



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 25, 2024 – 03:21 PM EST

PDB ID : 1IVG
Title : STRUCTURES OF AROMATIC INHIBITORS OF INFLUENZA VIRUS
NEURAMINIDASE
Authors : Jedrzejewski, M.J.; Luo, M.
Deposited on : 1994-12-12
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

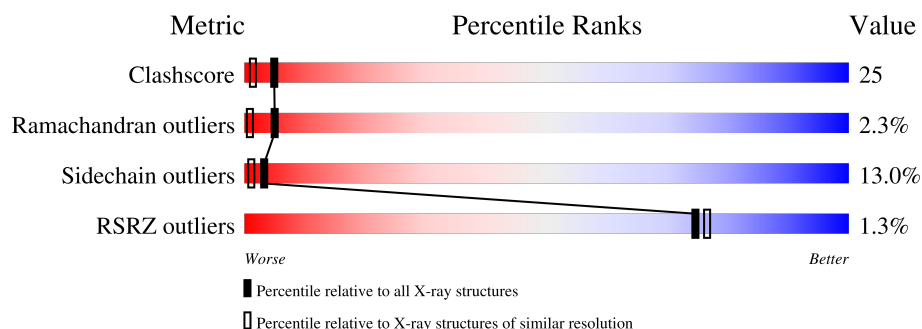
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 1.90 Å.

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






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	388	 61% 31% 7% •
1	B	388	 63% 29% 7% •
2	C	2	 100%
2	E	2	 50% 50%
2	G	2	 100%
2	J	2	 50% 50%
3	D	4	 75% 25%

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Mol	Chain	Length	Quality of chain
4	F	6	 100%
4	I	6	 100%
5	H	4	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	F	1	-	-	X	-
4	MAN	F	4	-	-	X	-
4	MAN	F	6	-	-	X	-
4	MAN	I	4	-	-	X	-
4	MAN	I	5	-	-	X	-
5	FUC	H	4	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8557 atoms, of which 2032 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 INFLUENZA A SUBTYPE N2 NEURAMINIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	388	Total	C	H	N	O	S	0	0	0
			3745	1866	723	545	588	23			
1	B	388	Total	C	H	N	O	S	0	0	0
			3745	1866	723	545	588	23			

There are 2 discrepancies between the modelled and reference sequences:

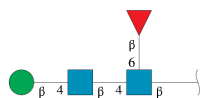
Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	ASN	conflict	UNP P06820
B	339	ASP	ASN	conflict	UNP P06820

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



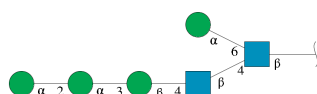
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	2	Total	C	H	N	O		0	0	0
			55	16	27	2	10				
2	E	2	Total	C	H	N	O		0	0	0
			55	16	27	2	10				
2	G	2	Total	C	H	N	O		0	0	0
			55	16	27	2	10				
2	J	2	Total	C	H	N	O		0	0	0
			55	16	27	2	10				

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



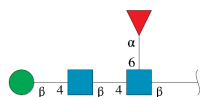
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	4	Total	C	H	N	O	0	0	0
			96	28	47	2	19			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	6	Total	C	H	N	O	0	0	0
			139	40	67	2	30			
4	I	6	Total	C	H	N	O	0	0	0
			139	40	67	2	30			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-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
5	H	4	Total	C	H	N	O	0	0	0
			96	28	47	2	19			

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

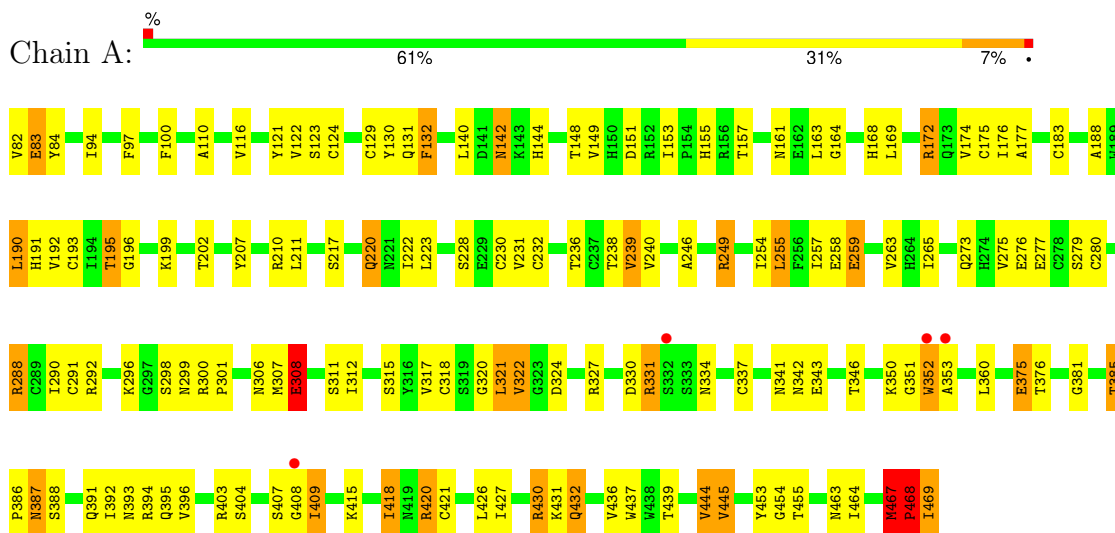
- Molecule 7 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	120	Total	H	O	0	0
			360	240	120		
7	B	5	Total	H	O	0	0
			15	10	5		

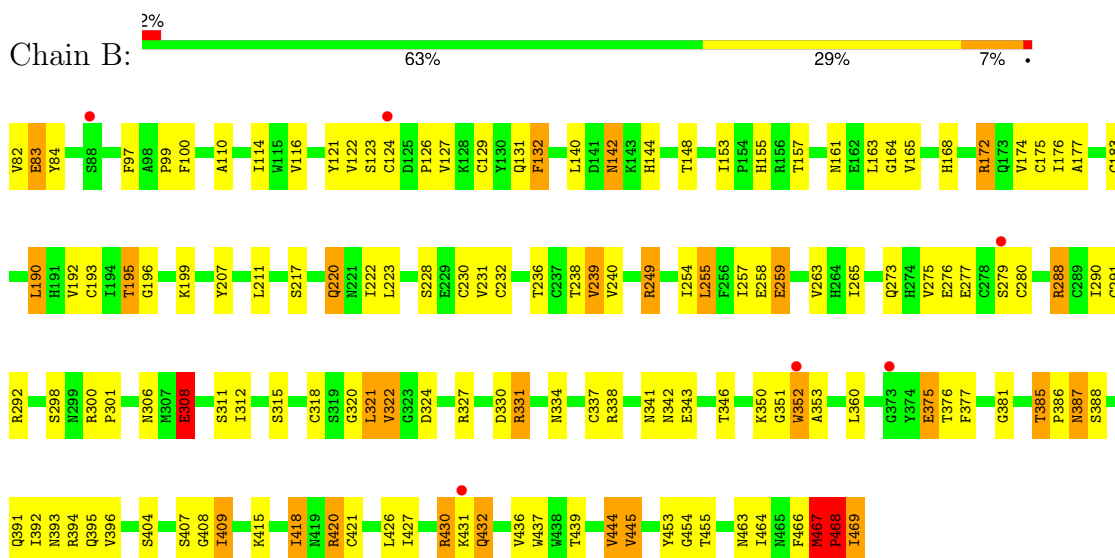
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: INFLUENZA A SUBTYPE N2 NEURAMINIDASE



• Molecule 1: INFLUENZA A SUBTYPE N2 NEURAMINIDASE



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



MAG1
MAG2


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

Chain E:  50% 50%MAG1
MAG2

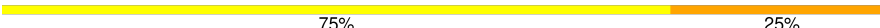
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%MAG1
MAG2

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

Chain J:  50% 50%MAG1
MAG2

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

Chain D:  75% 25%MAG1
MAG2
BMA3
FUL4

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

Chain F:  100%MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

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

Chain I:  100%MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

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

Chain H:

100%

MAG1
MAG2
BMA3
FUC4

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	120.97Å 141.14Å 142.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 1.90 5.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (5.00-1.90) 35.1 (5.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 1.80Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.205 , (Not available) 0.256 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.54 , 91.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8557	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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: BMA, MAN, FUL, FUC, CA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.55	0/3092	0.84	3/4194 (0.1%)
1	B	0.55	0/3092	0.84	3/4194 (0.1%)
All	All	0.55	0/6184	0.84	6/8388 (0.1%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	467	MET	N-CA-C	6.16	127.63	111.00
1	B	467	MET	N-CA-C	6.16	127.63	111.00
1	A	468	PRO	CA-N-CD	-5.38	103.96	111.50
1	B	468	PRO	CA-N-CD	-5.38	103.96	111.50
1	A	190	LEU	CA-CB-CG	5.15	127.15	115.30

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	3022	723	2851	136	75
1	B	3022	723	2850	167	4
2	C	28	27	25	2	0
2	E	28	27	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	28	27	25	2	0
2	J	28	27	25	1	0
3	D	49	47	43	1	0
4	F	72	67	49	49	0
4	I	72	67	59	2	74
5	H	49	47	43	0	0
6	A	1	0	0	1	0
6	B	1	0	0	0	0
7	A	120	240	0	18	3
7	B	5	10	0	2	0
All	All	6525	2032	5995	306	78

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 25.

The worst 5 of 306 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:TYR:HD1	4:F:1:NAG:C8	1.33	1.41
1:B:453:TYR:CD1	4:F:1:NAG:C8	2.04	1.38
1:B:453:TYR:CD1	4:F:1:NAG:H81	1.64	1.27
1:B:377:PHE:HB3	4:F:4:MAN:H3	1.25	1.14
1:B:394:ARG:HD3	4:F:3:BMA:H3	1.14	1.14

The worst 5 of 78 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ARG:CB	4:I:4:MAN:C2[4_555]	0.65	1.55
1:A:394:ARG:N	4:I:5:MAN:C1[4_555]	0.82	1.38
1:A:394:ARG:CA	4:I:4:MAN:O2[4_555]	0.91	1.29
1:A:394:ARG:CA	4:I:5:MAN:C1[4_555]	1.10	1.10
1:A:391:GLN:OE1	4:I:4:MAN:C4[4_555]	1.11	1.09

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	386/388 (100%)	344 (89%)	33 (8%)	9 (2%)	5	1
1	B	386/388 (100%)	344 (89%)	33 (8%)	9 (2%)	5	1
All	All	772/776 (100%)	688 (89%)	66 (8%)	18 (2%)	5	1

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	VAL
1	A	467	MET
1	A	468	PRO
1	B	322	VAL
1	B	467	MET

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	338/338 (100%)	294 (87%)	44 (13%)	3	1
1	B	338/338 (100%)	294 (87%)	44 (13%)	3	1
All	All	676/676 (100%)	588 (87%)	88 (13%)	3	1

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	231	VAL

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Mol	Chain	Res	Type
1	B	346	THR
1	B	239	VAL
1	B	288	ARG
1	B	387	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	142	ASN
1	B	393	ASN
1	B	387	ASN
1	B	395	GLN
1	A	393	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

28 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	1,2	14,14,15	1.41	3 (21%)	17,19,21	2.43	8 (47%)
2	NAG	C	2	2	14,14,15	1.63	3 (21%)	17,19,21	2.87	6 (35%)
3	NAG	D	1	3,1	14,14,15	1.29	1 (7%)	17,19,21	3.56	5 (29%)
3	NAG	D	2	3	14,14,15	1.48	2 (14%)	17,19,21	2.90	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	D	3	3	11,11,12	1.25	1 (9%)	15,15,17	1.66	4 (26%)
3	FUL	D	4	3	10,10,11	1.24	1 (10%)	14,14,16	1.15	1 (7%)
2	NAG	E	1	1,2	14,14,15	1.39	2 (14%)	17,19,21	2.05	5 (29%)
2	NAG	E	2	2	14,14,15	1.09	2 (14%)	17,19,21	2.06	3 (17%)
4	NAG	F	1	4,1	14,14,15	1.58	3 (21%)	17,19,21	3.57	6 (35%)
4	NAG	F	2	4	14,14,15	2.35	7 (50%)	17,19,21	3.84	9 (52%)
4	BMA	F	3	4	11,11,12	3.64	8 (72%)	15,15,17	2.04	5 (33%)
4	MAN	F	4	4	11,11,12	2.19	4 (36%)	15,15,17	2.37	5 (33%)
4	MAN	F	5	4	11,11,12	1.39	1 (9%)	15,15,17	1.19	2 (13%)
4	MAN	F	6	4	11,11,12	1.73	2 (18%)	15,15,17	2.93	8 (53%)
2	NAG	G	1	1,2	14,14,15	1.41	3 (21%)	17,19,21	2.43	8 (47%)
2	NAG	G	2	2	14,14,15	1.63	3 (21%)	17,19,21	2.87	6 (35%)
5	NAG	H	1	5,1	14,14,15	1.29	1 (7%)	17,19,21	3.56	5 (29%)
5	NAG	H	2	5	14,14,15	1.48	2 (14%)	17,19,21	2.90	6 (35%)
5	BMA	H	3	5	11,11,12	1.25	1 (9%)	15,15,17	1.66	4 (26%)
5	FUC	H	4	5	10,10,11	1.24	1 (10%)	14,14,16	1.15	1 (7%)
4	NAG	I	1	4,1	14,14,15	1.58	3 (21%)	17,19,21	3.57	6 (35%)
4	NAG	I	2	4	14,14,15	2.35	7 (50%)	17,19,21	3.84	9 (52%)
4	BMA	I	3	4	11,11,12	3.64	8 (72%)	15,15,17	2.04	5 (33%)
4	MAN	I	4	4	11,11,12	2.19	4 (36%)	15,15,17	2.37	5 (33%)
4	MAN	I	5	4	11,11,12	1.39	1 (9%)	15,15,17	1.19	2 (13%)
4	MAN	I	6	4	11,11,12	1.73	2 (18%)	15,15,17	2.93	8 (53%)
2	NAG	J	1	1,2	14,14,15	1.39	2 (14%)	17,19,21	2.05	5 (29%)
2	NAG	J	2	2	14,14,15	1.09	2 (14%)	17,19,21	2.06	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	FUL	D	4	3	-	-	0/1/1/1

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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	-	3/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	3/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	1/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	MAN	F	5	4	-	2/2/19/22	0/1/1/1
4	MAN	F	6	4	-	2/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	3/6/23/26	0/1/1/1
5	NAG	H	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	H	2	5	-	1/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	FUC	H	4	5	1/1/5/5	-	0/1/1/1
4	NAG	I	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	I	2	4	-	3/6/23/26	0/1/1/1
4	BMA	I	3	4	-	1/2/19/22	1/1/1/1
4	MAN	I	4	4	-	0/2/19/22	0/1/1/1
4	MAN	I	5	4	-	2/2/19/22	0/1/1/1
4	MAN	I	6	4	-	2/2/19/22	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	3/6/23/26	0/1/1/1

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	3	BMA	C2-C3	6.29	1.62	1.52
4	I	3	BMA	C2-C3	6.29	1.62	1.52
4	F	3	BMA	C4-C5	6.23	1.66	1.53
4	I	3	BMA	C4-C5	6.23	1.66	1.53
4	F	2	NAG	C4-C3	4.80	1.64	1.52

The worst 5 of 146 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	NAG	C1-C2-N2	10.90	127.61	110.43
5	H	1	NAG	C1-C2-N2	10.90	127.61	110.43
4	F	1	NAG	C6-C5-C4	10.12	137.86	113.02
4	I	1	NAG	C6-C5-C4	10.12	137.86	113.02
4	F	2	NAG	C1-C2-N2	8.60	123.98	110.43

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	H	4	FUC	C1

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C1-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7
2	G	2	NAG	C1-C2-N2-C7
2	J	2	NAG	C3-C2-N2-C7
3	D	1	NAG	C1-C2-N2-C7

All (2) ring outliers are listed below:

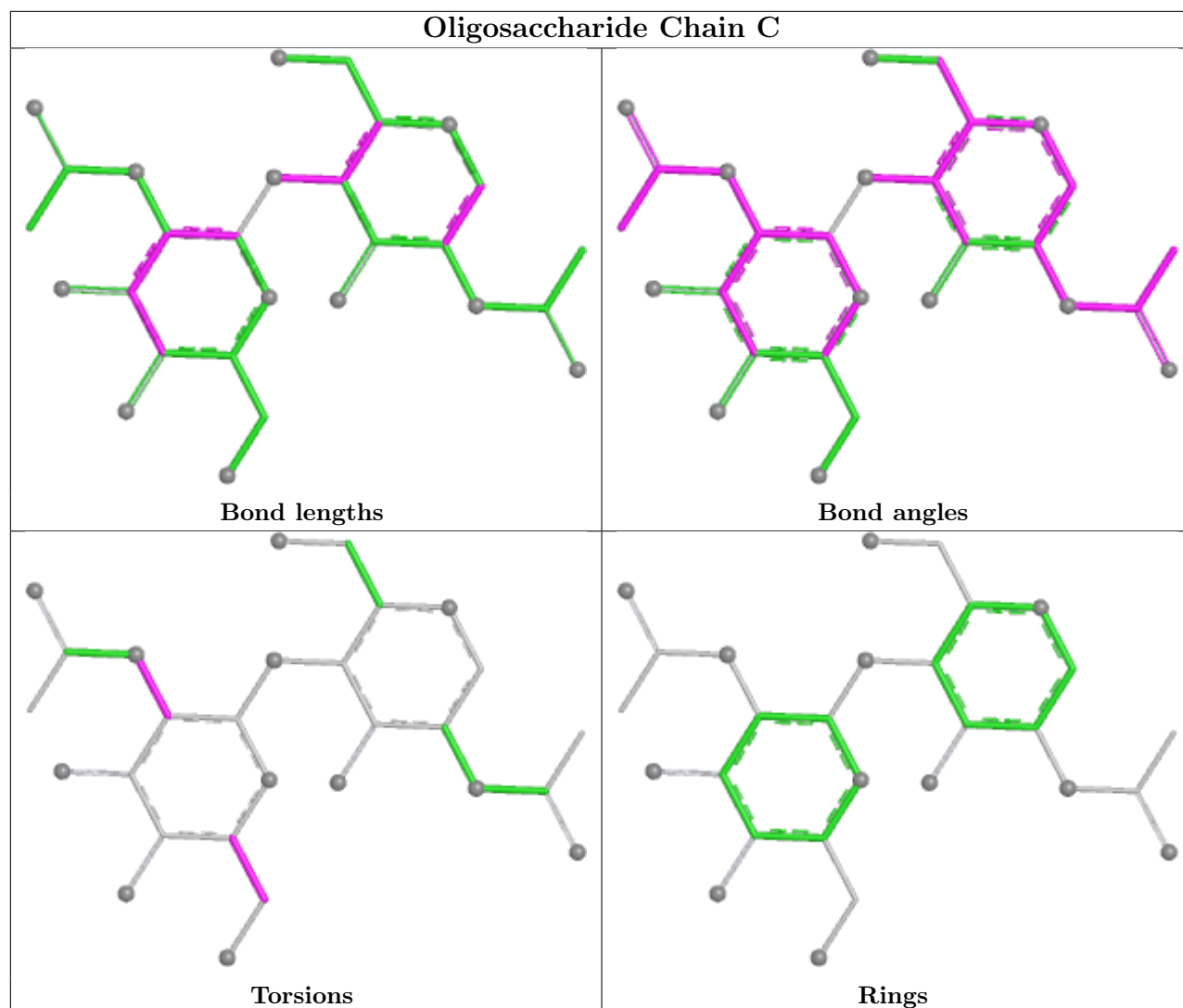
Mol	Chain	Res	Type	Atoms
4	F	3	BMA	C1-C2-C3-C4-C5-O5
4	I	3	BMA	C1-C2-C3-C4-C5-O5

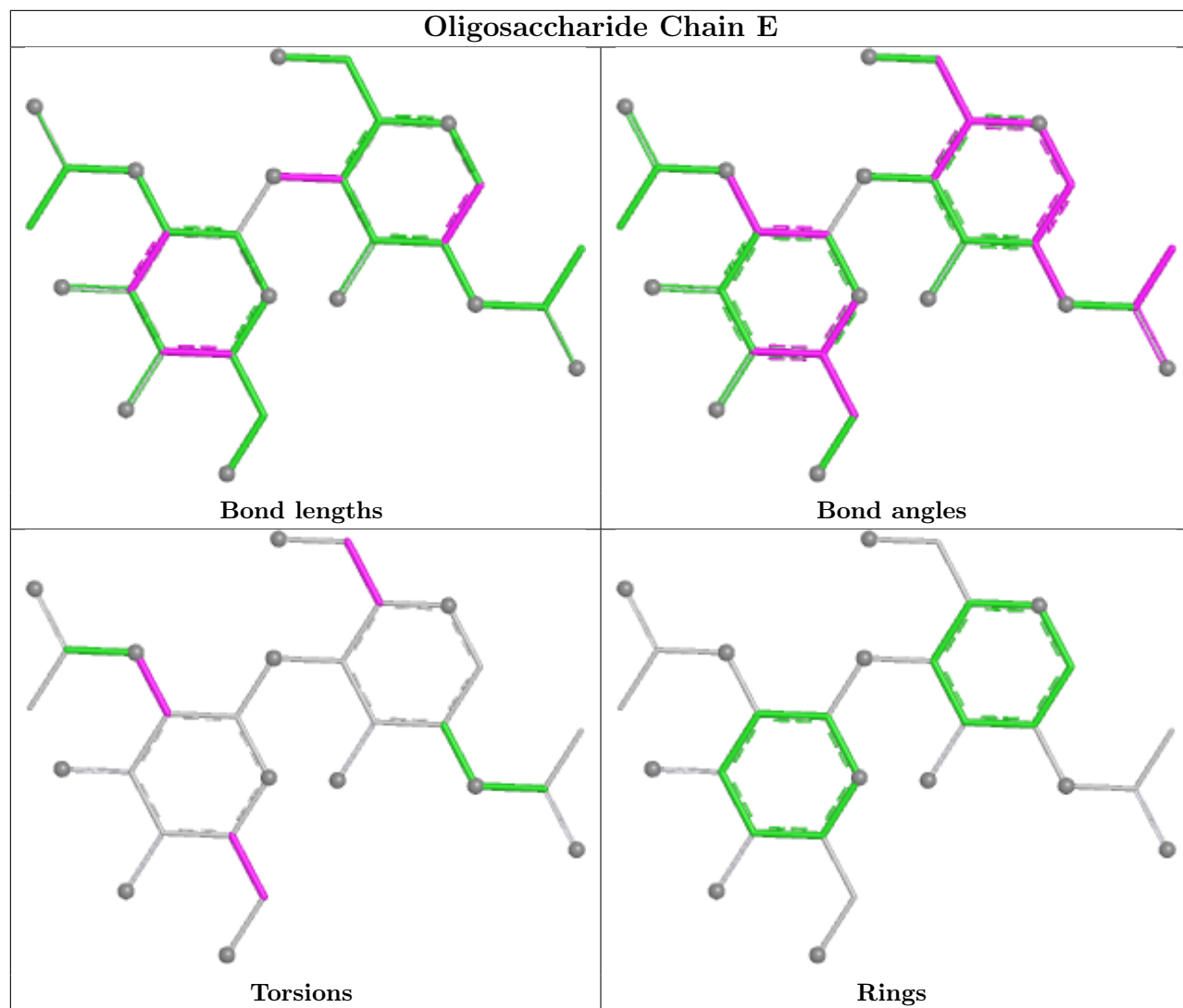
19 monomers are involved in 132 short contacts:

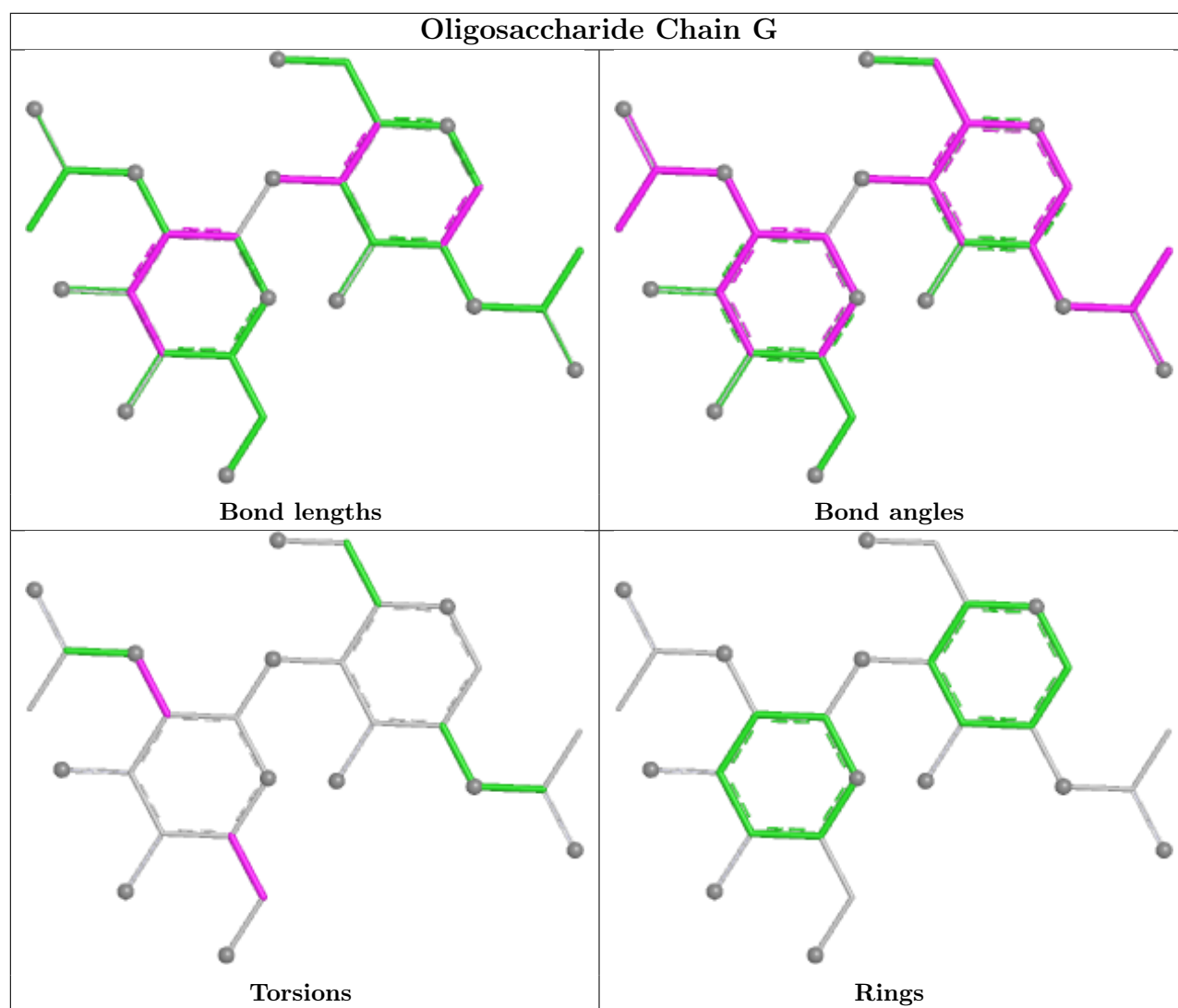
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	NAG	2	0
4	F	2	NAG	2	0
2	G	1	NAG	2	0
4	F	5	MAN	4	0
4	I	6	MAN	0	2
3	D	4	FUL	1	0
4	F	4	MAN	12	0
4	I	4	MAN	0	28
4	F	3	BMA	4	0
4	F	6	MAN	9	0
4	I	3	BMA	1	0
2	C	1	NAG	2	0
4	F	1	NAG	20	0
4	I	1	NAG	1	3
2	E	2	NAG	1	0
4	I	2	NAG	2	0
2	J	2	NAG	1	0
4	I	5	MAN	0	41
2	C	2	NAG	2	0

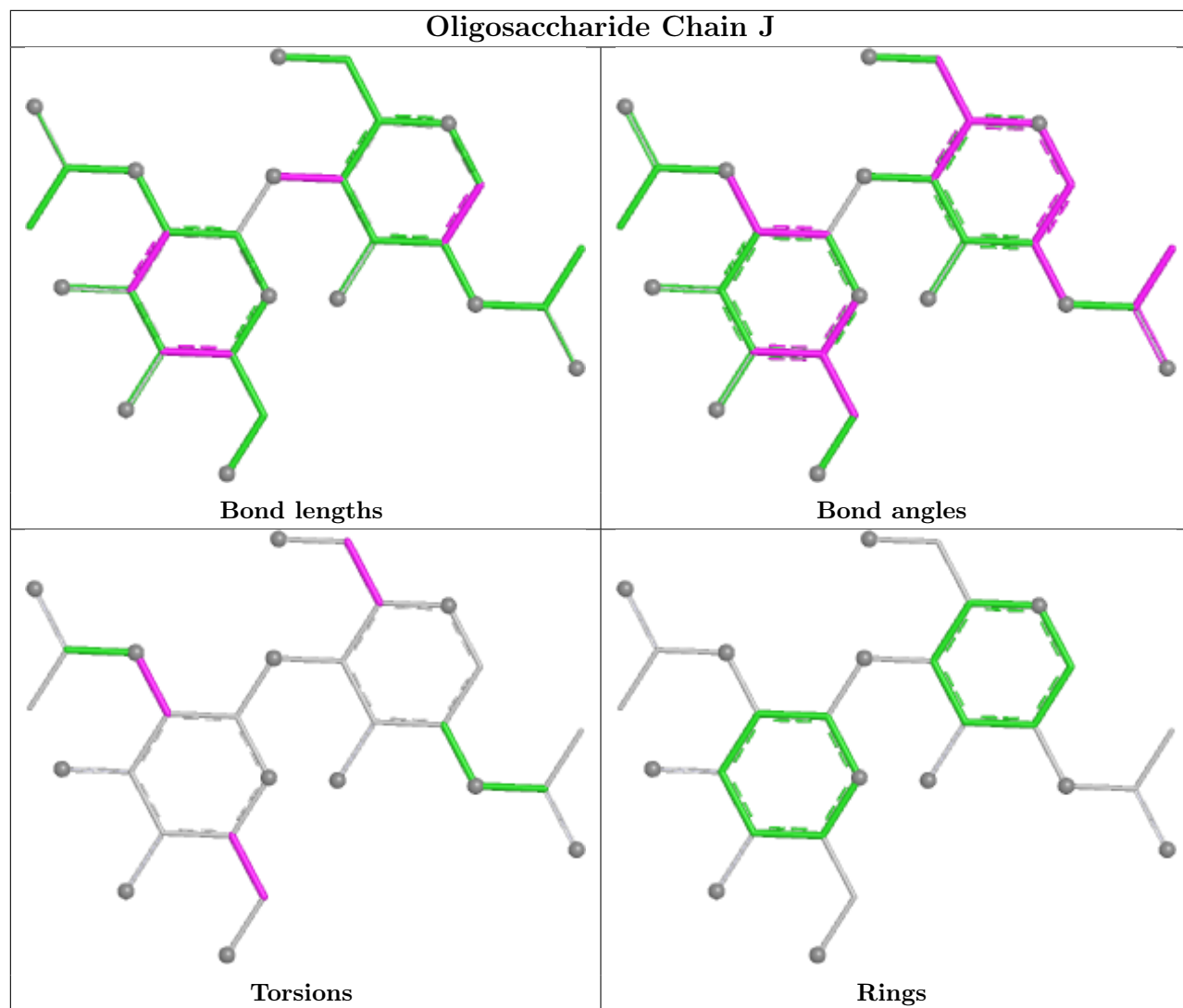
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

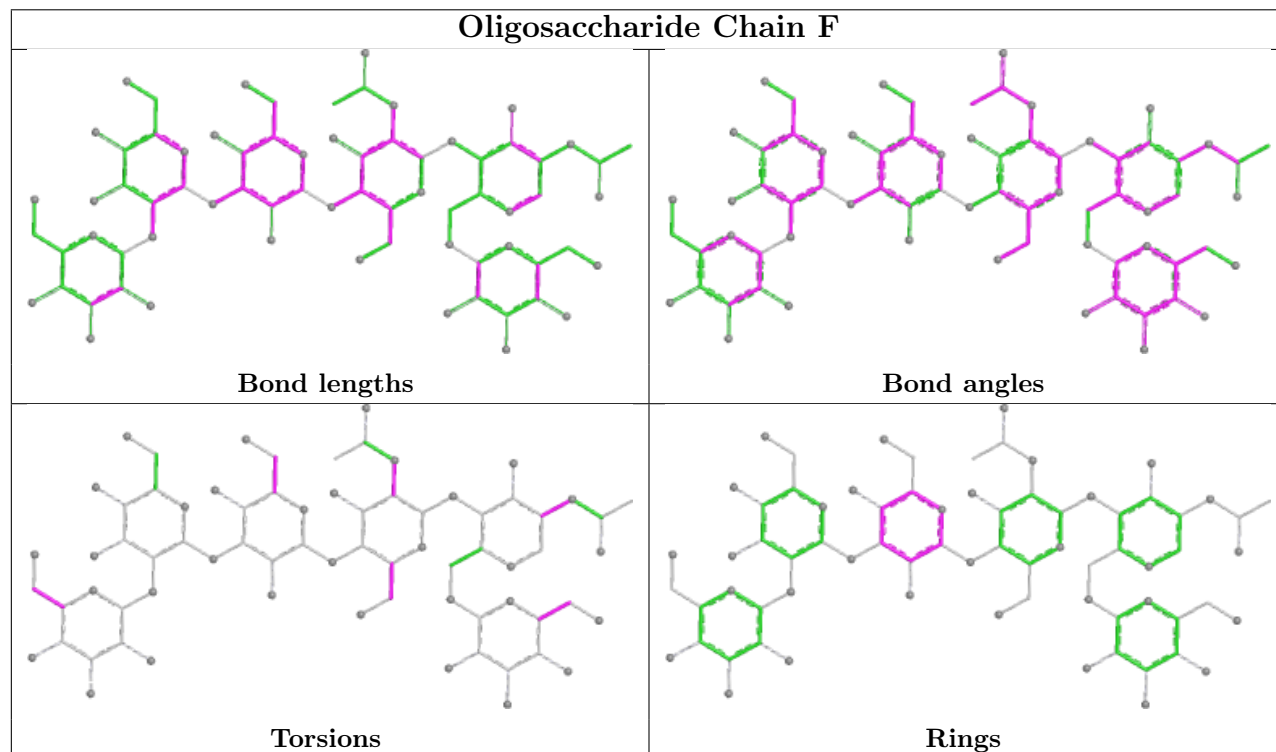
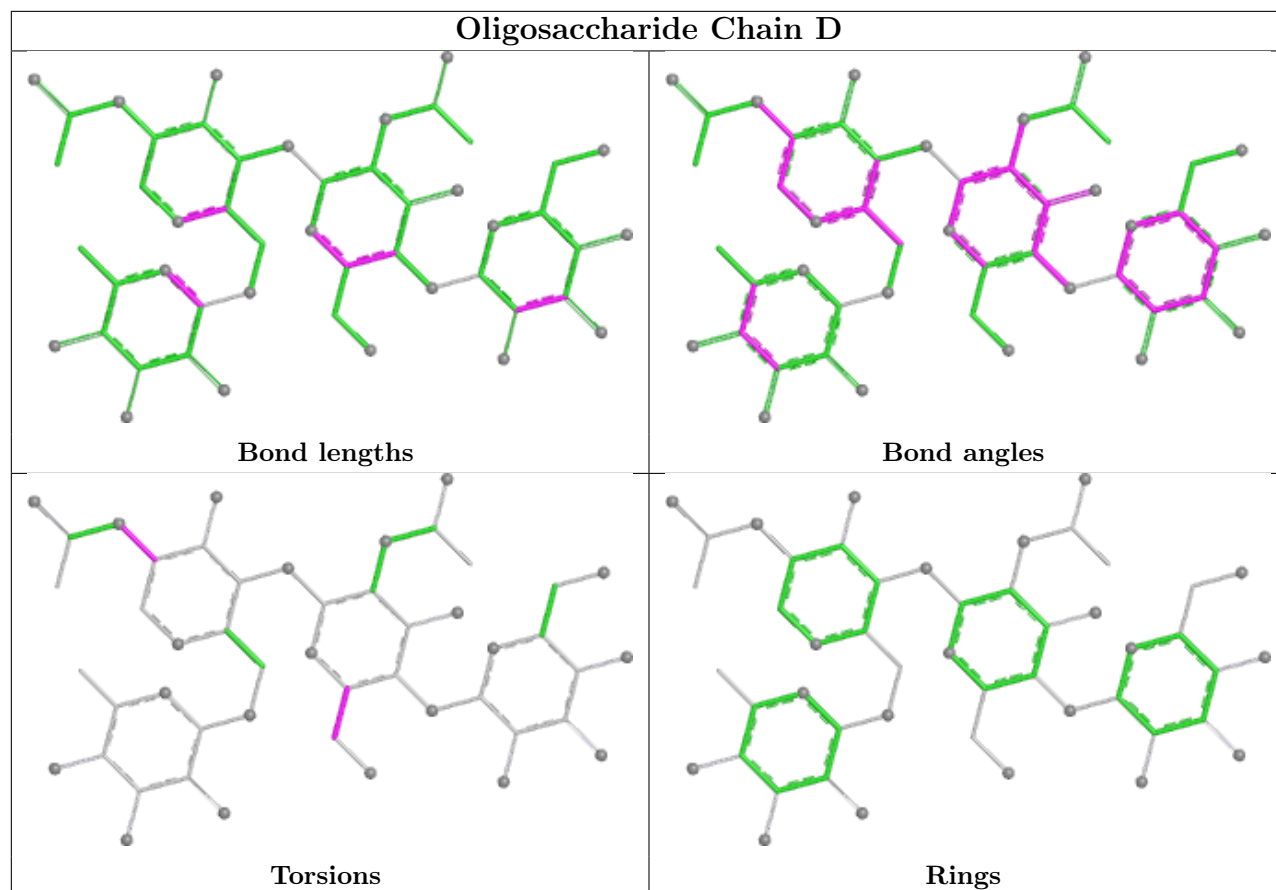
bond angles, torsion angles, and ring geometry for oligosaccharide.

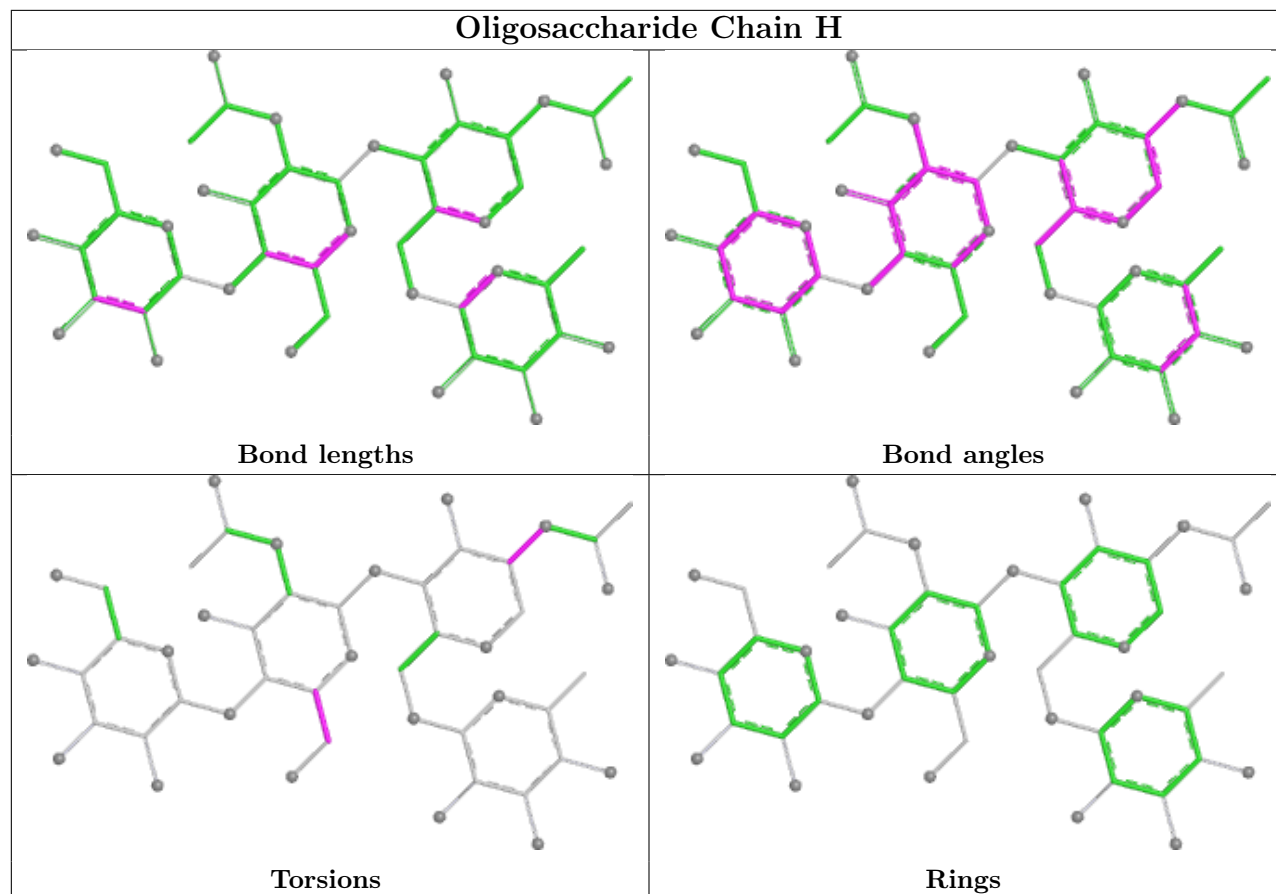
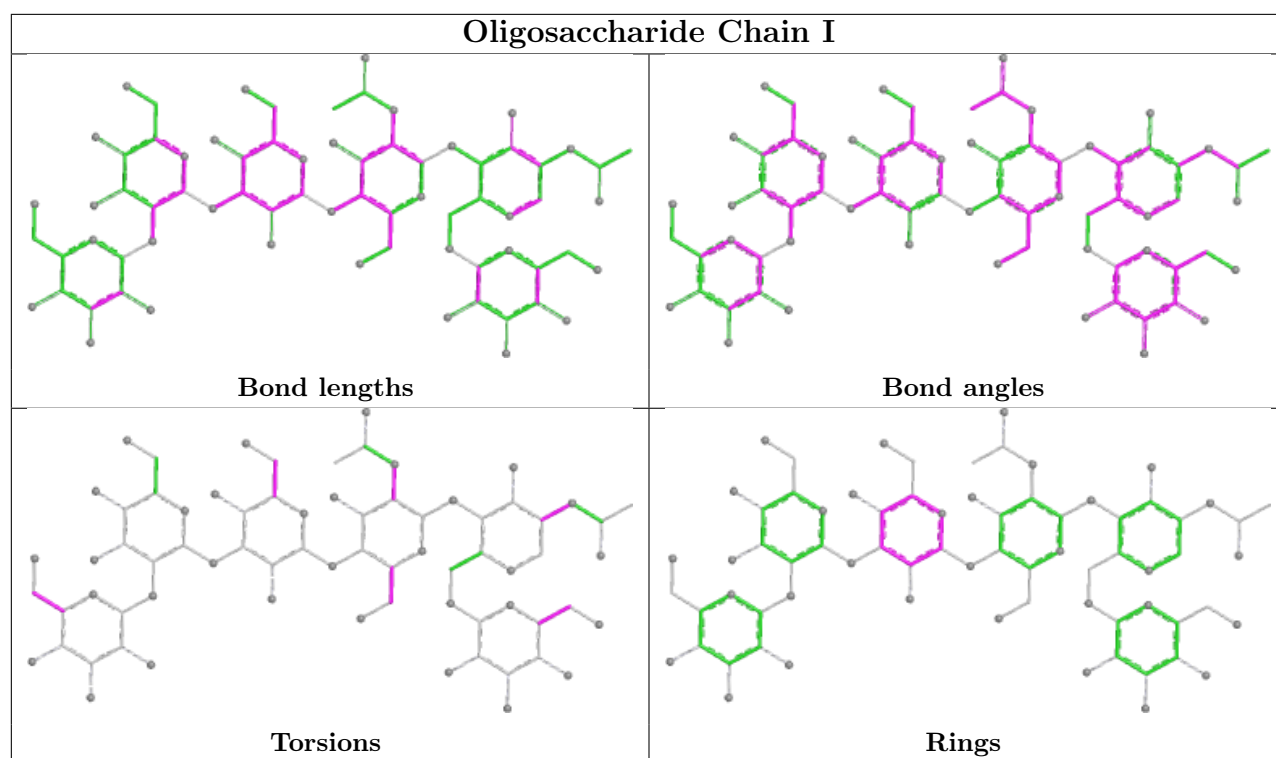












5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

Warning: The R factor obtained from EDS is 0.2628, which does not match the depositor's R factor of 0.205. Please interpret the results in this section carefully.

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	388/388 (100%)	0.03	4 (1%) 79 81	9, 20, 30, 41	0
1	B	388/388 (100%)	0.06	6 (1%) 71 74	9, 20, 30, 41	0
All	All	776/776 (100%)	0.05	10 (1%) 74 76	9, 20, 30, 41	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	352	TRP	6.1
1	B	431	LYS	3.2
1	A	352	TRP	3.0
1	B	373	GLY	2.3
1	A	408	GLY	2.3

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	BMA	D	3	11/12	0.57	0.19	15,15,55,57	0
3	FUL	D	4	10/11	0.58	0.15	15,15,49,52	0

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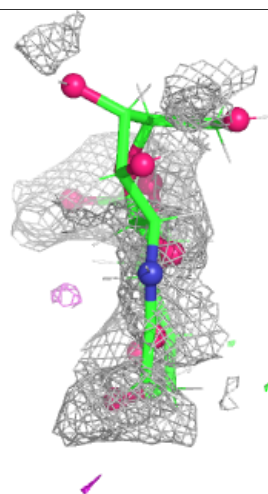
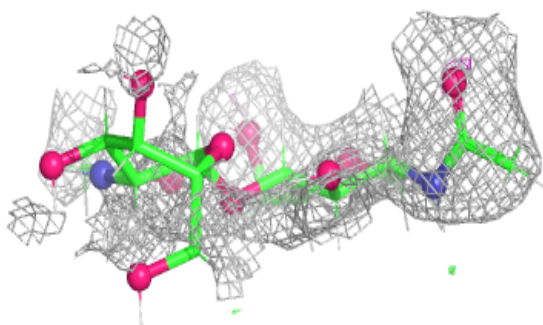
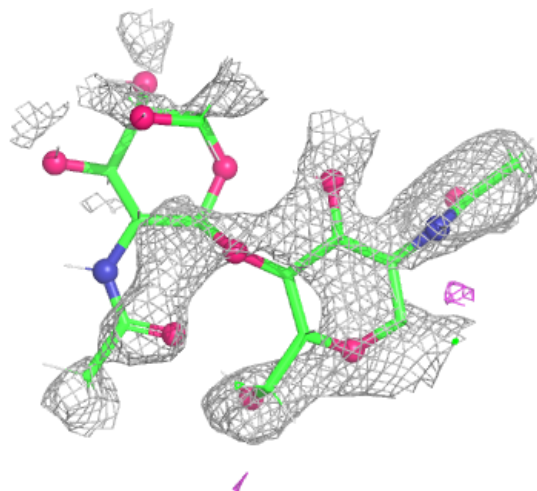
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	C	2	14/15	0.61	0.17	15,15,52,53	0
5	BMA	H	3	11/12	0.62	0.17	15,15,55,57	0
4	MAN	I	6	11/12	0.68	0.18	15,15,48,50	0
3	NAG	D	2	14/15	0.69	0.15	15,15,49,50	0
4	NAG	F	2	14/15	0.69	0.21	15,15,49,49	0
5	NAG	H	2	14/15	0.76	0.15	15,15,49,50	0
2	NAG	E	1	14/15	0.76	0.14	15,15,46,47	0
2	NAG	G	2	14/15	0.78	0.14	15,15,52,53	0
4	BMA	I	3	11/12	0.79	0.15	15,15,50,51	0
4	MAN	F	6	11/12	0.80	0.15	15,15,48,50	0
4	NAG	I	2	14/15	0.80	0.14	15,15,49,49	0
2	NAG	C	1	14/15	0.85	0.12	15,15,36,37	0
4	NAG	I	1	14/15	0.86	0.11	15,27,40,45	0
4	BMA	F	3	11/12	0.86	0.12	15,15,50,51	0
2	NAG	J	2	14/15	0.86	0.11	15,15,50,52	0
4	NAG	F	1	14/15	0.87	0.13	15,27,40,45	0
2	NAG	E	2	14/15	0.87	0.12	15,15,50,52	0
2	NAG	J	1	14/15	0.88	0.10	15,15,46,47	0
2	NAG	G	1	14/15	0.89	0.09	15,15,36,37	0
5	FUC	H	4	10/11	0.89	0.11	15,15,49,52	0
4	MAN	F	5	11/12	0.90	0.20	15,15,57,61	0
4	MAN	I	4	11/12	0.90	0.12	15,15,51,53	0
4	MAN	F	4	11/12	0.92	0.13	15,15,51,53	0
5	NAG	H	1	14/15	0.93	0.11	15,29,42,47	0
4	MAN	I	5	11/12	0.93	0.17	15,15,57,61	0
3	NAG	D	1	14/15	0.94	0.11	15,29,42,47	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.

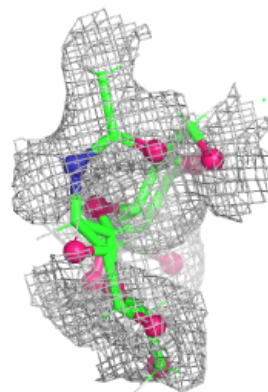
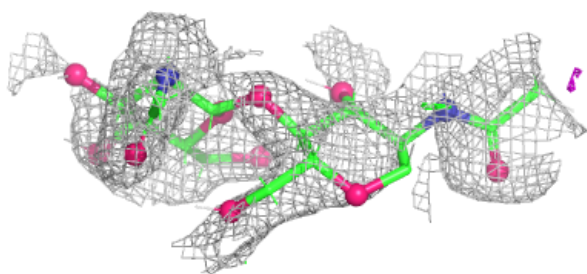
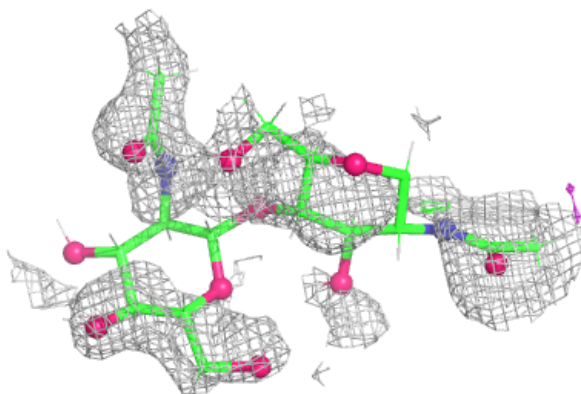
Electron density around Chain C:

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



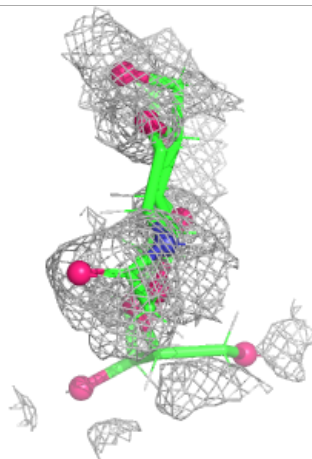
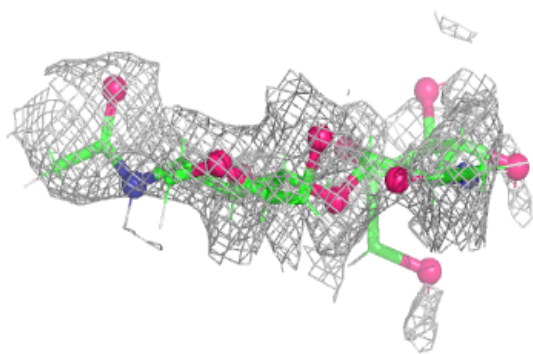
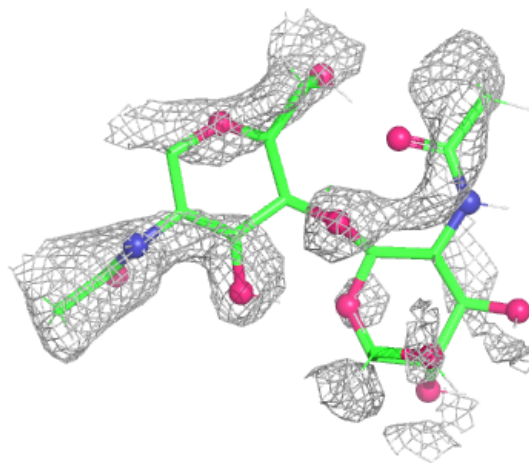
Electron density around Chain E:

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



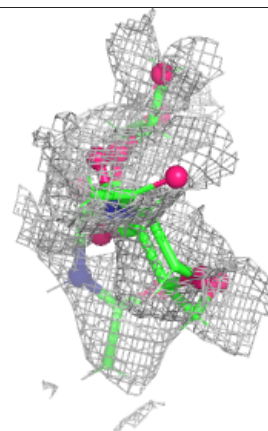
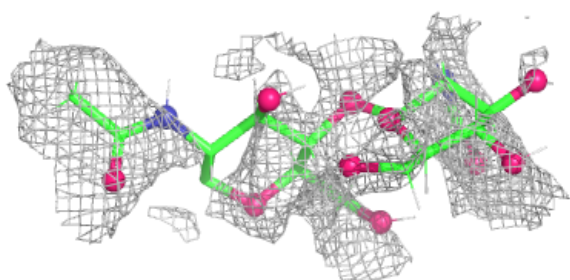
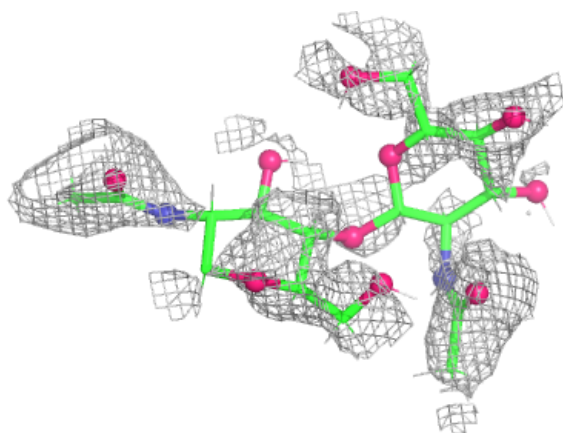
Electron density around Chain G:

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



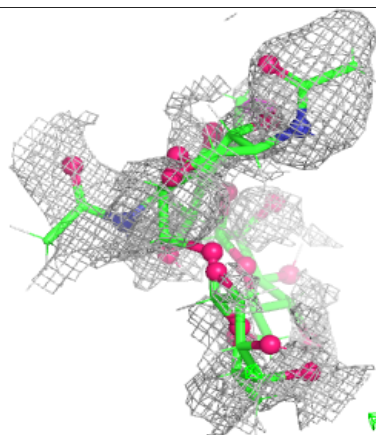
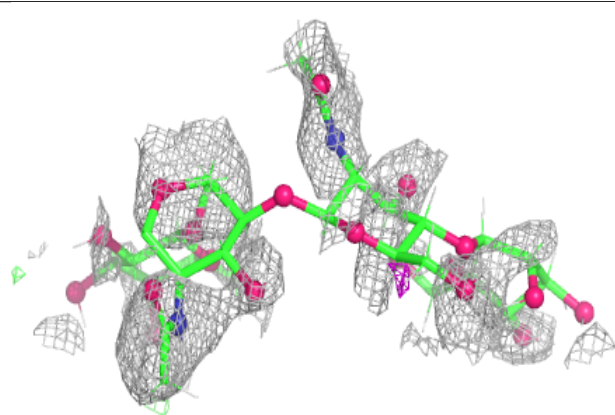
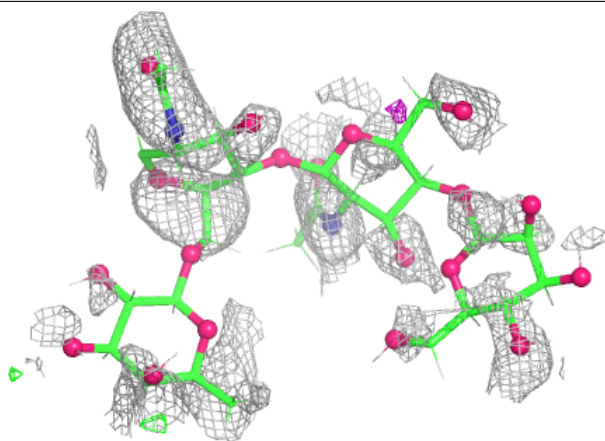
Electron density around Chain J:

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



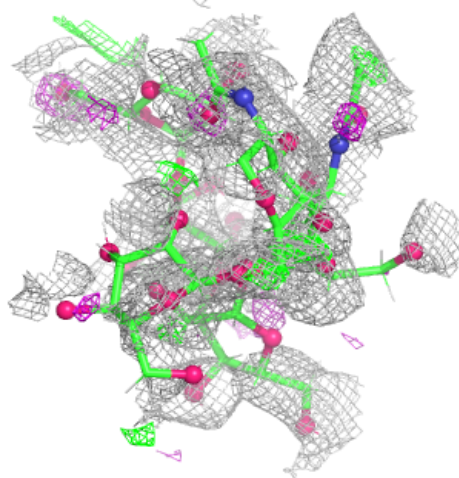
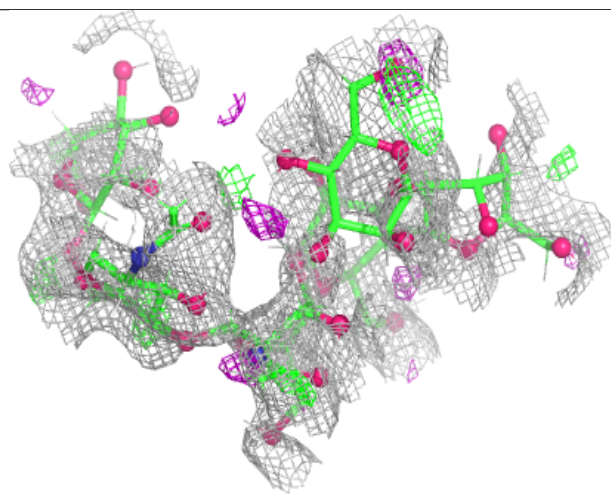
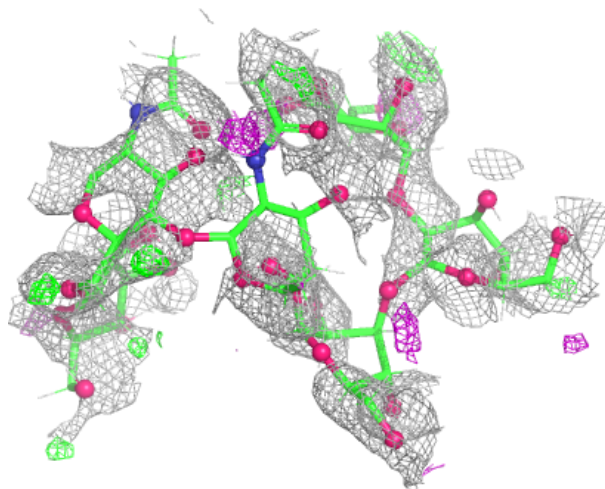
Electron density around Chain D:

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



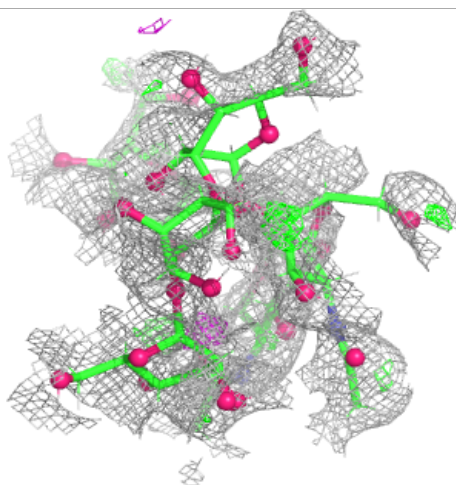
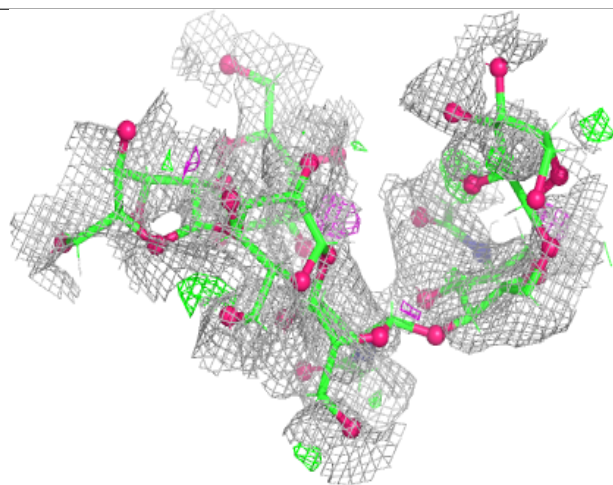
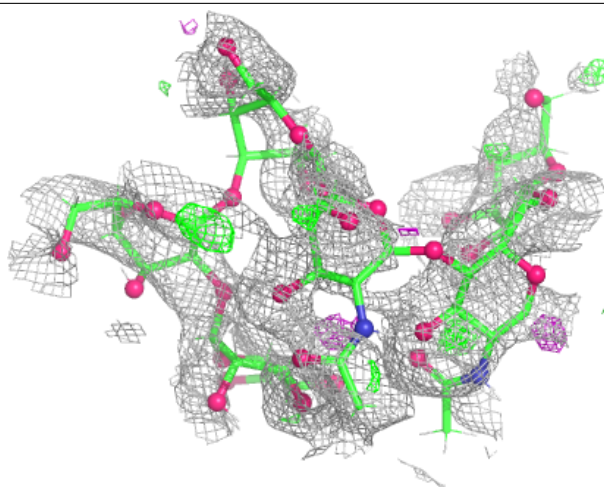
Electron density around Chain F:

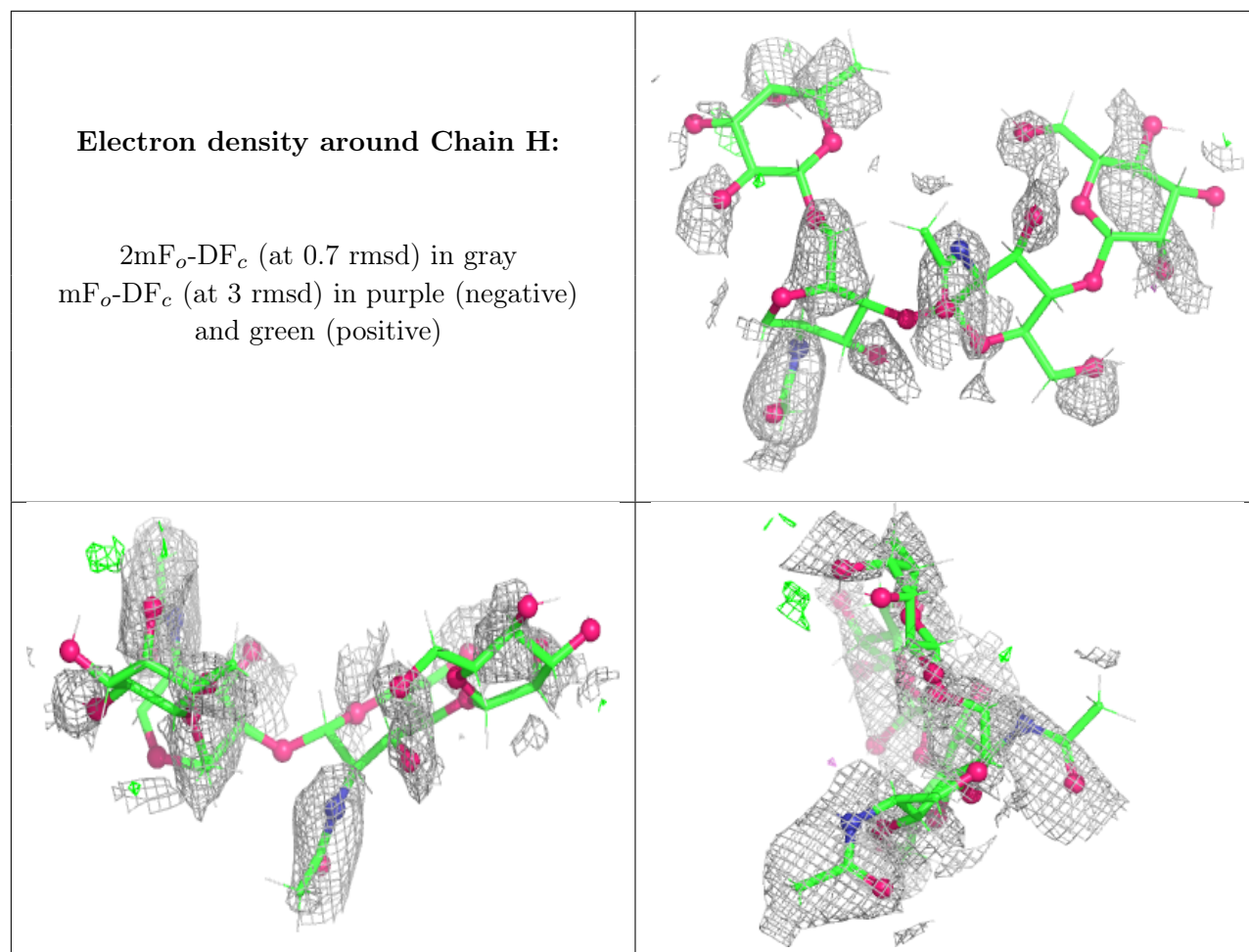
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain I:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	CA	B	470	1/1	0.89	0.04	29,29,29,29	0
6	CA	A	470	1/1	0.95	0.05	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.