



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 30, 2023 – 04:45 PM JST

PDB ID : 4WEF  
Title : Structure of the Hemagglutinin-neuraminidase from Human parainfluenza virus type III: complex with difluorosialic acid  
Authors : Streltsov, V.A.; Pilling, P.; Barrett, S.; McKimm-Breschkin, J.  
Deposited on : 2014-09-10  
Resolution : 2.50 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](mailto: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>.

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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 : 2.36  
buster-report : 1.1.7 (2018)  
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) : 2.36

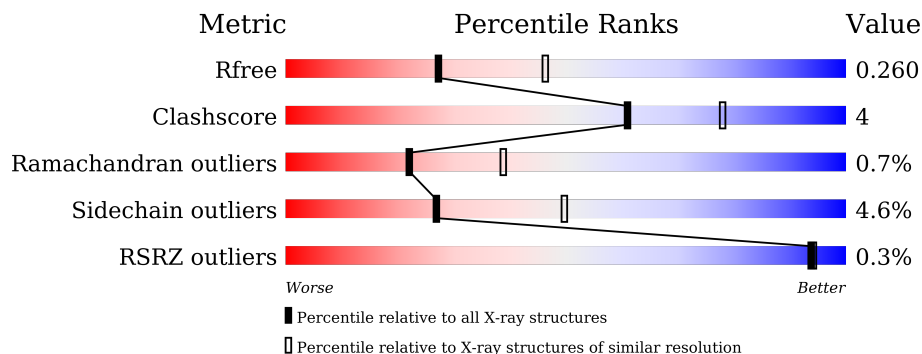
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	431	87% (green), 12% (yellow), 1% (orange), 2% (red)
1	B	431	86% (green), 13% (yellow), 1% (orange)
2	C	4	100% (yellow)
2	E	4	75% (yellow), 25% (orange)
3	D	3	67% (yellow), 33% (orange)
3	F	3	33% (yellow), 67% (orange)

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 7765 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.

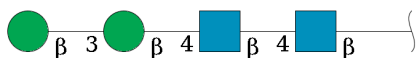
- Molecule 1 is a protein called Hemagglutinin-neuraminidase glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	431	3378	2138	580	640	20	0	1	0
1	B	431	3375	2137	579	639	20	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

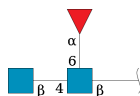
Chain	Residue	Modelled	Actual	Comment	Reference
A	408	GLY	SER	engineered mutation	UNP Q6WJ03
B	408	GLY	SER	engineered mutation	UNP Q6WJ03

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



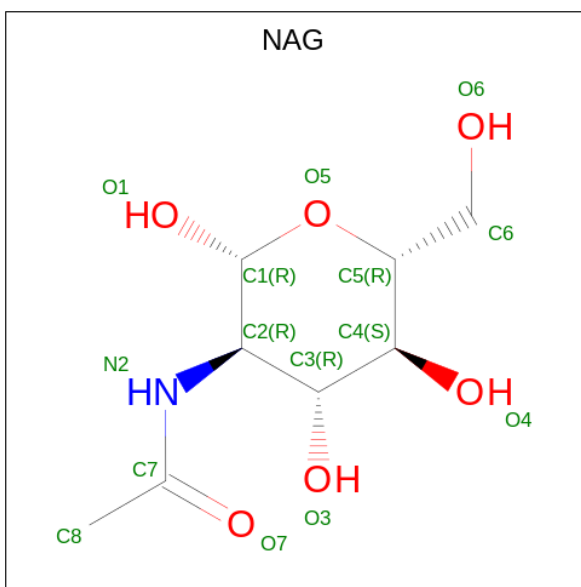
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	4	50	28	2	20	0	0	0
2	E	4	50	28	2	20	0	0	0

- Molecule 3 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.



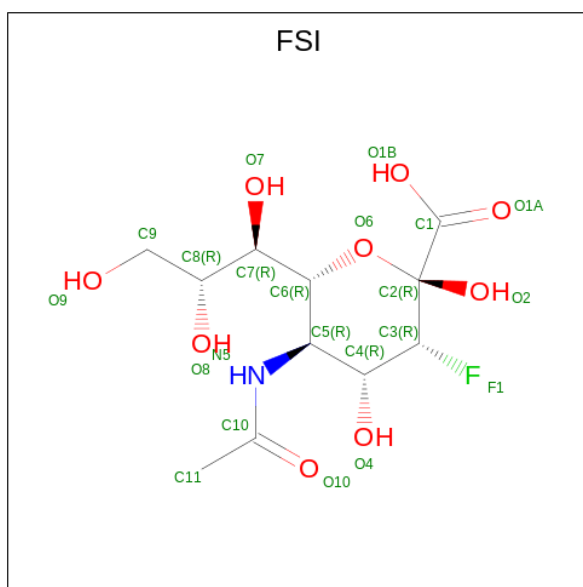
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	3	38	22	2	14	0	0	0
3	F	3	38	22	2	14	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



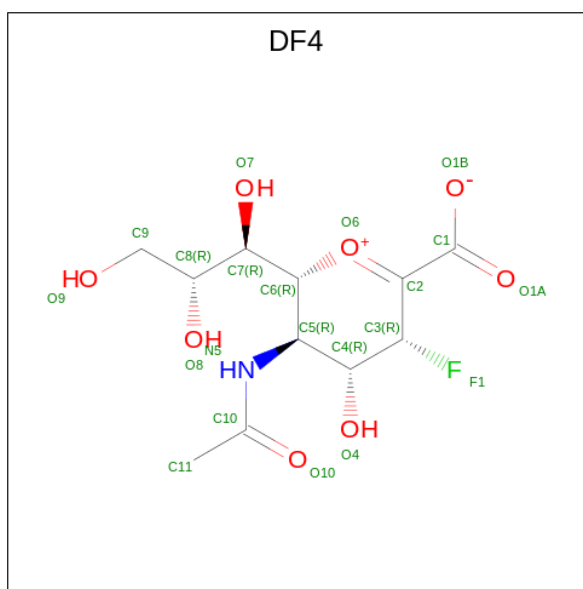
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0

- Molecule 5 is 5-acetamido-3,5-dideoxy-3-fluoro-D-erythro-alpha-L-manno-non-2-ulopyranosonic acid (three-letter code: FSI) (formula:  $C_{11}H_{18}FNO_9$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
5	A	1	Total	C	F	N	O	0	1
			21	11	1	1	8		
5	B	1	Total	C	F	N	O	0	1
			21	11	1	1	8		

- Molecule 6 is (3R,4R,5R,6R)-5-(acetamino)-3-fluoro-4-hydroxy-6-[(1R,2R)-1,2,3-trihydroxypropyl]-3,4,5,6-tetrahydropyranium-2-carboxylate (three-letter code: DF4) (formula: C<sub>11</sub>H<sub>16</sub>FNO<sub>8</sub>).



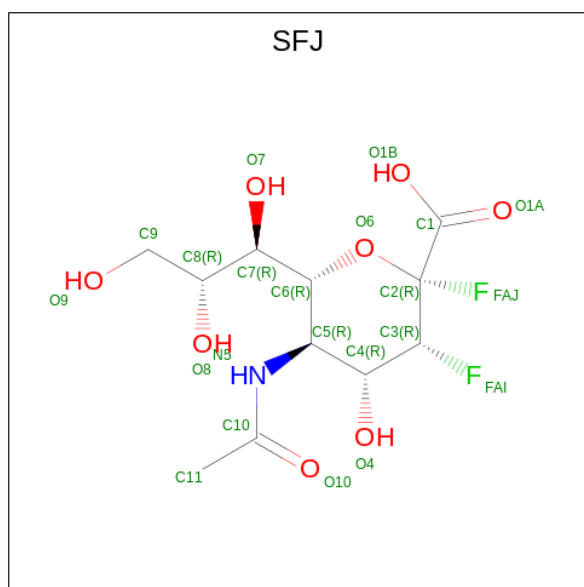
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
6	A	1	Total	C	F	N	O	0	1
			21	11	1	1	8		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
6	B	1	21	11	1	1	8	0	1

- Molecule 7 is (2R,3R,4R,5R,6R)-5-acetamido-2,3-difluoro-4-hydroxy-6-[(1R,2R)-1,2,3-trihydroxypropyl]tetrahydro-2H-pyran-2-carboxylic acid (three-letter code: SFJ) (formula: C<sub>11</sub>H<sub>17</sub>F<sub>2</sub>NO<sub>8</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
7	A	1	22	11	2	1	8	0	0
7	A	1	22	11	2	1	8	0	0
7	B	1	22	11	2	1	8	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 10 is water.

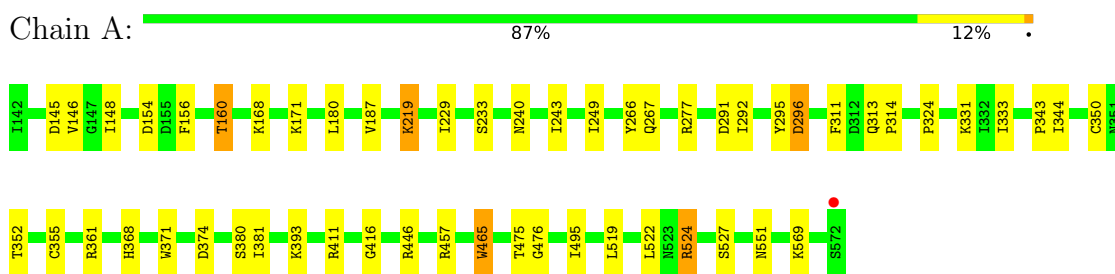
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	293	Total O 293 293	0	0
10	B	298	Total O 298 298	0	0



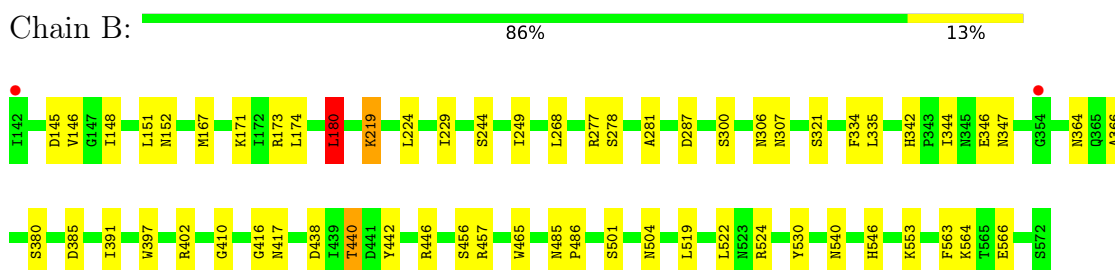
### 3 Residue-property plots [i](#)

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.

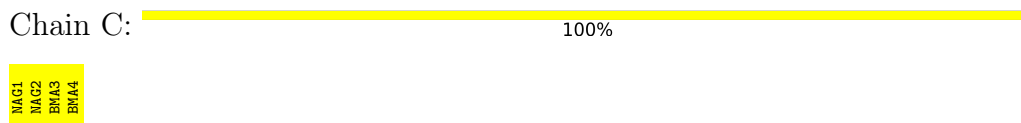
- Molecule 1: Hemagglutinin-neuraminidase glycoprotein



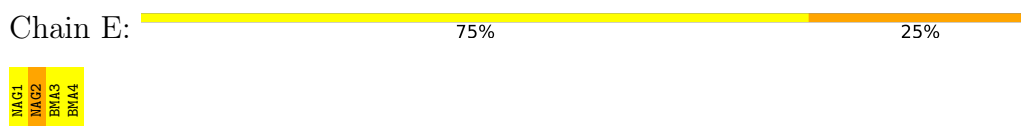
- Molecule 1: Hemagglutinin-neuraminidase glycoprotein




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



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



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

Chain D:  67% 33%

MAG1  
MAG2  
FUC3

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

Chain F:  33% 67%

MAG1  
MAG2  
FUC3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	218.67Å 218.67Å 109.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	77.46 – 2.50 77.46 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (77.46-2.50) 99.9 (77.46-2.50)	Depositor EDS
$R_{merge}$	0.29	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.189 , 0.258 0.196 , 0.260	Depositor DCC
$R_{free}$ test set	2666 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.4	Xtrriage
Anisotropy	0.042	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 52.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7765	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAG, CA, BMA, FSI, SFJ, SO4, FUC, DF4

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	0.73	1/3464 (0.0%)	0.84	1/4723 (0.0%)
1	B	0.69	0/3456	0.84	1/4712 (0.0%)
All	All	0.71	1/6920 (0.0%)	0.84	2/9435 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	465	TRP	CB-CG	-5.07	1.41	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	180	LEU	CB-CG-CD2	5.29	120.00	111.00

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	3378	0	3344	23	0
1	B	3375	0	3342	34	0
2	C	50	0	43	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	50	0	43	1	0
3	D	38	0	34	1	0
3	F	38	0	34	2	0
4	A	14	0	13	1	0
4	B	14	0	13	0	0
5	A	21	0	16	0	0
5	B	21	0	16	0	0
6	A	21	0	16	1	0
6	B	21	0	16	1	0
7	A	44	0	0	0	0
7	B	22	0	0	3	0
8	A	30	0	0	0	0
8	B	35	0	0	1	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	293	0	0	3	0
10	B	298	0	0	16	0
All	All	7765	0	6930	63	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 63 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:540:ASN:HB2	10:B:843:HOH:O	1.85	0.77
1:B:416:GLY:HA3	10:B:716:HOH:O	1.92	0.69
1:B:277:ARG:HD2	10:B:703:HOH:O	1.94	0.68
1:B:530:TYR:OH	6:B:611[B]:DF4:C2	2.45	0.64
7:B:612:SFJ:O9	10:B:701:HOH:O	2.15	0.64

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	430/431 (100%)	401 (93%)	25 (6%)	4 (1%)	17	31
1	B	429/431 (100%)	399 (93%)	28 (6%)	2 (0%)	29	48
All	All	859/862 (100%)	800 (93%)	53 (6%)	6 (1%)	22	39

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	SER
1	A	160	THR
1	A	416	GLY
1	B	287	ASP
1	A	350	CYS

### 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	390/389 (100%)	373 (96%)	17 (4%)	28	52
1	B	389/389 (100%)	370 (95%)	19 (5%)	25	47
All	All	779/778 (100%)	743 (95%)	36 (5%)	27	50

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	391	ILE
1	B	566	GLU
1	B	417	ASN
1	B	501	SER
1	A	446	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	294	ASN
1	B	551	ASN
1	B	345	ASN
1	B	556	ASN
1	B	417	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](#)

8 non-standard protein/DNA/RNA residues 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	2	2	14,14,15	0.42	0	17,19,21	1.42	4 (23%)
2	NAG	E	1	1,2	14,14,15	0.62	0	17,19,21	1.92	4 (23%)
3	NAG	F	2	3	14,14,15	0.87	1 (7%)	17,19,21	2.39	4 (23%)
2	NAG	C	2	2	14,14,15	0.51	0	17,19,21	1.78	4 (23%)
3	NAG	D	1	3,1	14,14,15	0.99	1 (7%)	17,19,21	1.46	3 (17%)
4	NAG	A	601	1	14,14,15	0.52	0	17,19,21	2.00	3 (17%)
3	NAG	D	2	3	14,14,15	0.57	0	17,19,21	1.71	4 (23%)
2	NAG	C	1	1,2	14,14,15	0.88	0	17,19,21	1.92	4 (23%)

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	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
4	NAG	A	601	1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
2	NAG	C	1	1,2	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	NAG	C1-C2	2.39	1.55	1.52
3	D	1	NAG	O5-C1	-2.10	1.40	1.43

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	NAG	C1-O5-C5	5.99	120.31	112.19
4	A	601	NAG	C1-O5-C5	5.62	119.81	112.19
2	E	1	NAG	C1-O5-C5	5.17	119.20	112.19
3	F	2	NAG	C1-C2-N2	5.00	119.03	110.49
2	C	1	NAG	C2-N2-C7	4.43	129.20	122.90

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0
3	D	1	NAG	1	0
4	A	601	NAG	1	0



## 5.5 Carbohydrates i

14 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	0.88	0	17,19,21	1.92	4 (23%)
2	NAG	C	2	2	14,14,15	0.51	0	17,19,21	1.78	4 (23%)
2	BMA	C	3	2	11,11,12	0.57	0	15,15,17	1.26	2 (13%)
2	BMA	C	4	2	11,11,12	0.79	0	15,15,17	1.46	3 (20%)
3	NAG	D	1	3,1	14,14,15	0.99	1 (7%)	17,19,21	1.46	3 (17%)
3	NAG	D	2	3	14,14,15	0.57	0	17,19,21	1.71	4 (23%)
3	FUC	D	3	3	10,10,11	0.68	0	14,14,16	2.70	6 (42%)
2	NAG	E	1	1,2	14,14,15	0.62	0	17,19,21	1.92	4 (23%)
2	NAG	E	2	2	14,14,15	0.42	0	17,19,21	1.42	4 (23%)
2	BMA	E	3	2	11,11,12	0.67	0	15,15,17	1.21	2 (13%)
2	BMA	E	4	2	11,11,12	0.86	0	15,15,17	2.68	7 (46%)
3	NAG	F	1	3,1	14,14,15	1.10	1 (7%)	17,19,21	2.36	4 (23%)
3	NAG	F	2	3	14,14,15	0.87	1 (7%)	17,19,21	2.39	4 (23%)
3	FUC	F	3	3	10,10,11	1.09	1 (10%)	14,14,16	2.41	5 (35%)

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	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	BMA	C	4	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	O5-C1	-3.37	1.38	1.43
3	F	3	FUC	C1-C2	2.83	1.58	1.52
3	F	2	NAG	C1-C2	2.39	1.55	1.52
3	D	1	NAG	O5-C1	-2.10	1.40	1.43

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	FUC	C1-C2-C3	7.94	119.42	109.67
3	F	1	NAG	O5-C5-C6	-6.05	97.71	107.20
3	F	2	NAG	C1-O5-C5	5.99	120.31	112.19
3	F	1	NAG	O5-C1-C2	-5.42	102.73	111.29
3	F	3	FUC	C1-C2-C3	5.36	116.25	109.67

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

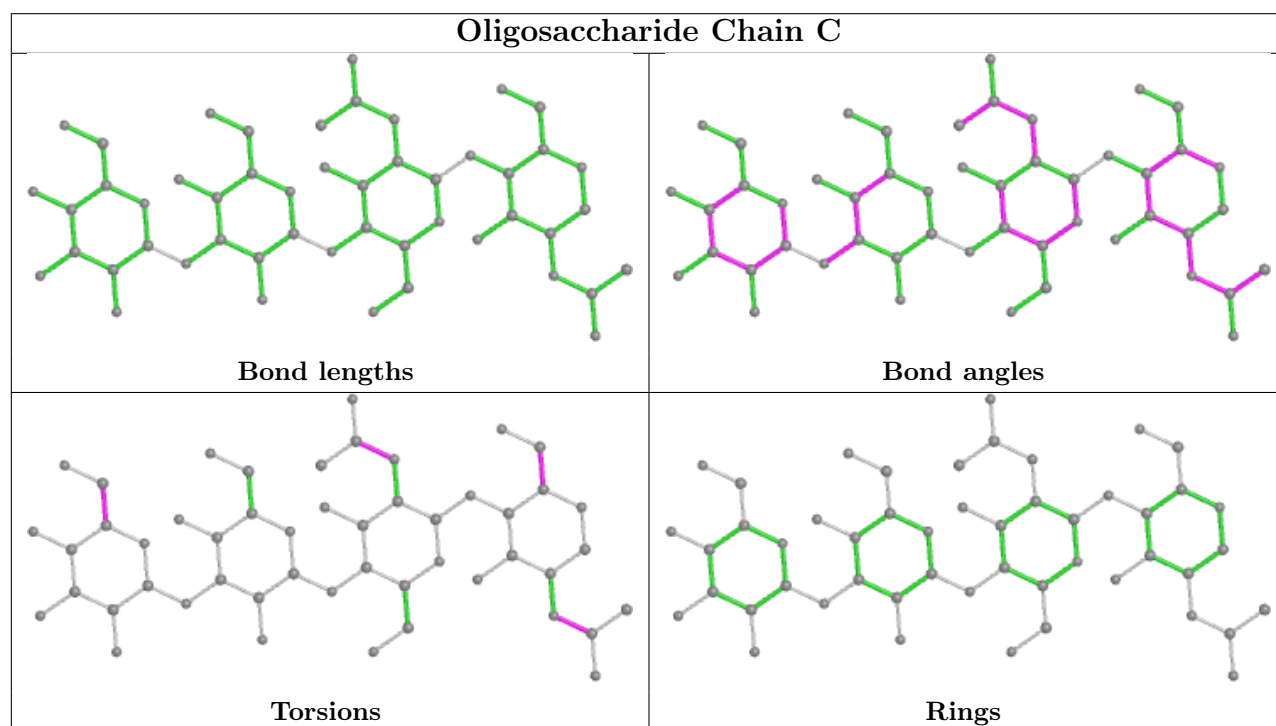
Mol	Chain	Res	Type	Atoms
2	E	3	BMA	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6

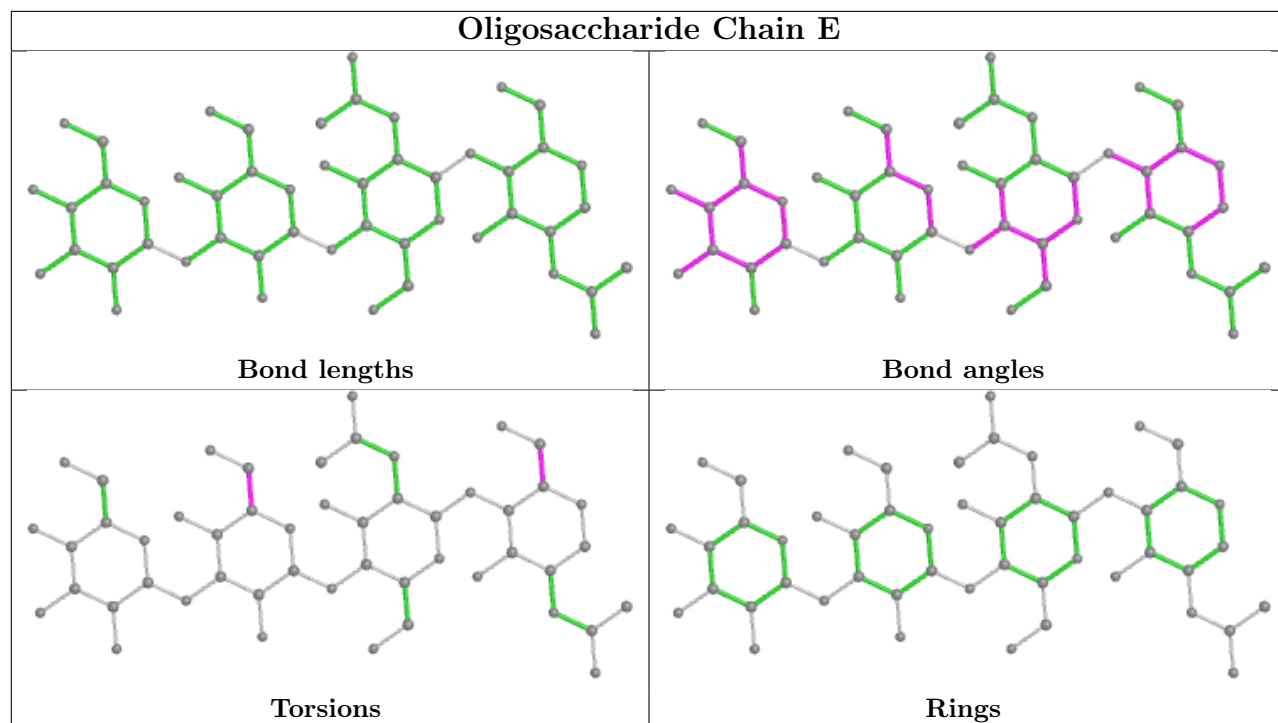
There are no ring outliers.

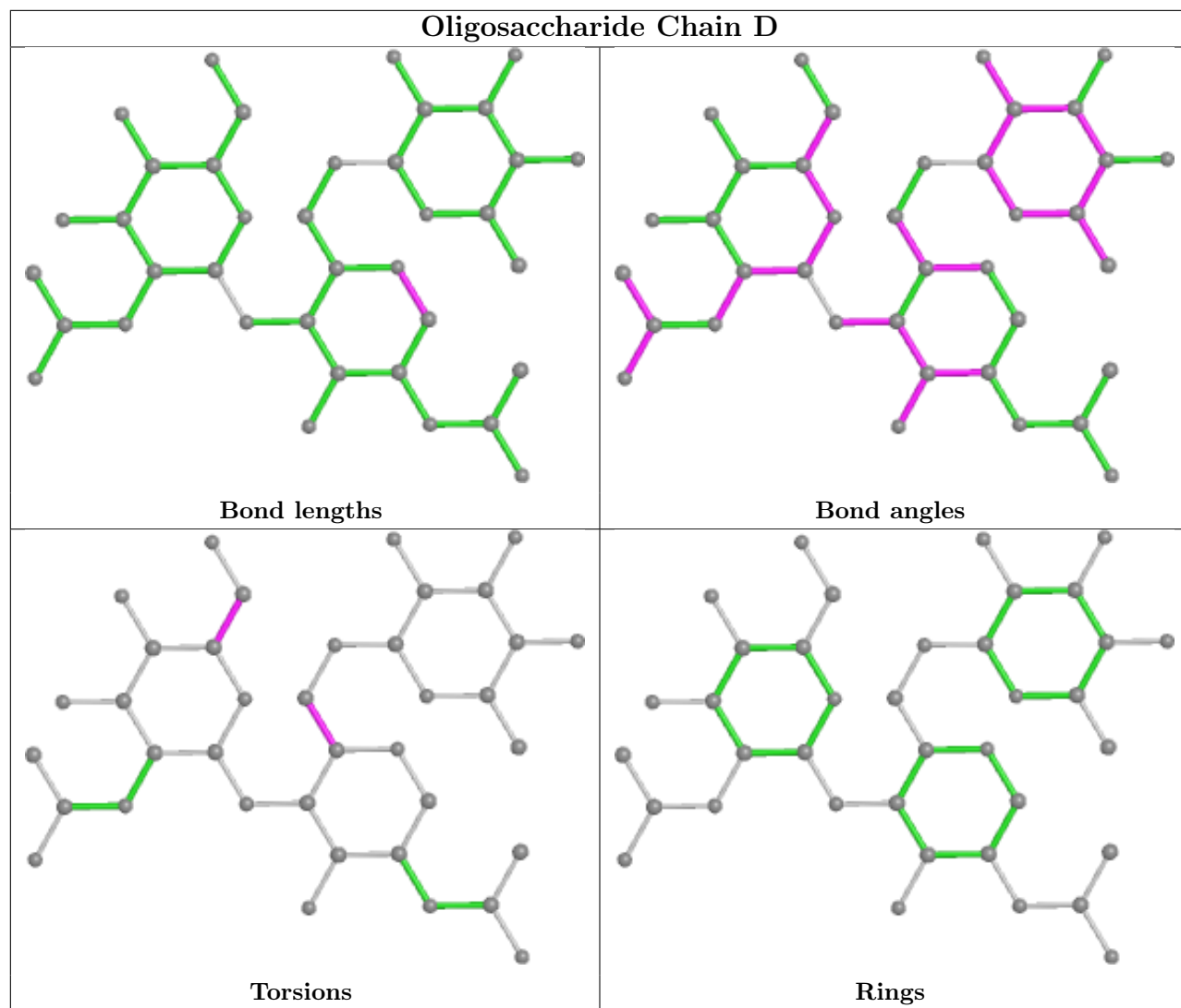
4 monomers are involved in 4 short contacts:

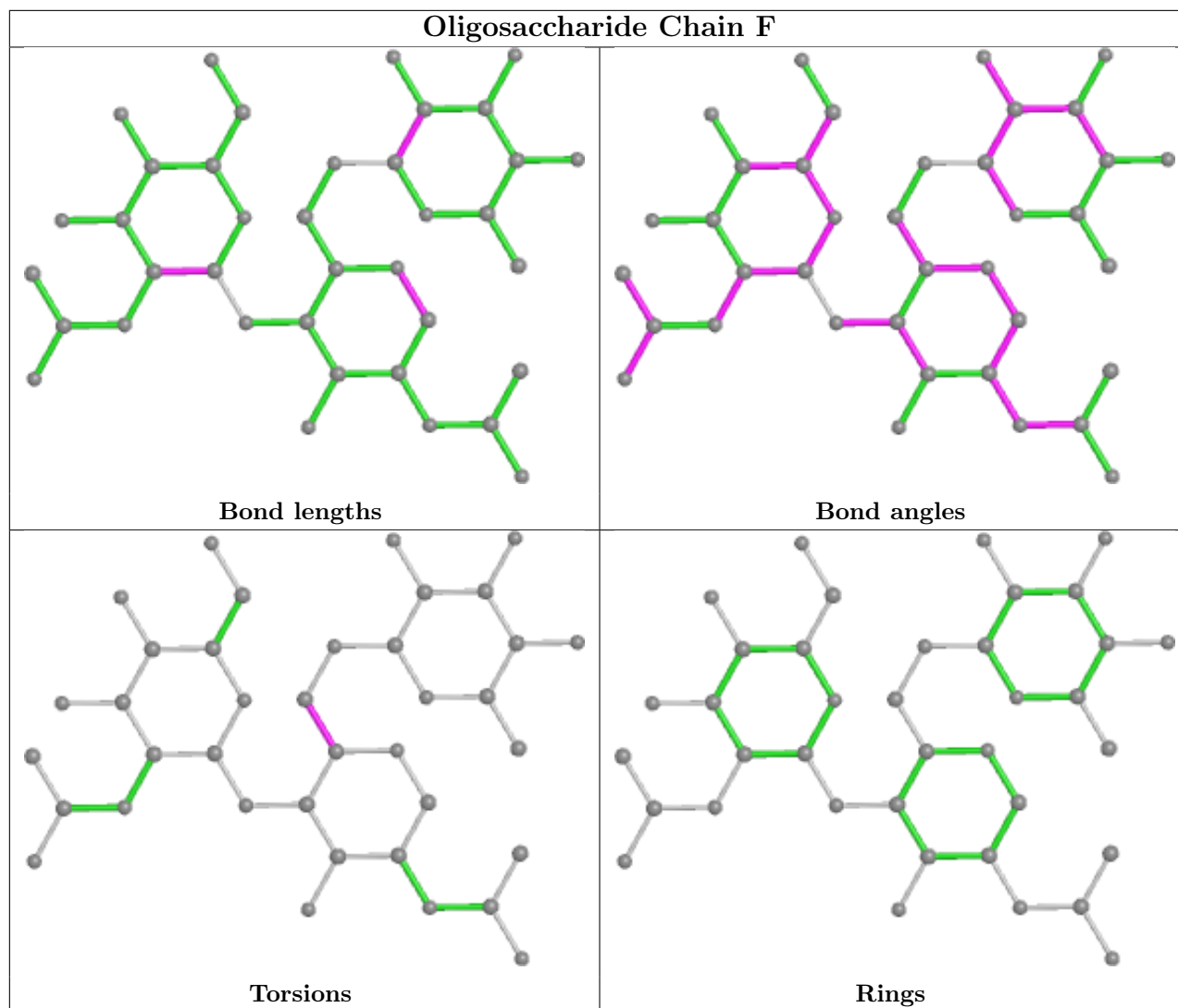
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0
3	F	1	NAG	2	0
3	D	1	NAG	1	0
3	F	3	FUC	1	0

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









## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 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	$\# Z  > 2$
8	SO4	B	615	-	4,4,4	0.44	0	6,6,6	0.38	0
8	SO4	A	614	-	4,4,4	0.58	0	6,6,6	0.72	0
8	SO4	A	617	-	4,4,4	0.35	0	6,6,6	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	SO4	A	615	-	4,4,4	0.48	0	6,6,6	0.56	0
8	SO4	B	617	-	4,4,4	0.42	0	6,6,6	0.21	0
8	SO4	A	618	-	4,4,4	0.41	0	6,6,6	0.33	0
8	SO4	A	616	-	4,4,4	0.39	0	6,6,6	0.91	0
6	DF4	B	611[B]	-	16,21,21	1.04	1 (6%)	19,30,30	1.00	0
8	SO4	B	618	-	4,4,4	0.31	0	6,6,6	0.31	0
8	SO4	A	613	-	4,4,4	0.42	0	6,6,6	0.21	0
5	FSI	B	610[A]	1	21,21,22	0.98	1 (4%)	23,30,33	1.18	3 (13%)
8	SO4	B	616	-	4,4,4	0.50	0	6,6,6	0.25	0
8	SO4	B	614	-	4,4,4	0.38	0	6,6,6	0.38	0
8	SO4	B	613	-	4,4,4	0.47	0	6,6,6	0.31	0
4	NAG	B	602	1	14,14,15	0.49	0	17,19,21	1.52	4 (23%)
8	SO4	B	601	-	4,4,4	0.37	0	6,6,6	0.23	0
5	FSI	A	609[A]	1	21,21,22	0.77	0	23,30,33	1.50	4 (17%)
7	SFJ	B	612	-	18,22,22	1.73	2 (11%)	20,33,33	3.12	7 (35%)
6	DF4	A	610[B]	-	16,21,21	1.02	1 (6%)	19,30,30	1.27	2 (10%)
7	SFJ	A	612	-	18,22,22	0.97	1 (5%)	20,33,33	2.40	8 (40%)
4	NAG	A	601	1	14,14,15	0.52	0	17,19,21	2.00	3 (17%)
7	SFJ	A	611	-	18,22,22	0.93	1 (5%)	20,33,33	1.47	4 (20%)

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
7	SFJ	B	612	-	-	6/15/43/43	0/1/1/1
6	DF4	A	610[B]	-	-	2/14/38/38	0/0/1/1
5	FSI	B	610[A]	1	-	2/18/38/43	0/1/1/1
7	SFJ	A	612	-	-	4/15/43/43	0/1/1/1
4	NAG	B	602	1	-	0/6/23/26	0/1/1/1
4	NAG	A	601	1	-	0/6/23/26	0/1/1/1
7	SFJ	A	611	-	-	2/15/43/43	0/1/1/1
5	FSI	A	609[A]	1	-	2/18/38/43	0/1/1/1
6	DF4	B	611[B]	-	-	3/14/38/38	0/0/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	612	SFJ	C7-C6	4.74	1.59	1.53
7	B	612	SFJ	C3-C4	3.99	1.56	1.52
6	A	610[B]	DF4	O1A-C1	3.78	1.32	1.22
6	B	611[B]	DF4	O1A-C1	3.73	1.32	1.22
7	A	612	SFJ	C3-C4	2.51	1.54	1.52

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	612	SFJ	FAI-C3-C4	8.17	116.11	108.85
7	B	612	SFJ	C3-C4-C5	6.86	118.68	109.83
7	A	612	SFJ	C3-C4-C5	6.22	117.85	109.83
4	A	601	NAG	C1-O5-C5	5.62	119.81	112.19
7	B	612	SFJ	O7-C7-C6	4.95	120.18	109.50

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	610[B]	DF4	C7-C8-C9-O9
6	A	610[B]	DF4	O8-C8-C9-O9
7	A	612	SFJ	O8-C8-C9-O9
7	B	612	SFJ	C6-C7-C8-O8
7	B	612	SFJ	O7-C7-C8-C9

There are no ring outliers.

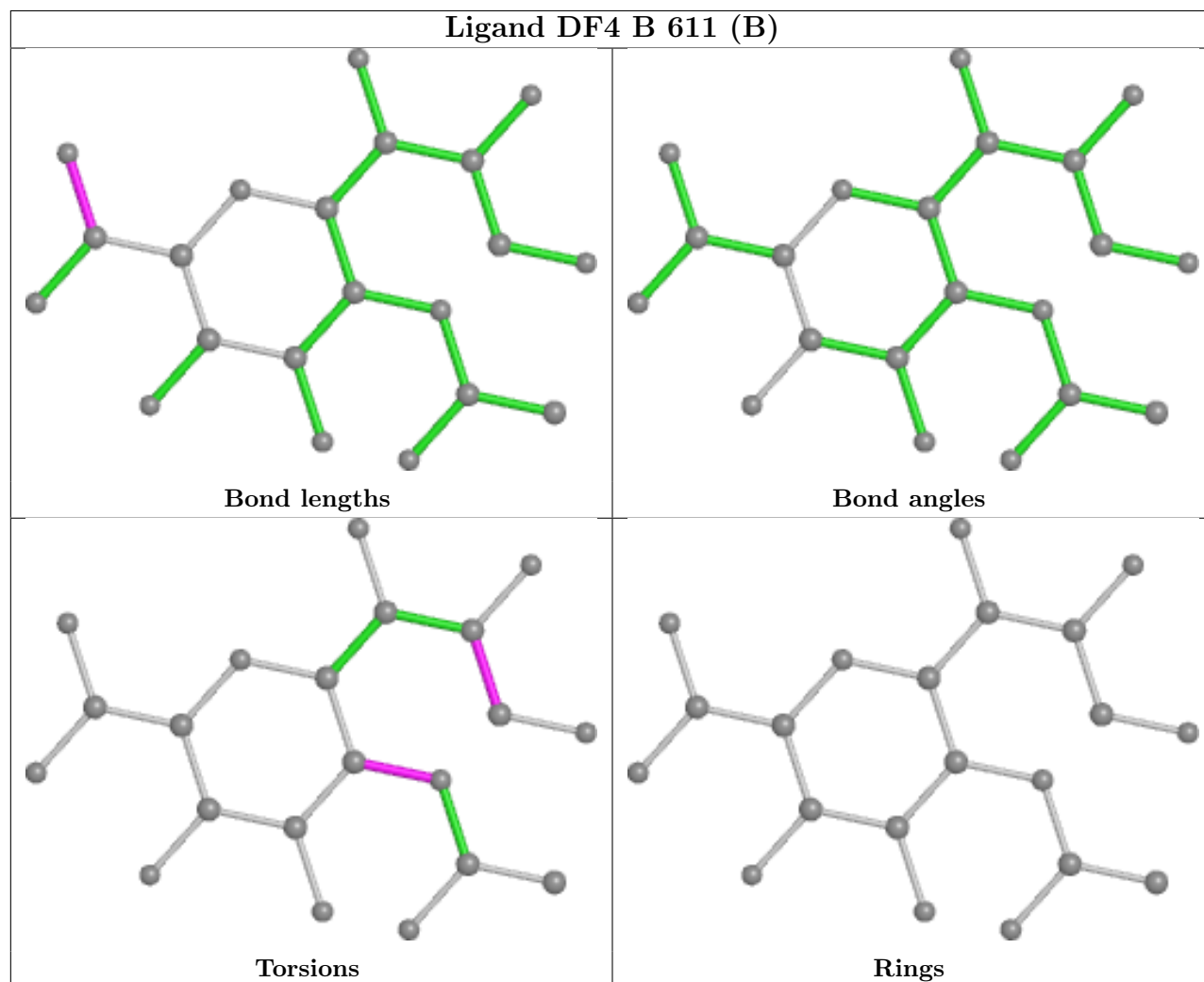
5 monomers are involved in 7 short contacts:

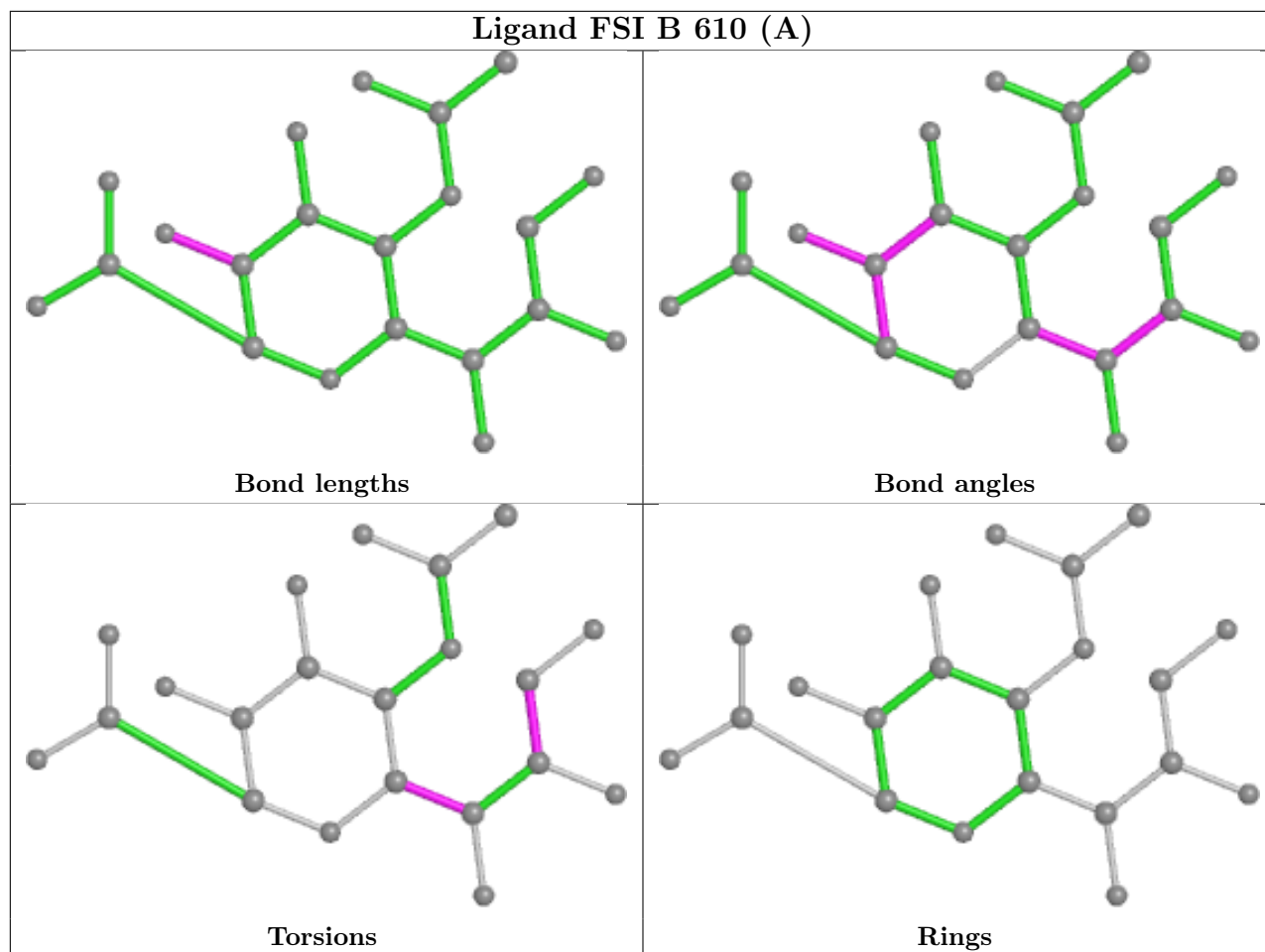
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	611[B]	DF4	1	0
8	B	618	SO4	1	0
7	B	612	SFJ	3	0
6	A	610[B]	DF4	1	0
4	A	601	NAG	1	0

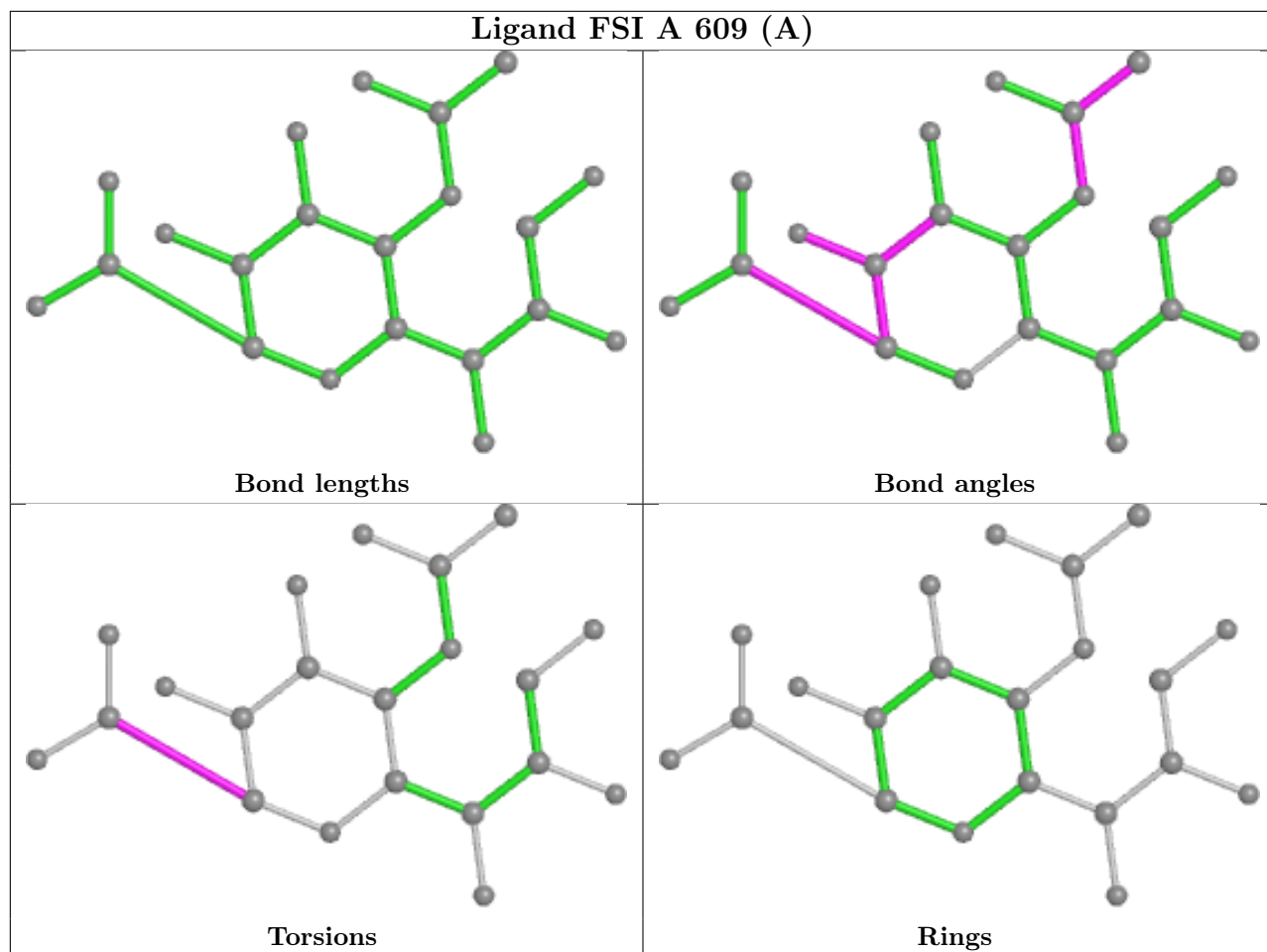
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

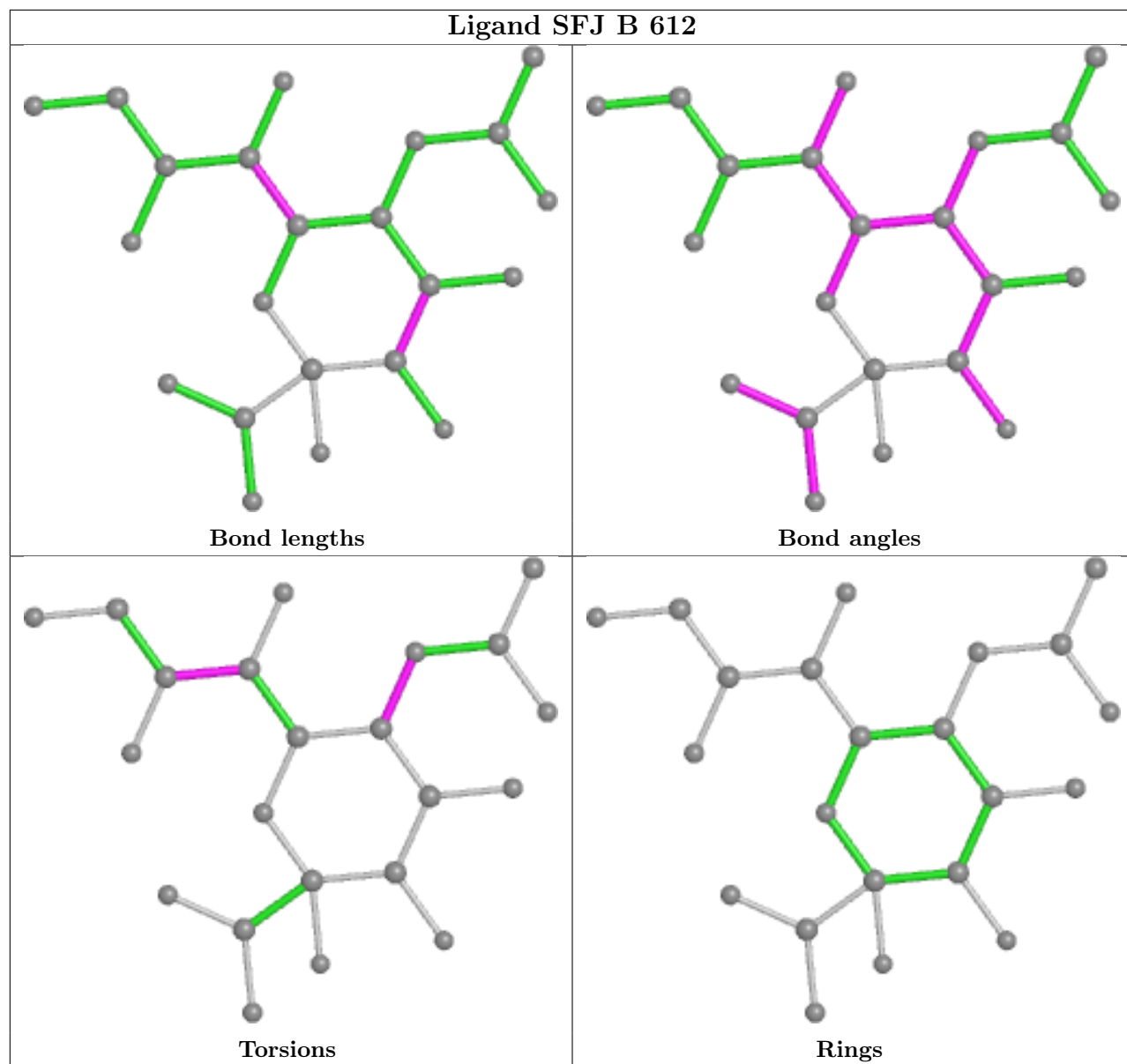


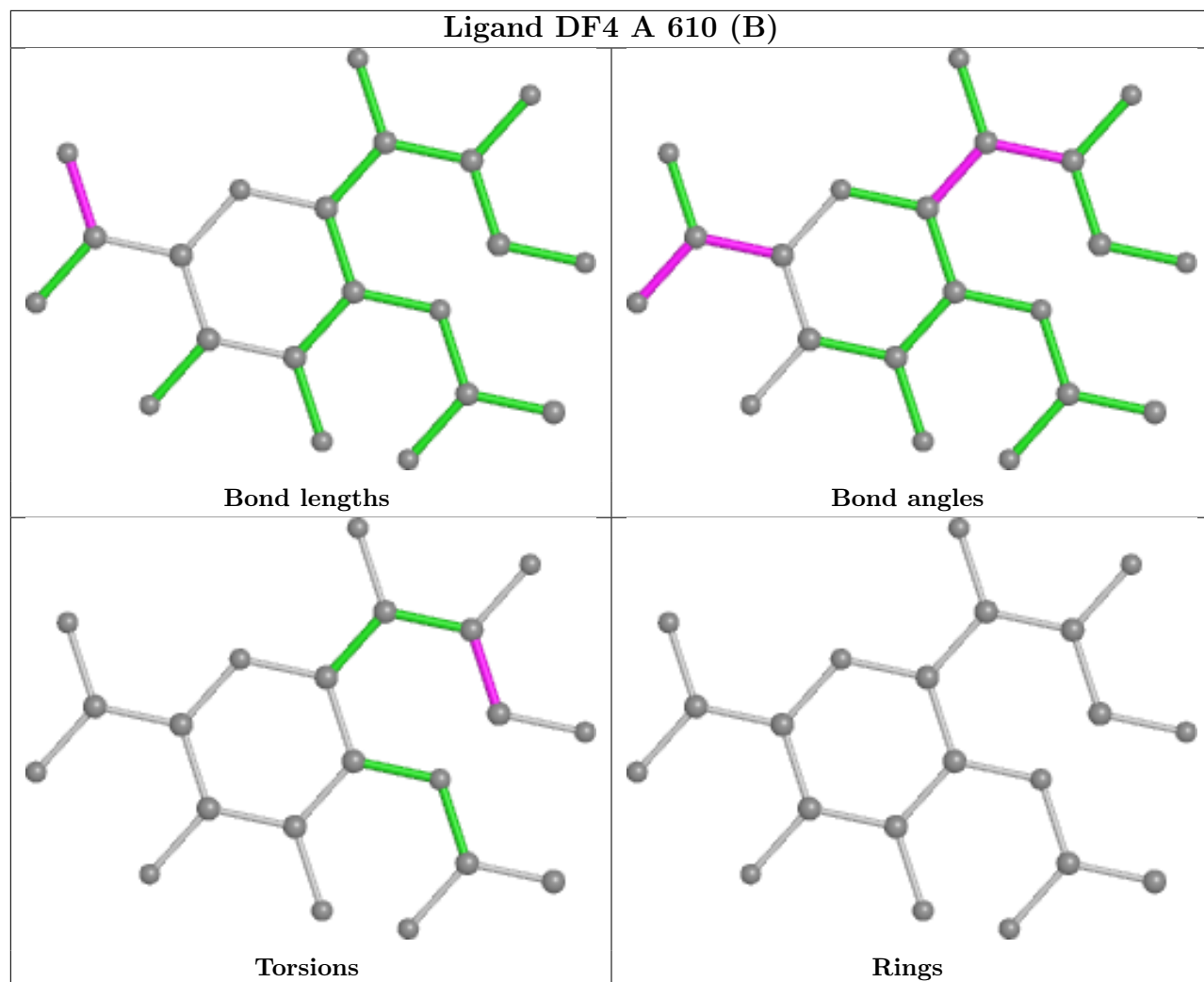
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

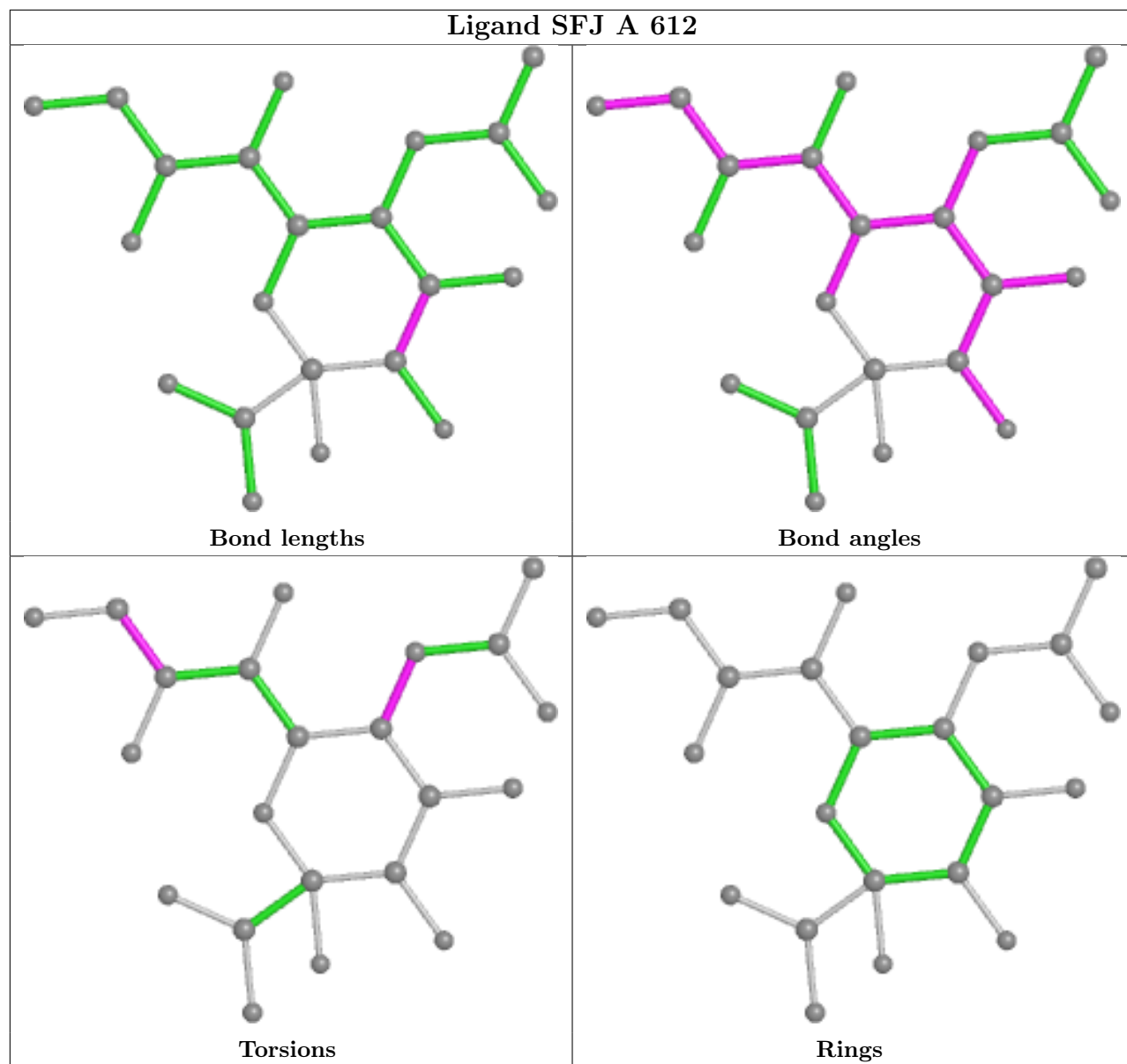


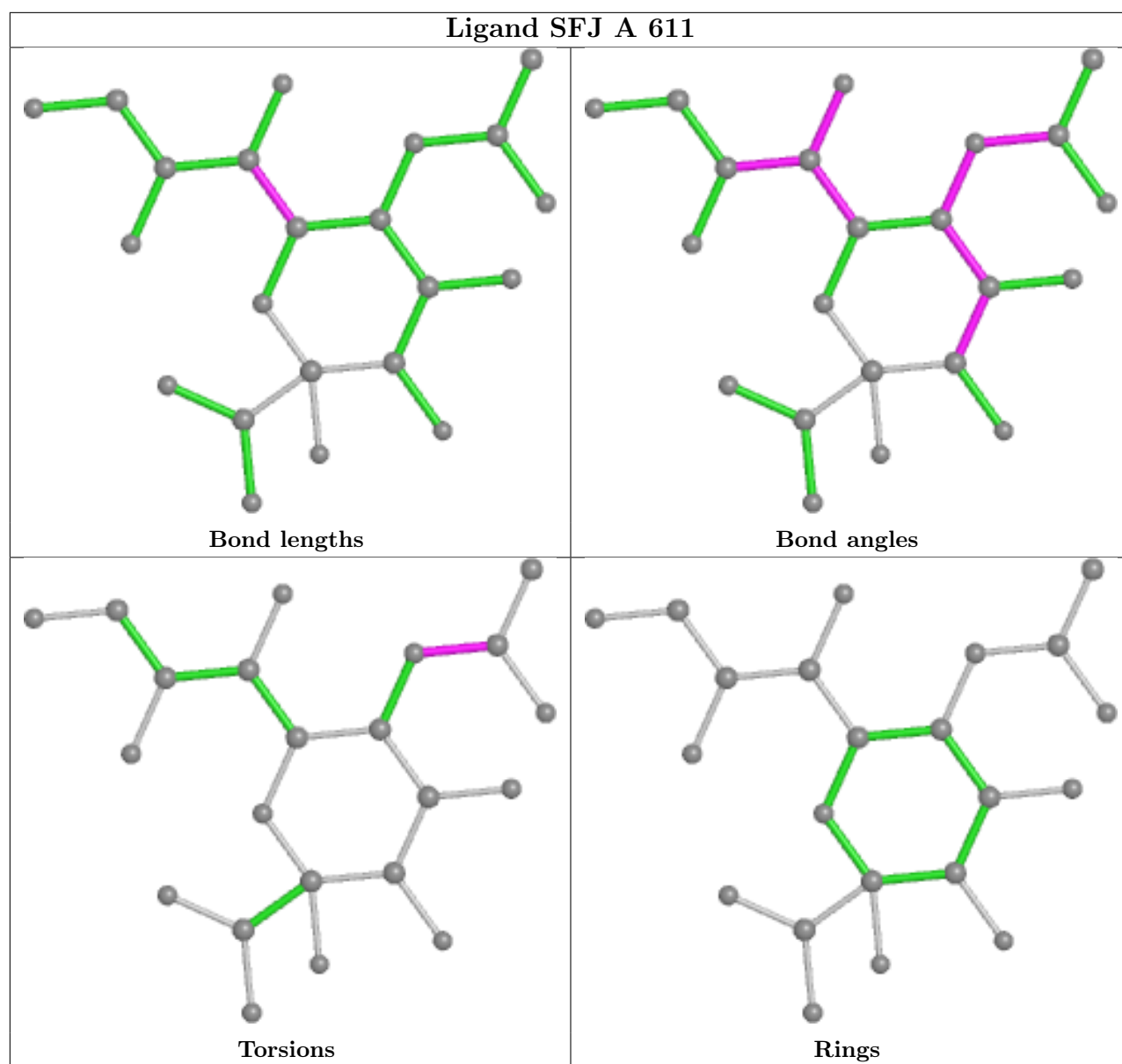












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	431/431 (100%)	-0.20	1 (0%) 95 95	17, 32, 55, 86	0
1	B	431/431 (100%)	-0.18	2 (0%) 91 91	19, 32, 58, 90	0
All	All	862/862 (100%)	-0.19	3 (0%) 94 94	17, 32, 56, 90	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	572	SER	3.8
1	B	142	ILE	2.8
1	B	354	GLY	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAG	D	1	14/15	0.69	0.17	70,81,97,99	0
3	NAG	D	2	14/15	0.72	0.29	96,114,124,129	0
4	NAG	A	601	14/15	0.75	0.26	82,92,101,105	0
2	NAG	C	1	14/15	0.83	0.23	72,84,90,94	0
3	NAG	F	2	14/15	0.85	0.27	72,80,94,99	0
2	NAG	E	2	14/15	0.88	0.21	58,75,79,99	0
2	NAG	C	2	14/15	0.90	0.22	73,85,90,97	0
2	NAG	E	1	14/15	0.93	0.21	71,74,86,92	0



### 6.3 Carbohydrates

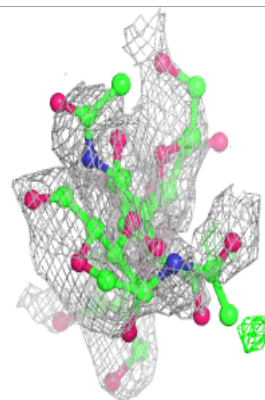
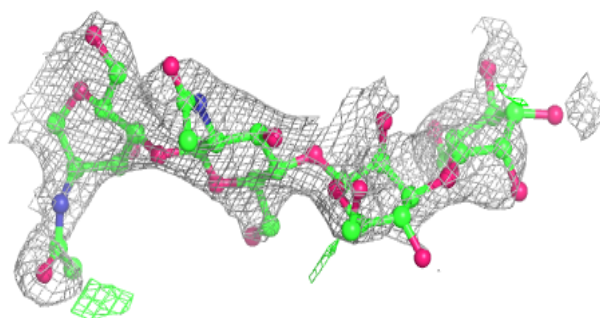
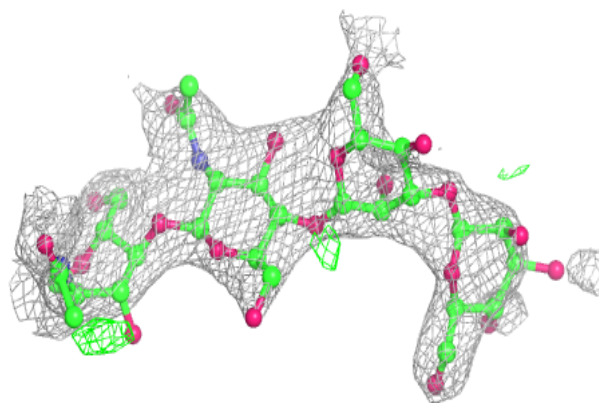
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	D	1	14/15	0.69	0.17	70,81,97,99	0
3	NAG	D	2	14/15	0.72	0.29	96,114,124,129	0
2	BMA	E	4	11/12	0.73	0.29	84,98,102,105	0
2	BMA	C	3	11/12	0.74	0.27	94,102,106,108	0
2	BMA	C	4	11/12	0.75	0.28	70,93,102,104	0
2	BMA	E	3	11/12	0.76	0.36	98,111,114,115	0
3	FUC	D	3	10/11	0.79	0.34	97,105,111,111	0
3	FUC	F	3	10/11	0.81	0.22	57,62,64,66	0
2	NAG	C	1	14/15	0.83	0.23	72,84,90,94	0
3	NAG	F	2	14/15	0.85	0.27	72,80,94,99	0
2	NAG	E	2	14/15	0.88	0.21	58,75,79,99	0
2	NAG	C	2	14/15	0.90	0.22	73,85,90,97	0
3	NAG	F	1	14/15	0.90	0.15	52,60,71,72	0
2	NAG	E	1	14/15	0.93	0.21	71,74,86,92	0

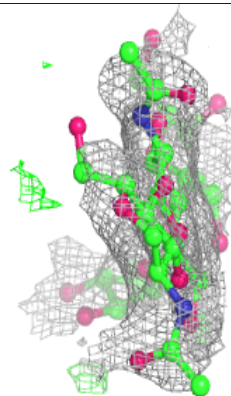
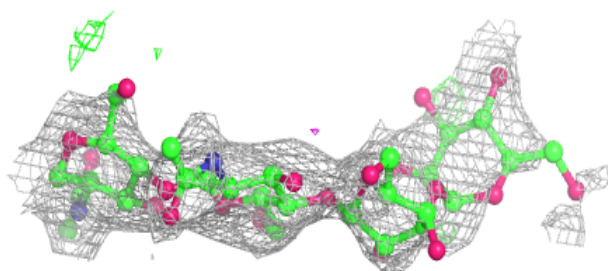
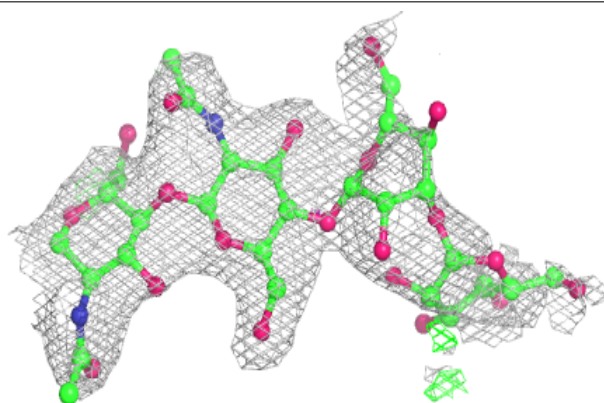
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**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)

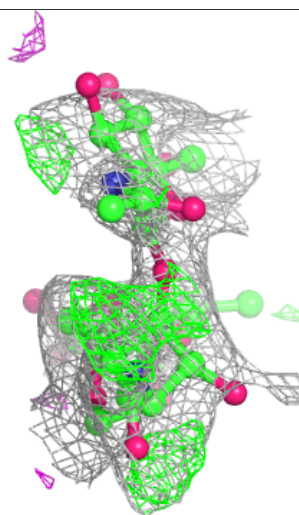
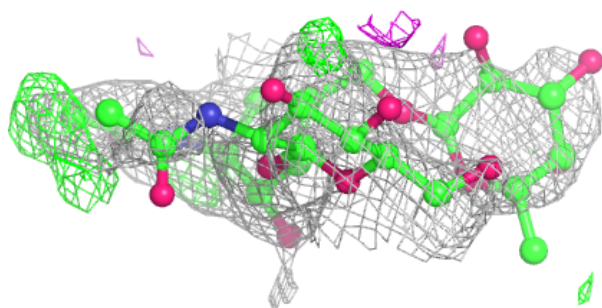
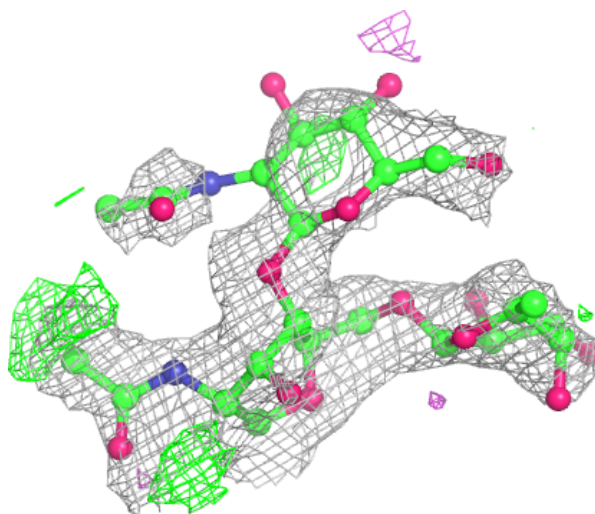
**Electron density around Chain E:**

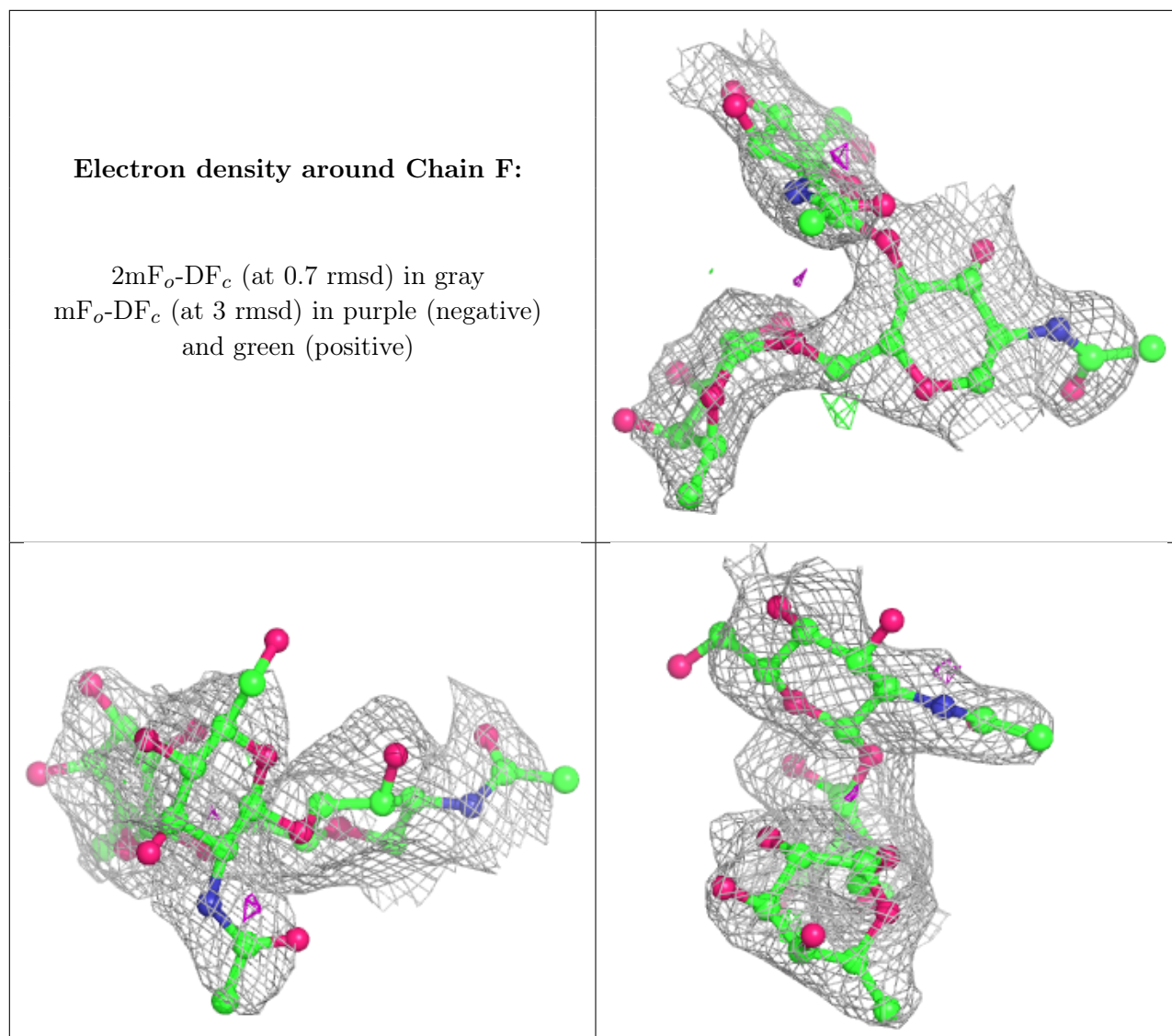
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain D:**

$2mF_o-DF_c$  (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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	A	601	14/15	0.75	0.26	82,92,101,105	0
7	SFJ	A	612	22/22	0.80	0.29	54,76,87,91	0
7	SFJ	B	612	22/22	0.85	0.31	51,67,74,80	0
8	SO4	B	616	5/5	0.90	0.26	77,77,84,92	0
7	SFJ	A	611	22/22	0.91	0.14	36,49,55,57	0
8	SO4	A	613	5/5	0.91	0.19	64,80,83,84	0
8	SO4	A	615	5/5	0.91	0.23	79,79,87,88	0

*Continued on next page...*

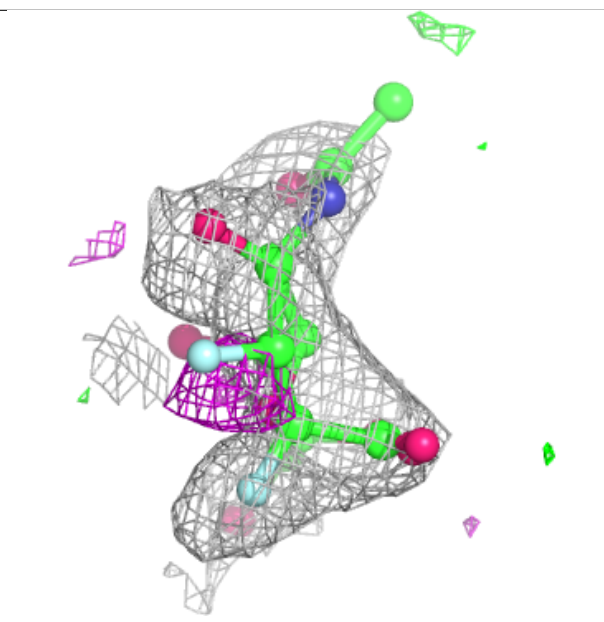
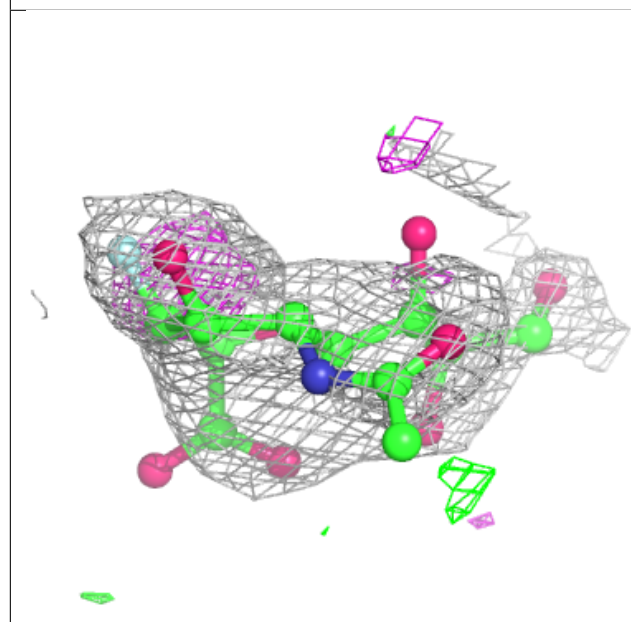
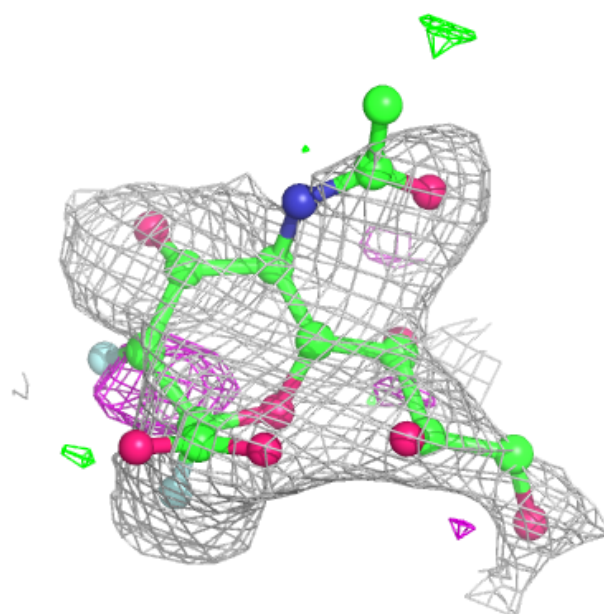
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	SO4	B	615	5/5	0.91	0.15	79,82,85,89	0
4	NAG	B	602	14/15	0.91	0.14	46,66,79,80	0
8	SO4	B	613	5/5	0.92	0.24	75,77,87,88	0
8	SO4	B	617	5/5	0.92	0.24	72,79,82,93	0
8	SO4	B	614	5/5	0.95	0.16	70,71,73,77	0
8	SO4	A	616	5/5	0.95	0.16	64,65,69,70	0
8	SO4	B	618	5/5	0.95	0.22	85,85,89,91	0
8	SO4	A	614	5/5	0.96	0.18	52,54,62,69	0
8	SO4	A	617	5/5	0.96	0.18	77,83,83,92	0
5	FSI	A	609[A]	21/22	0.97	0.12	21,24,29,30	21
6	DF4	A	610[B]	21/21	0.97	0.15	17,18,19,20	21
8	SO4	B	601	5/5	0.97	0.11	70,71,75,75	0
6	DF4	B	611[B]	21/21	0.98	0.14	13,13,14,14	21
8	SO4	A	618	5/5	0.98	0.13	61,61,64,64	0
5	FSI	B	610[A]	21/22	0.98	0.14	23,25,30,31	21
9	CA	A	619	1/1	0.98	0.07	37,37,37,37	0
9	CA	B	619	1/1	0.99	0.07	32,32,32,32	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

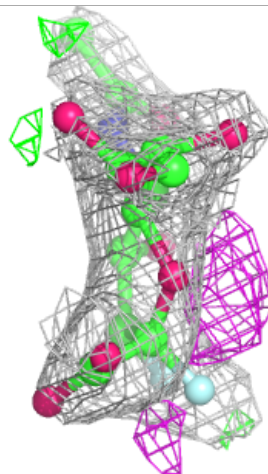
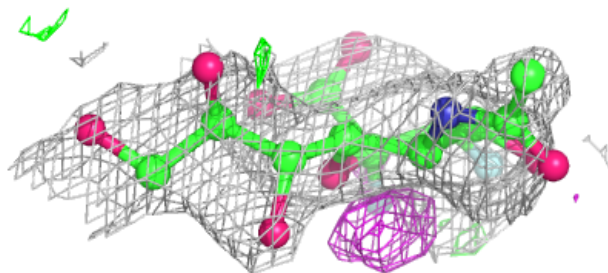
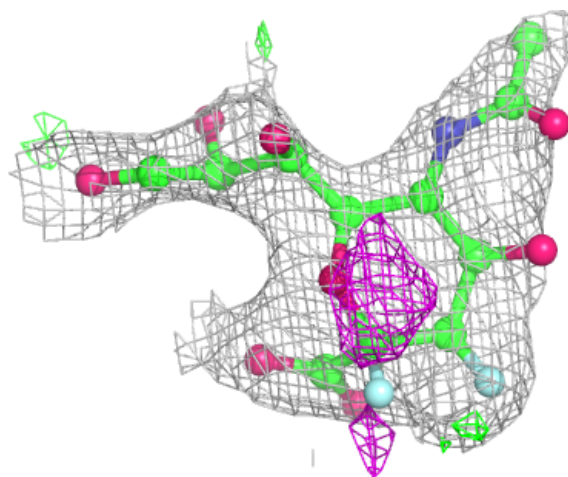
**Electron density around SFJ A 612:**

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



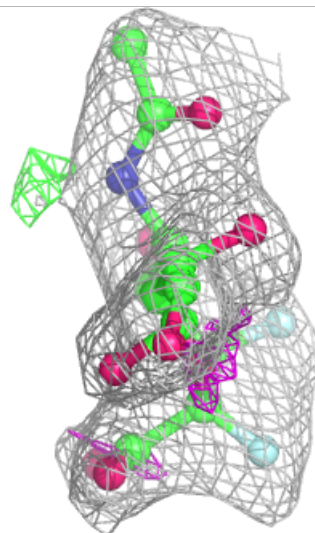
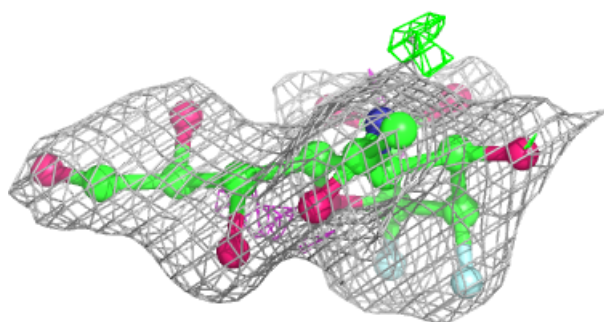
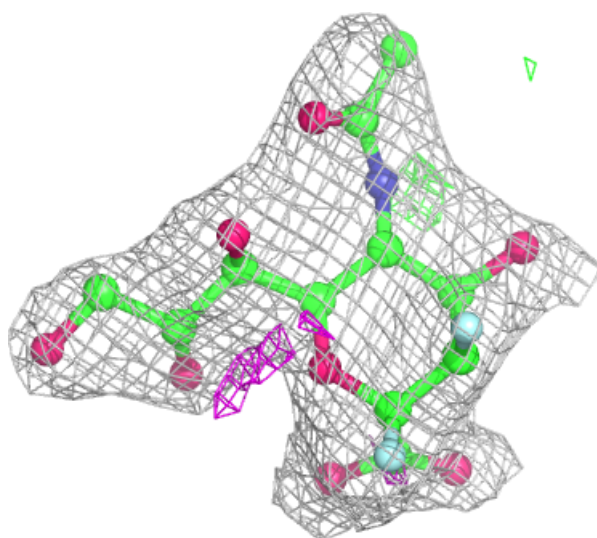
**Electron density around SFJ B 612:**

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



**Electron density around SFJ A 611:**

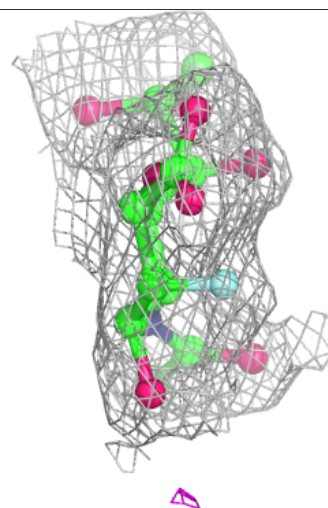
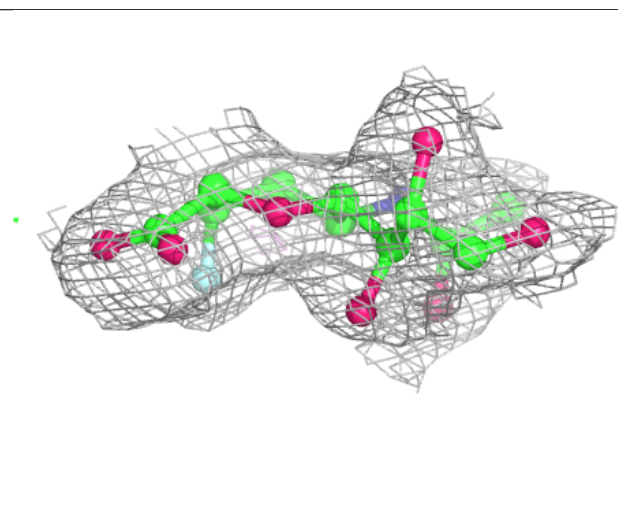
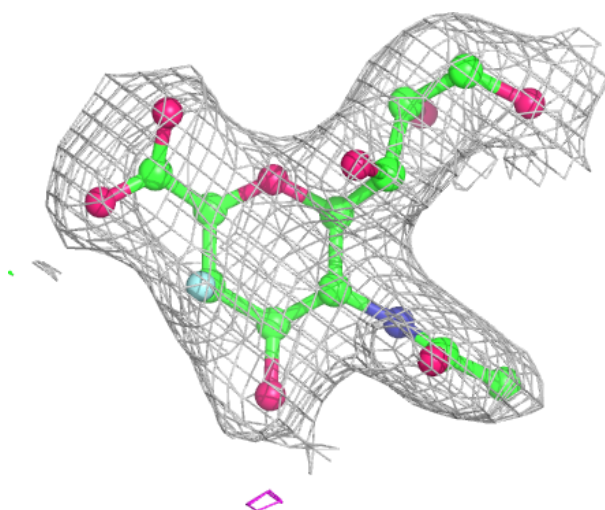
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





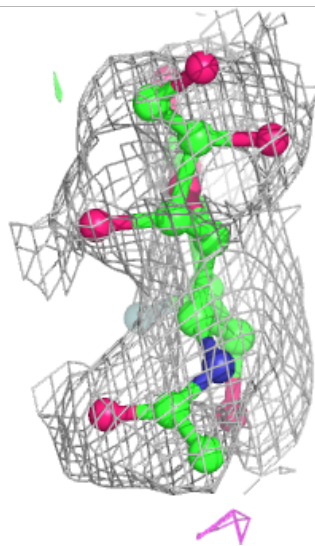
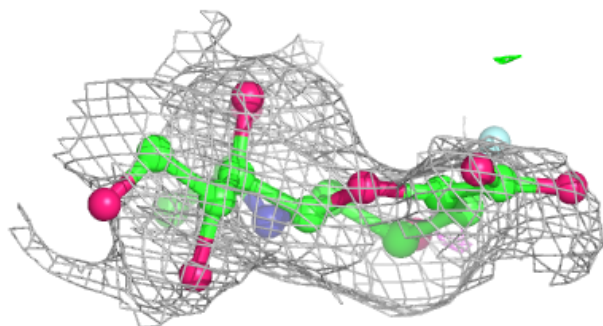
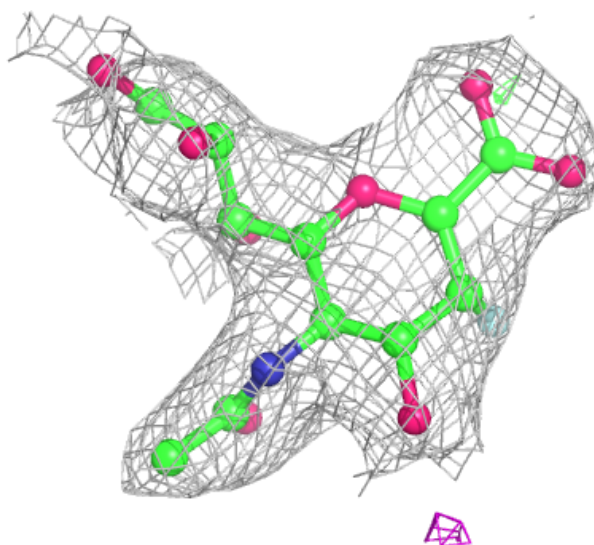
**Electron density around FSI A 609 (A):**

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



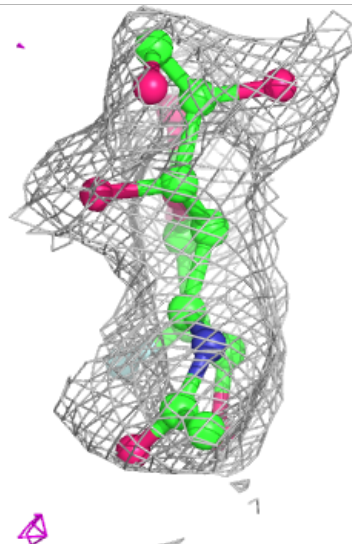
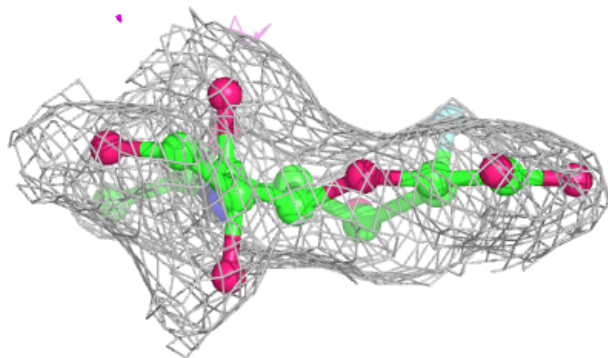
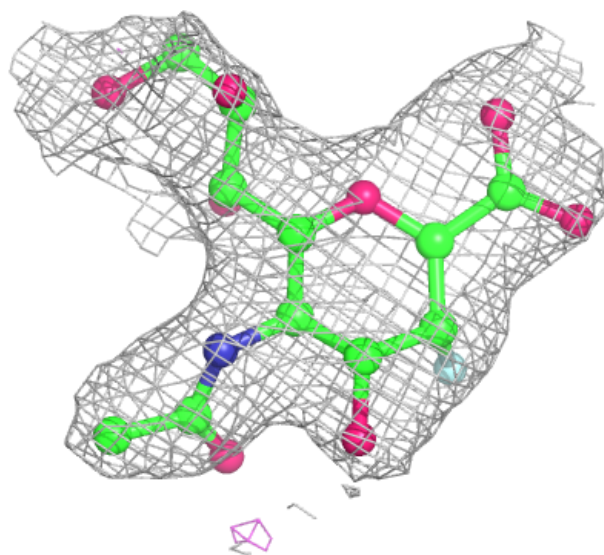
**Electron density around DF4 A 610 (B):**

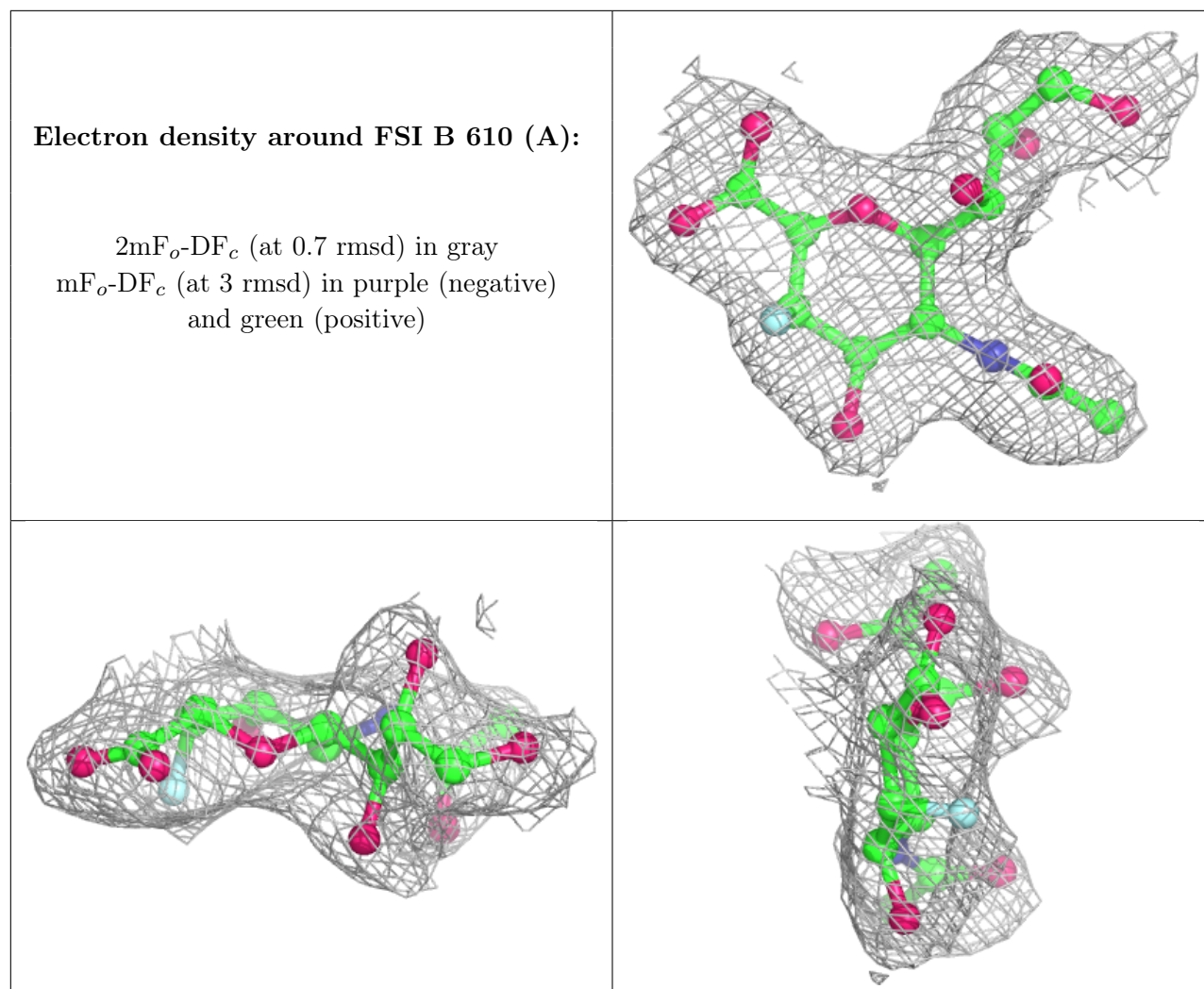
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around DF4 B 611 (B):**

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





## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.