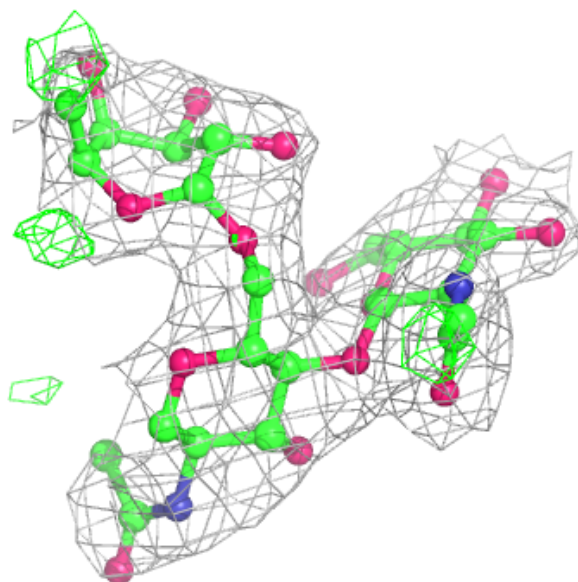
Electron density around Chain E:

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



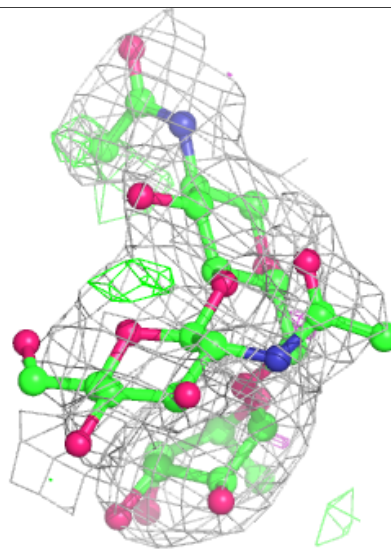
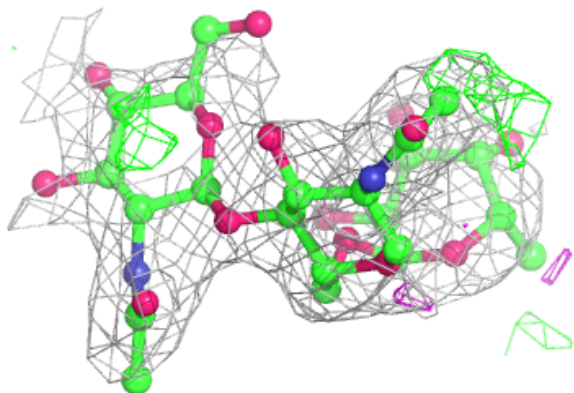
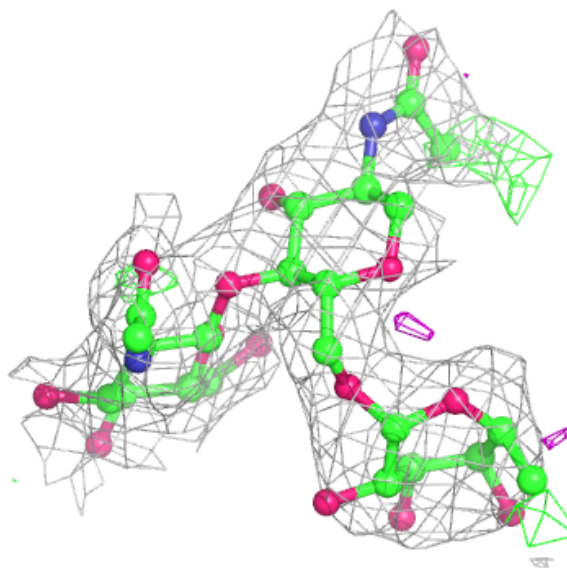
Electron density around Chain F:

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and green (positive)



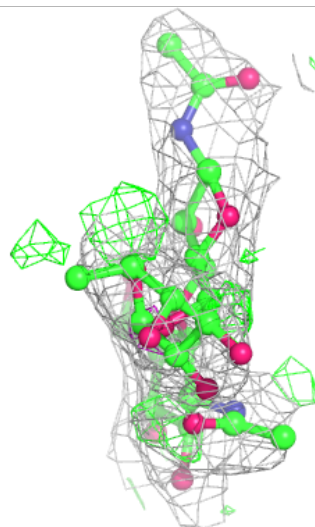
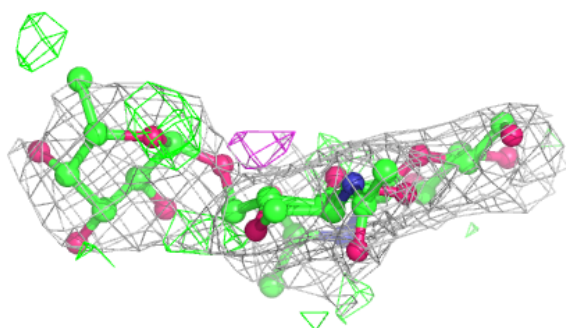
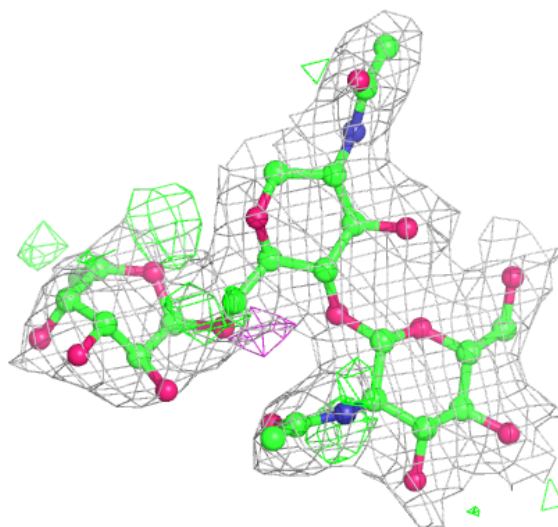
Electron density around Chain I:

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



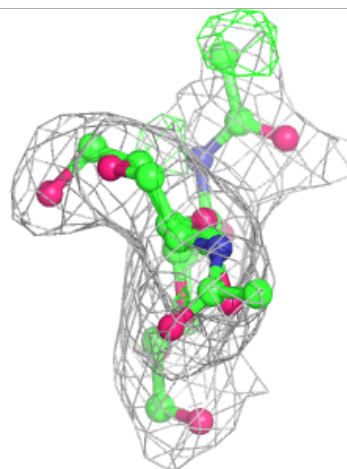
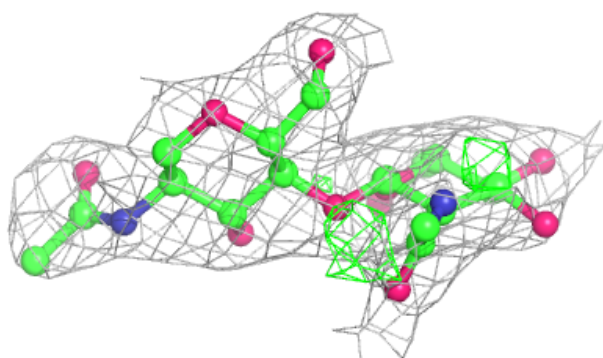
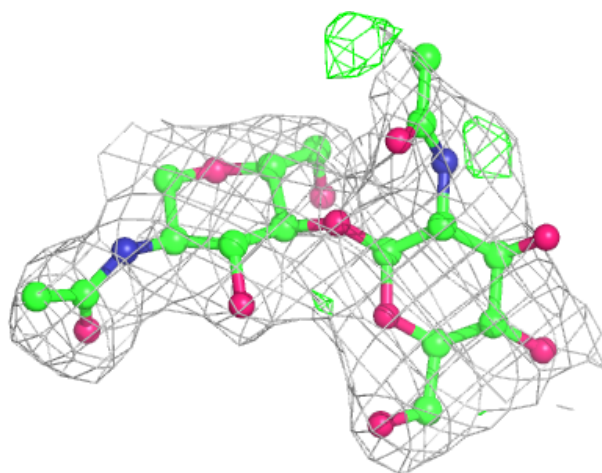
Electron density around Chain J:

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



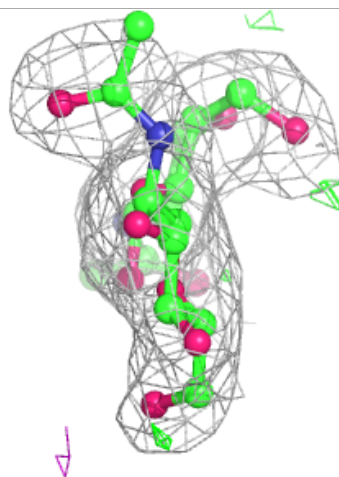
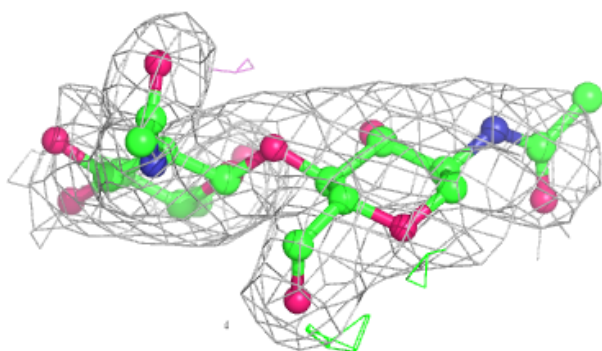
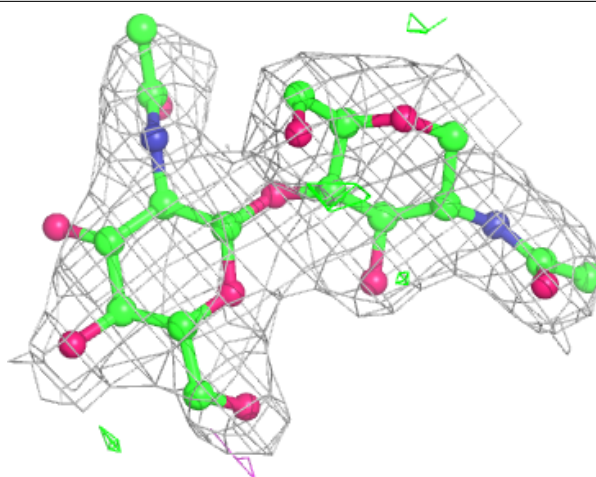
Electron density around Chain G:

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



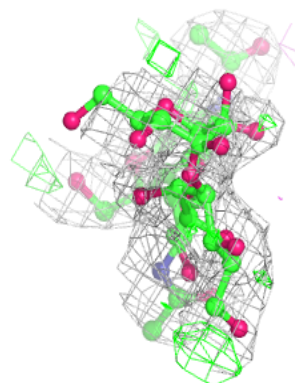
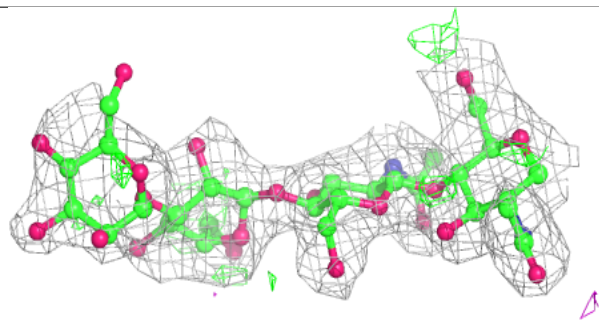
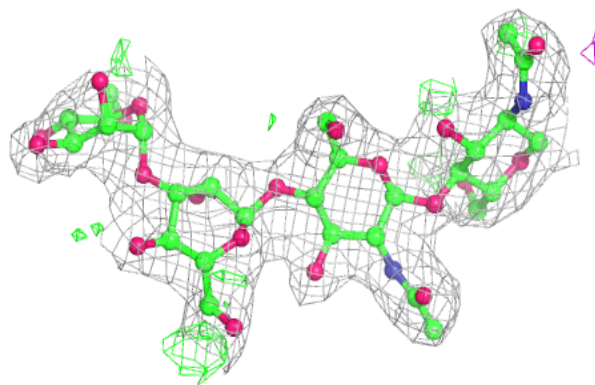
Electron density around Chain K:

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

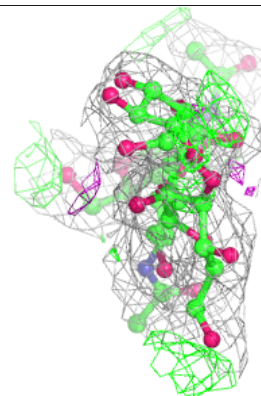
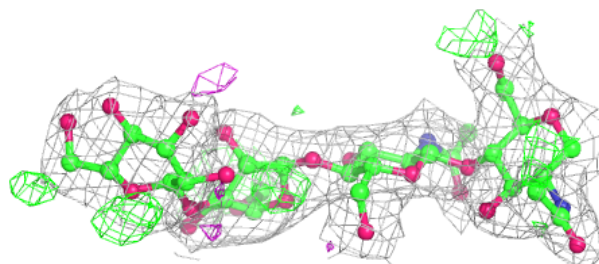
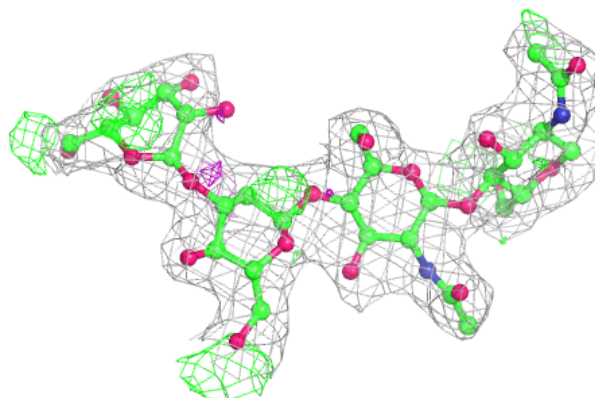


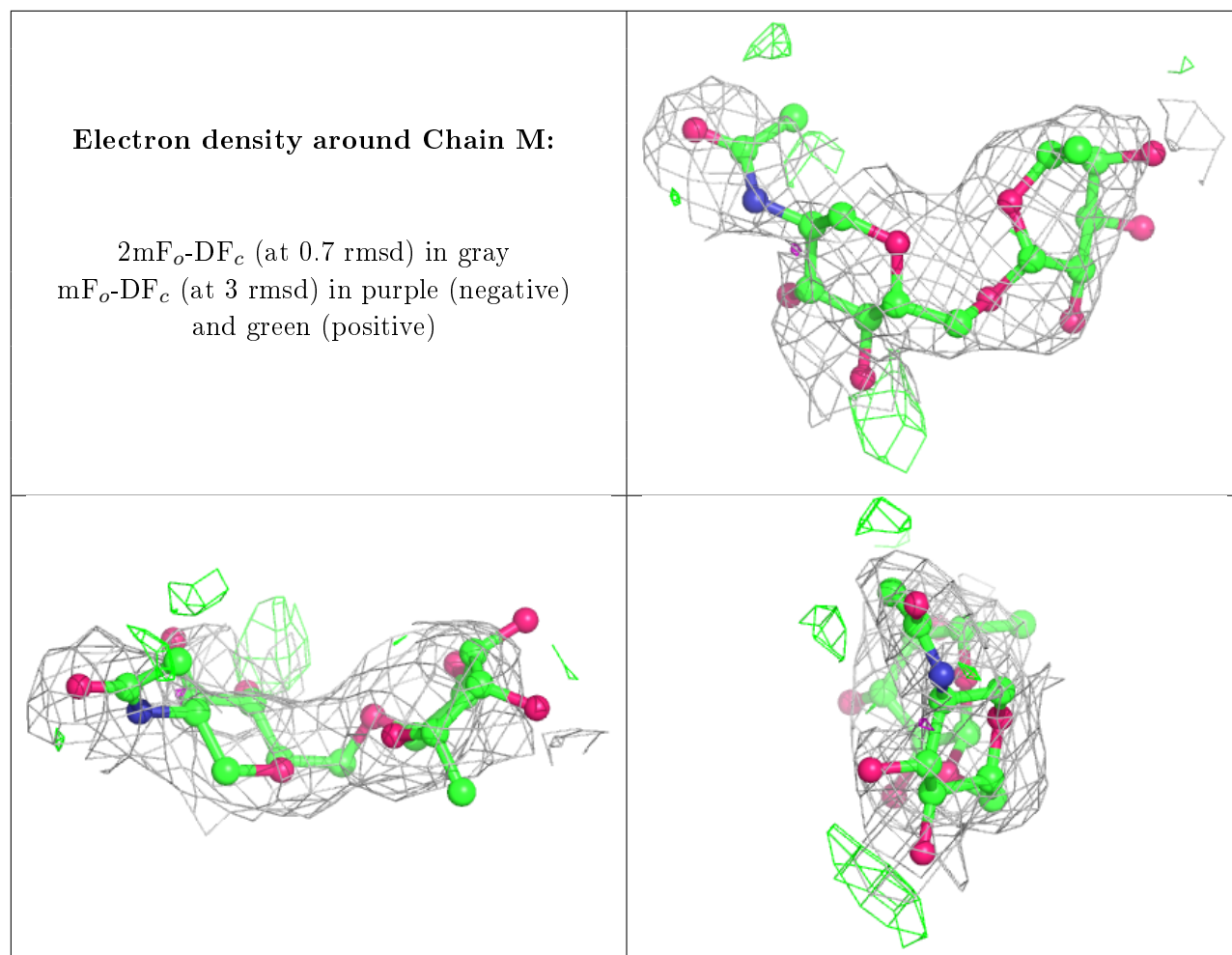
Electron density around Chain H:

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

**Electron density around Chain L:**

$2mF_o-DF_c$ (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
6	NAG	A	504	14/15	0.76	0.24	48,66,71,71	0
6	NAG	D	503	14/15	0.77	0.19	57,65,74,77	0
6	NAG	B	504	14/15	0.79	0.19	51,61,67,70	0
6	NAG	A	506	14/15	0.84	0.17	50,56,64,67	0
6	NAG	D	505	14/15	0.87	0.17	42,56,62,68	0
6	NAG	B	511	14/15	0.89	0.18	40,47,56,57	0
6	NAG	A	507	14/15	0.91	0.14	41,51,56,59	0
6	NAG	A	505	14/15	0.91	0.14	31,37,45,48	0
6	NAG	C	513	14/15	0.91	0.17	41,45,55,59	0
6	NAG	D	506	14/15	0.91	0.17	48,53,58,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NAG	D	504	14/15	0.94	0.18	44,48,51,55	0
8	MMS	C	516	14/14	0.95	0.12	27,33,44,44	0
8	MMS	D	509	14/14	0.95	0.15	34,41,46,46	0
8	MMS	B	514	14/14	0.96	0.12	22,27,34,40	0
8	MMS	A	511	14/14	0.96	0.15	28,31,40,41	0
7	ZN	D	508	1/1	0.99	0.14	31,31,31,31	0
7	ZN	B	513	1/1	1.00	0.13	23,23,23,23	0
7	ZN	D	507	1/1	1.00	0.15	32,32,32,32	0
7	ZN	B	512	1/1	1.00	0.14	24,24,24,24	0
7	ZN	A	510	1/1	1.00	0.12	46,46,46,46	0
7	ZN	C	515	1/1	1.00	0.14	23,23,23,23	0
7	ZN	A	508	1/1	1.00	0.16	28,28,28,28	0
7	ZN	C	514	1/1	1.00	0.12	24,24,24,24	0
7	ZN	A	509	1/1	1.00	0.16	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.