



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 22, 2022 – 06:35 pm GMT

PDB ID : 8BES
Title : Structure of D188A-fructofuranosidase from *Rhodotorula dairenensis* in complex with fructose
Authors : Jimenez-Ortega, E.; Sanz-Aparicio, J.
Deposited on : 2022-10-21
Resolution : 1.86 Å (reported)

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

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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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.3
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) : 2.31.3

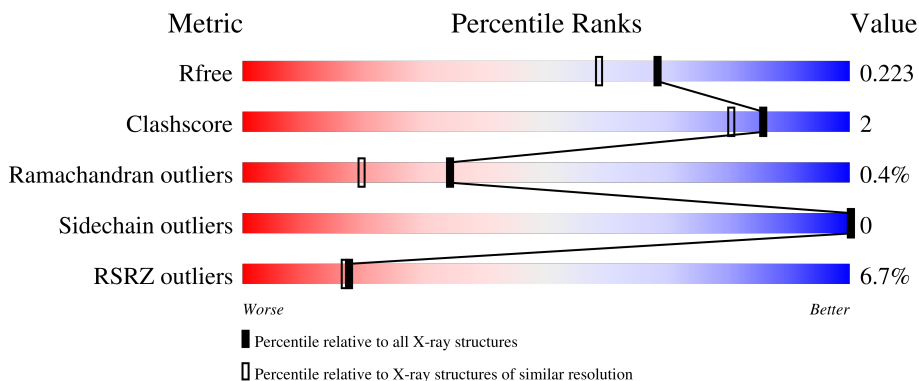
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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

Mol	Chain	Length	Quality of chain
1	A	675	
1	B	675	
1	C	675	
1	D	675	
2	E	4	

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Mol	Chain	Length	Quality of chain
3	F	3	
3	K	3	
4	G	2	
4	I	2	
4	J	2	
4	L	2	
5	H	6	

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
2	MAN	E	4	-	-	-	X
3	BMA	F	3	-	-	-	X
3	BMA	K	3	-	-	-	X
4	NAG	G	2	-	-	-	X
4	NAG	L	2	-	-	-	X
6	MAN	C	702	-	-	-	X
6	MAN	D	702	-	-	-	X

2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 19127 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 Beta-fructofuranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	526	Total 4085	C 2599	N 665	O 810	S 11	0	7	0
1	B	526	Total 4052	C 2579	N 659	O 803	S 11	0	2	0
1	C	524	Total 4034	C 2570	N 657	O 796	S 11	0	1	0
1	D	524	Total 4026	C 2566	N 655	O 794	S 11	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

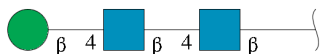
Chain	Residue	Modelled	Actual	Comment	Reference
A	188	ALA	ASP	engineered mutation	UNP A0A856TAI5
B	188	ALA	ASP	engineered mutation	UNP A0A856TAI5
C	188	ALA	ASP	engineered mutation	UNP A0A856TAI5
D	188	ALA	ASP	engineered mutation	UNP A0A856TAI5

- Molecule 2 is an oligosaccharide called alpha-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	E	4	Total 50	C 28	N 2	O 20	0	0	0

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



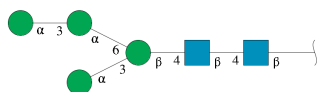
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	K	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



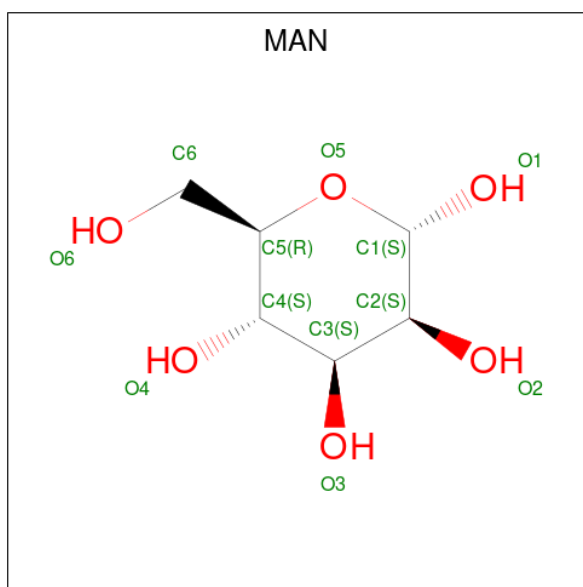
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-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
5	H	6	Total	C	N	O	0	0	0
			72	40	2	30			

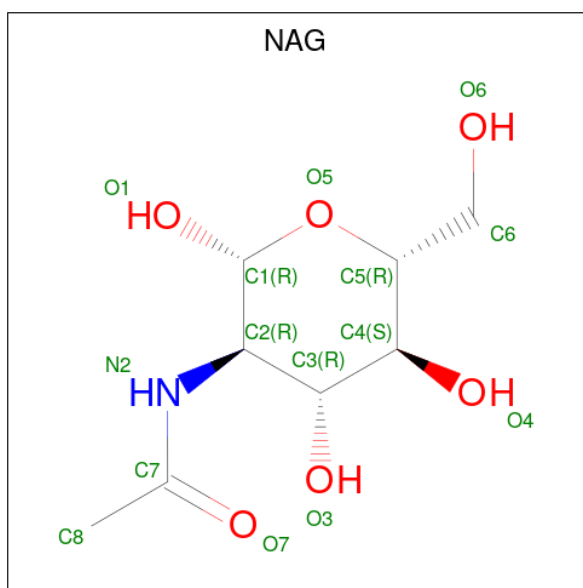
- Molecule 6 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 11 6 5	0	0
6	A	1	Total C O 11 6 5	0	0
6	A	1	Total C O 11 6 5	0	0
6	B	1	Total C O 11 6 5	0	0
6	B	1	Total C O 11 6 5	0	0
6	C	1	Total C O 11 6 5	0	0
6	C	1	Total C O 11 6 5	0	0
6	C	1	Total C O 11 6 5	0	0
6	C	1	Total C O 11 6 5	0	0
6	C	1	Total C O 11 6 5	0	0
6	D	1	Total C O 11 6 5	0	0
6	D	1	Total C O 11 6 5	0	0
6	D	1	Total C O 11 6 5	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

C₈H₁₅NO₆).



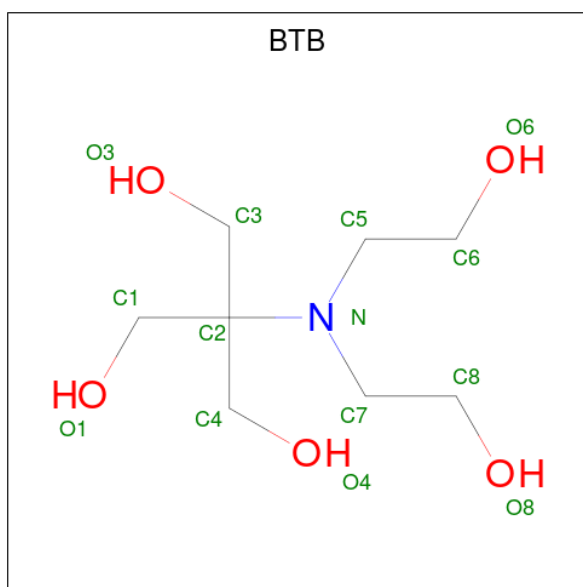
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1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

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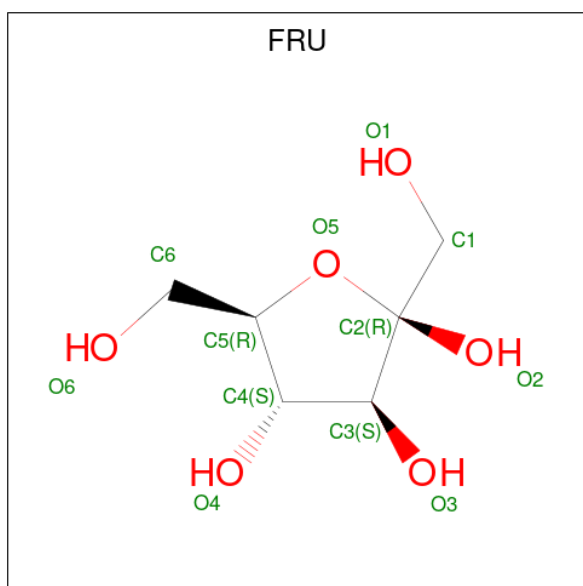
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1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

- Molecule 8 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C₈H₁₉NO₅).



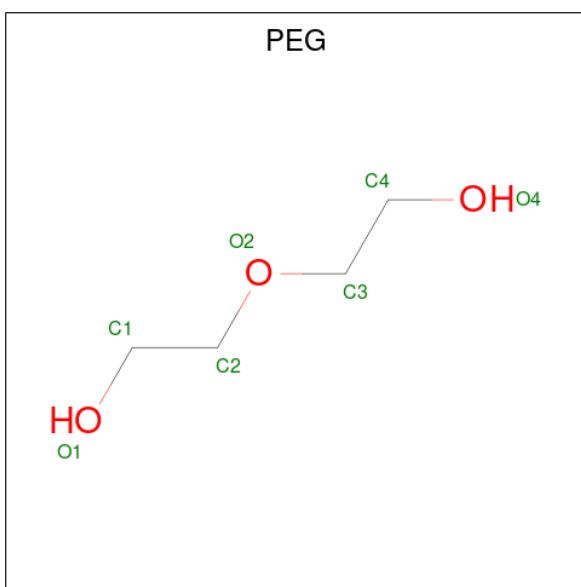
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	A	1	14	8	1	5	0	0
8	B	1	14	8	1	5	0	0
8	C	1	14	8	1	5	0	0
8	D	1	14	8	1	5	0	0

- Molecule 9 is beta-D-fructofuranose (three-letter code: FRU) (formula: C₆H₁₂O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			12	6	6		
9	B	1	Total	C	O	0	0
			12	6	6		
9	C	1	Total	C	O	0	0
			12	6	6		
9	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 10 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	C	O	0	0
			7	4	3		

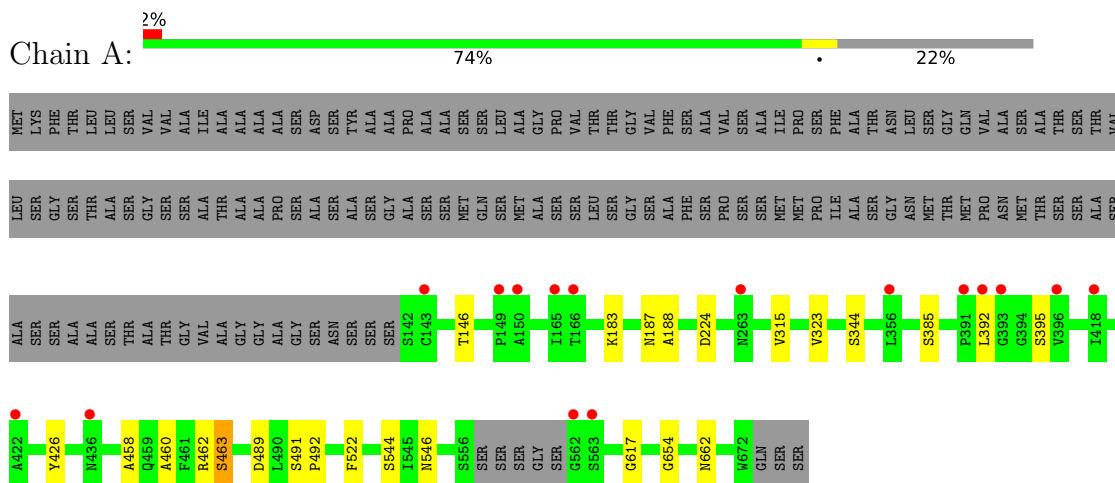
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	572	Total	O	0	0
			572	572		
11	B	502	Total	O	0	0
			502	502		
11	C	446	Total	O	0	0
			446	446		
11	D	452	Total	O	0	0
			452	452		

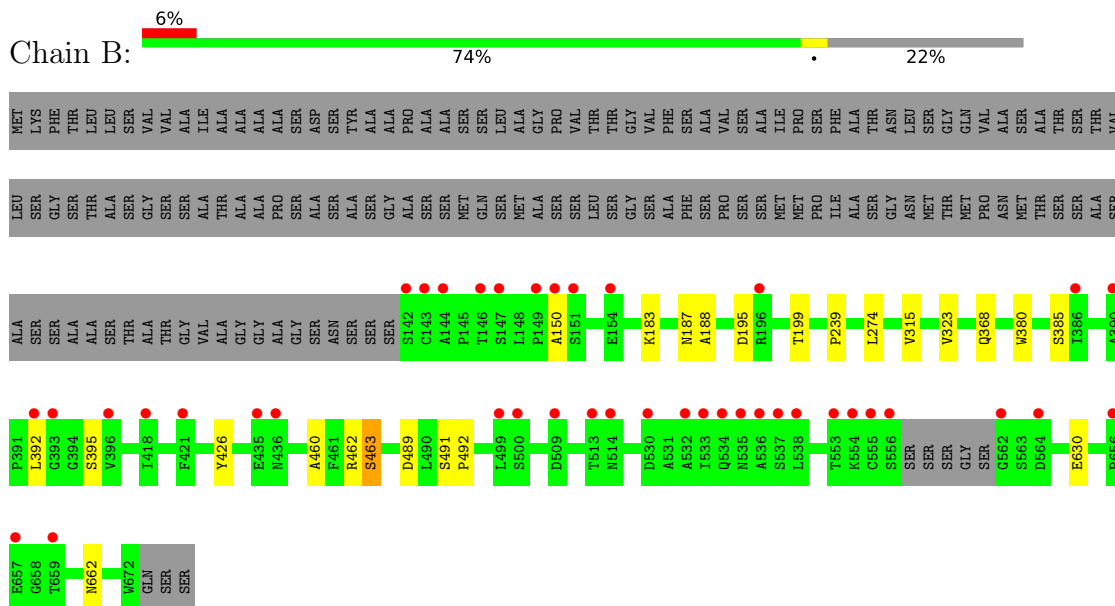
3 Residue-property plots i

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: Beta-fructofuranosidase

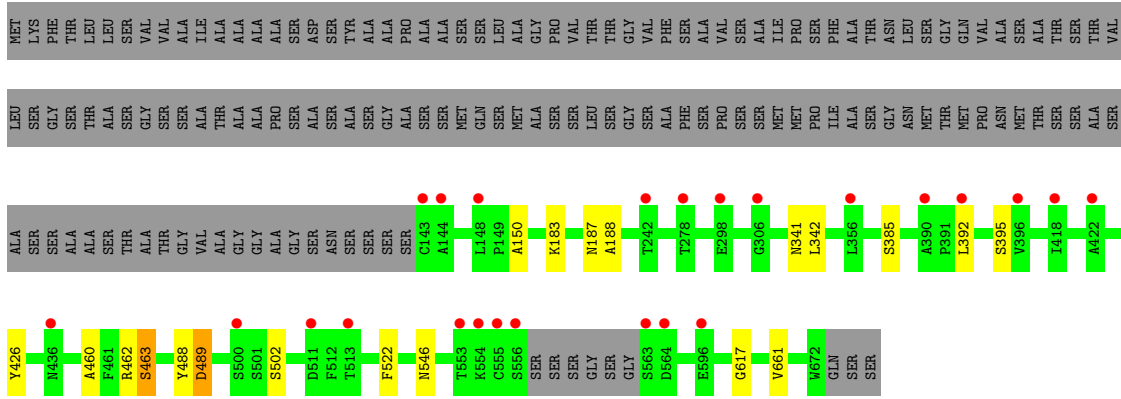


- Molecule 1: Beta-fructofuranosidase

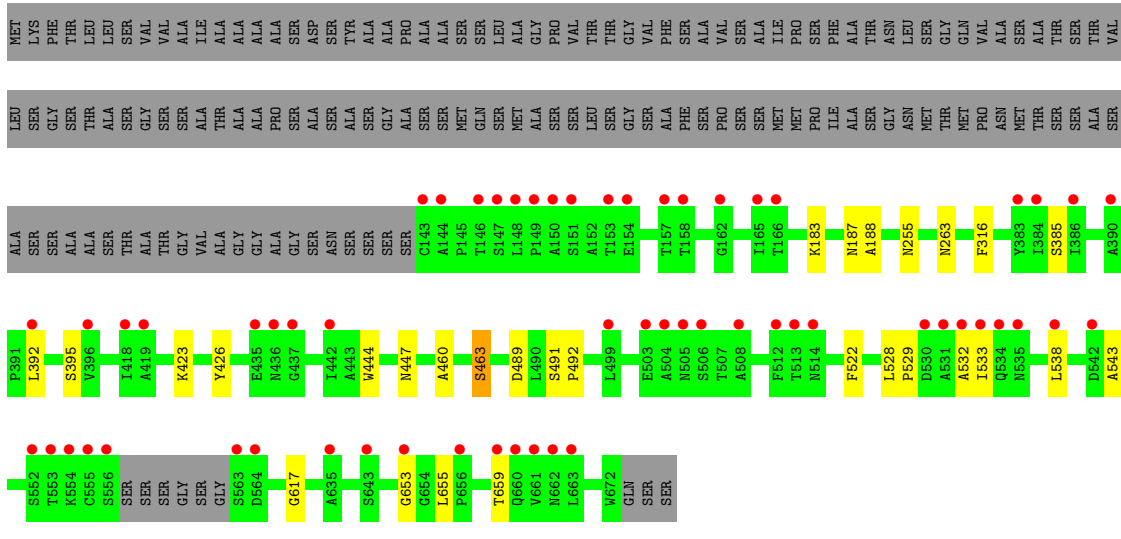
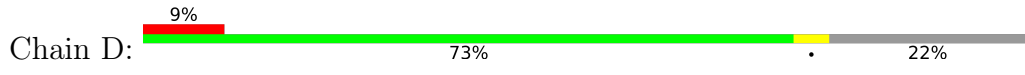


- Molecule 1: Beta-fructofuranosidase

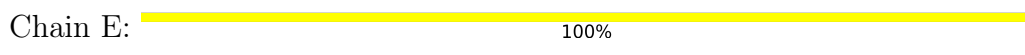




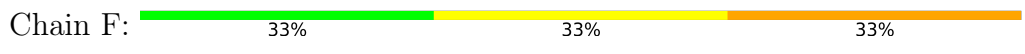
● Molecule 1: Beta-fructofuranosidase



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



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

Chain K:  67% 33%


MAG1
MAG2
BMA3

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

Chain G:  50% 50%



MAG1
MAG2

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

Chain I:  50% 50%


MAG1
MAG2

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

Chain J:  50% 50%

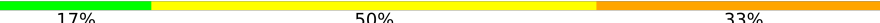

MAG1
MAG2

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

Chain L:  50% 50%


MAG1
MAG2

- Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-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

Chain H:  17% 50% 33%


MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.85Å 112.69Å 139.62Å 90.00° 104.90° 90.00°	Depositor
Resolution (Å)	45.74 – 1.86 45.70 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.74-1.86) 99.9 (45.70-1.86)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 1.86Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.184 , 0.217 0.192 , 0.223	Depositor DCC
R_{free} test set	10109 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtrriage
Anisotropy	0.245	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19127	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: BMA, MAN, NAG, BTB, FRU, PEG

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	0.61	0/4216	0.74	0/5797
1	B	0.62	0/4180	0.74	0/5748
1	C	0.62	0/4162	0.74	0/5724
1	D	0.62	0/4154	0.73	0/5713
All	All	0.62	0/16712	0.74	0/22982

There are no bond length outliers.

There are no bond angle outliers.

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	4085	0	3794	20	0
1	B	4052	0	3762	17	0
1	C	4034	0	3748	14	0
1	D	4026	0	3747	19	0
2	E	50	0	43	0	0
3	F	39	0	34	1	0
3	K	39	0	34	0	0
4	G	28	0	25	0	0
4	I	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	28	0	25	1	0
4	L	28	0	25	0	0
5	H	72	0	61	1	0
6	A	33	0	30	2	0
6	B	22	0	20	1	0
6	C	55	0	50	1	0
6	D	33	0	30	0	0
7	A	126	0	117	7	0
7	B	84	0	78	5	0
7	C	98	0	91	1	0
7	D	84	0	78	1	0
8	A	14	0	19	0	0
8	B	14	0	19	1	0
8	C	14	0	19	0	0
8	D	14	0	19	1	0
9	A	12	0	12	0	0
9	B	12	0	12	0	0
9	C	12	0	12	0	0
9	D	12	0	12	0	0
10	D	7	0	10	1	0
11	A	572	0	0	0	0
11	B	502	0	0	3	0
11	C	446	0	0	0	0
11	D	452	0	0	3	0
All	All	19127	0	15951	74	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 2.

The worst 5 of 74 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:ASN:HB3	11:D:1138:HOH:O	1.72	0.89
11:B:1302:HOH:O	3:F:3:BMA:H4	1.70	0.89
1:C:392:LEU:HD23	1:D:392:LEU:HD23	1.67	0.77
1:B:274:LEU:HD21	7:B:703:NAG:H62	1.73	0.70
1:C:150:ALA:HA	6:C:703:MAN:H3	1.74	0.70

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	529/675 (78%)	508 (96%)	19 (4%)	2 (0%)	34	19
1	B	524/675 (78%)	499 (95%)	23 (4%)	2 (0%)	34	19
1	C	521/675 (77%)	499 (96%)	20 (4%)	2 (0%)	34	19
1	D	520/675 (77%)	495 (95%)	23 (4%)	2 (0%)	34	19
All	All	2094/2700 (78%)	2001 (96%)	85 (4%)	8 (0%)	34	19

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	SER
1	B	463	SER
1	B	489	ASP
1	C	463	SER
1	D	463	SER

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	448/545 (82%)	448 (100%)	0	100	100
1	B	443/545 (81%)	443 (100%)	0	100	100
1	C	441/545 (81%)	441 (100%)	0	100	100
1	D	440/545 (81%)	440 (100%)	0	100	100
All	All	1772/2180 (81%)	1772 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	B	187	ASN
1	C	187	ASN
1	D	187	ASN
1	D	299	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

24 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	E	1	1,2	14,14,15	0.39	0	17,19,21	1.04	1 (5%)
2	NAG	E	2	2	14,14,15	0.34	0	17,19,21	0.97	1 (5%)
2	BMA	E	3	2	11,11,12	0.25	0	15,15,17	1.07	2 (13%)
2	MAN	E	4	2	11,11,12	0.32	0	15,15,17	0.80	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.33	0	17,19,21	0.90	0
3	NAG	F	2	3	14,14,15	0.31	0	17,19,21	1.11	1 (5%)
3	BMA	F	3	3	11,11,12	0.33	0	15,15,17	1.16	2 (13%)
4	NAG	G	1	1,4	14,14,15	0.35	0	17,19,21	0.62	0
4	NAG	G	2	4	14,14,15	0.26	0	17,19,21	1.08	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	H	1	1,5	14,14,15	0.45	0	17,19,21	0.81	1 (5%)
5	NAG	H	2	5	14,14,15	0.27	0	17,19,21	1.00	1 (5%)
5	BMA	H	3	5	11,11,12	0.27	0	15,15,17	1.54	1 (6%)
5	MAN	H	4	5	11,11,12	0.41	0	15,15,17	1.29	2 (13%)
5	MAN	H	5	5	11,11,12	0.38	0	15,15,17	0.87	1 (6%)
5	MAN	H	6	5	11,11,12	0.32	0	15,15,17	0.76	0
4	NAG	I	1	1,4	14,14,15	0.29	0	17,19,21	0.82	0
4	NAG	I	2	4	14,14,15	0.30	0	17,19,21	1.07	1 (5%)
4	NAG	J	1	1,4	14,14,15	0.27	0	17,19,21	0.77	1 (5%)
4	NAG	J	2	4	14,14,15	0.22	0	17,19,21	1.10	2 (11%)
3	NAG	K	1	1,3	14,14,15	0.34	0	17,19,21	0.66	0
3	NAG	K	2	3	14,14,15	0.27	0	17,19,21	0.83	0
3	BMA	K	3	3	11,11,12	0.38	0	15,15,17	1.29	2 (13%)
4	NAG	L	1	1,4	14,14,15	0.37	0	17,19,21	0.57	0
4	NAG	L	2	4	14,14,15	0.28	0	17,19,21	1.05	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1
5	NAG	H	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	MAN	H	4	5	-	1/2/19/22	0/1/1/1
5	MAN	H	5	5	-	2/2/19/22	0/1/1/1
5	MAN	H	6	5	-	2/2/19/22	0/1/1/1
4	NAG	I	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	J	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	1/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
4	NAG	L	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	3	BMA	C1-O5-C5	4.93	118.87	112.19
3	F	2	NAG	C1-O5-C5	3.78	117.31	112.19
4	L	2	NAG	C1-O5-C5	3.72	117.23	112.19
4	I	2	NAG	C1-O5-C5	3.71	117.21	112.19
3	K	3	BMA	C1-O5-C5	3.61	117.08	112.19

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

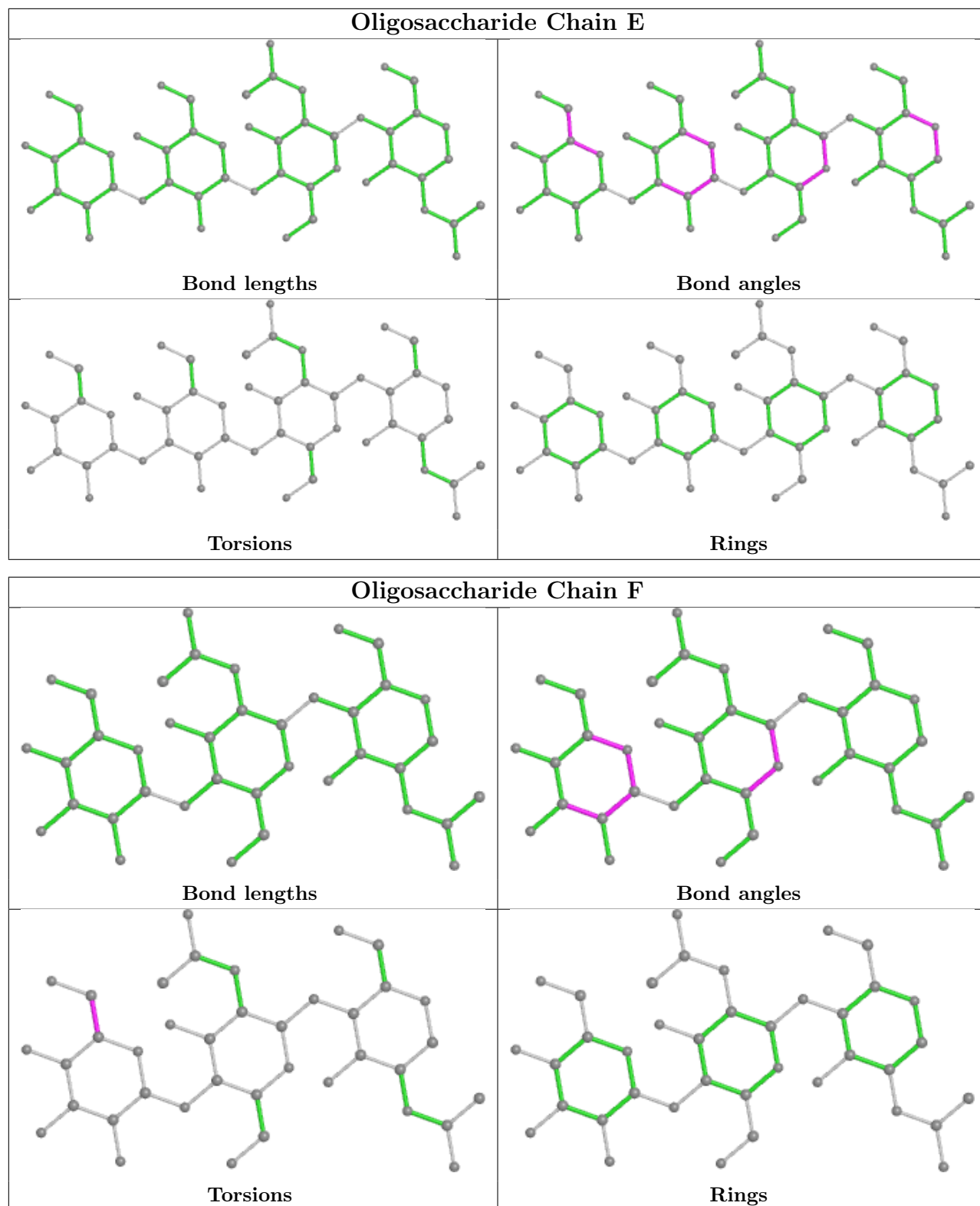
Mol	Chain	Res	Type	Atoms
5	H	6	MAN	C4-C5-C6-O6
5	H	5	MAN	O5-C5-C6-O6
5	H	5	MAN	C4-C5-C6-O6
5	H	6	MAN	O5-C5-C6-O6
5	H	4	MAN	O5-C5-C6-O6

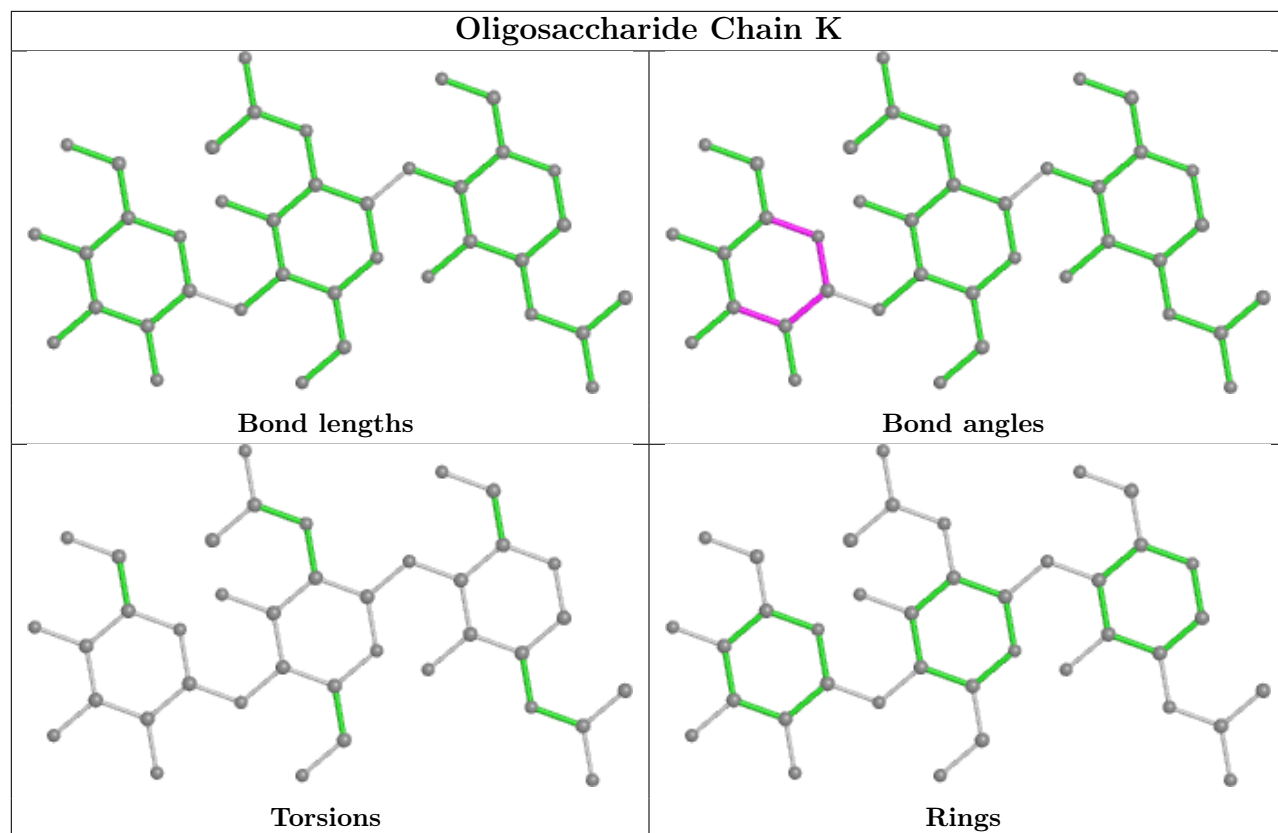
There are no ring outliers.

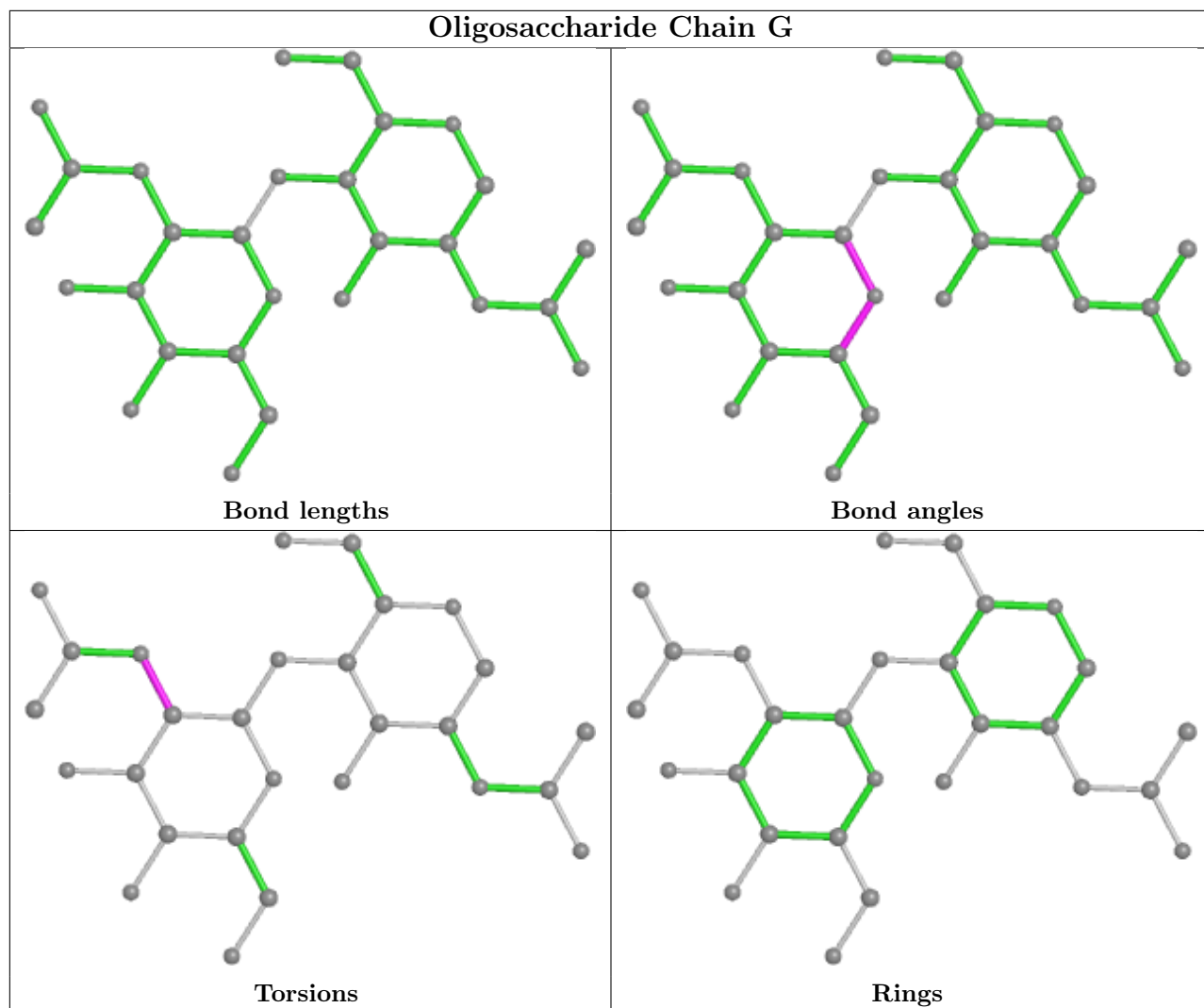
4 monomers are involved in 3 short contacts:

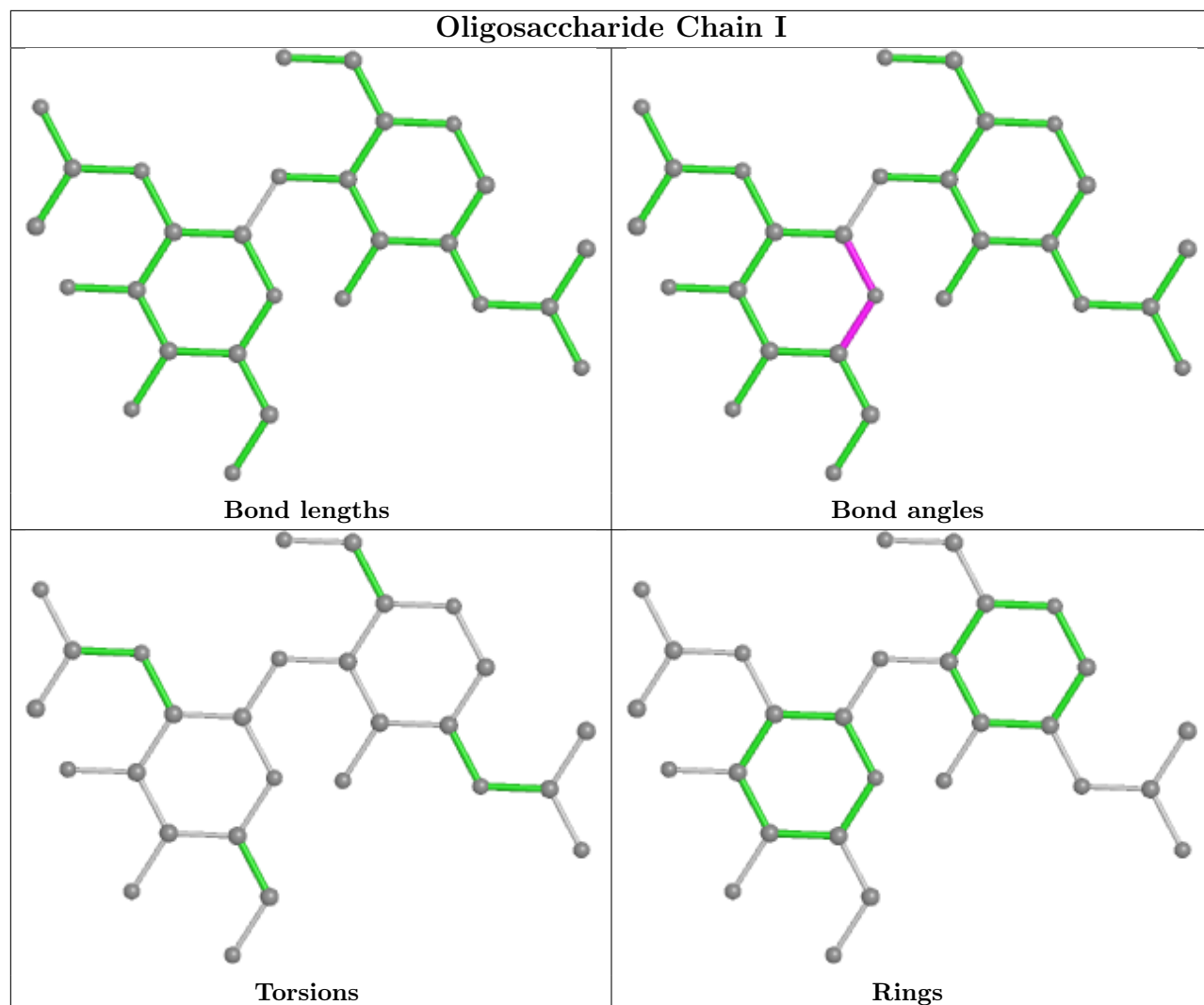
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	3	BMA	1	0
5	H	4	MAN	1	0
4	J	1	NAG	1	0
3	F	3	BMA	1	0

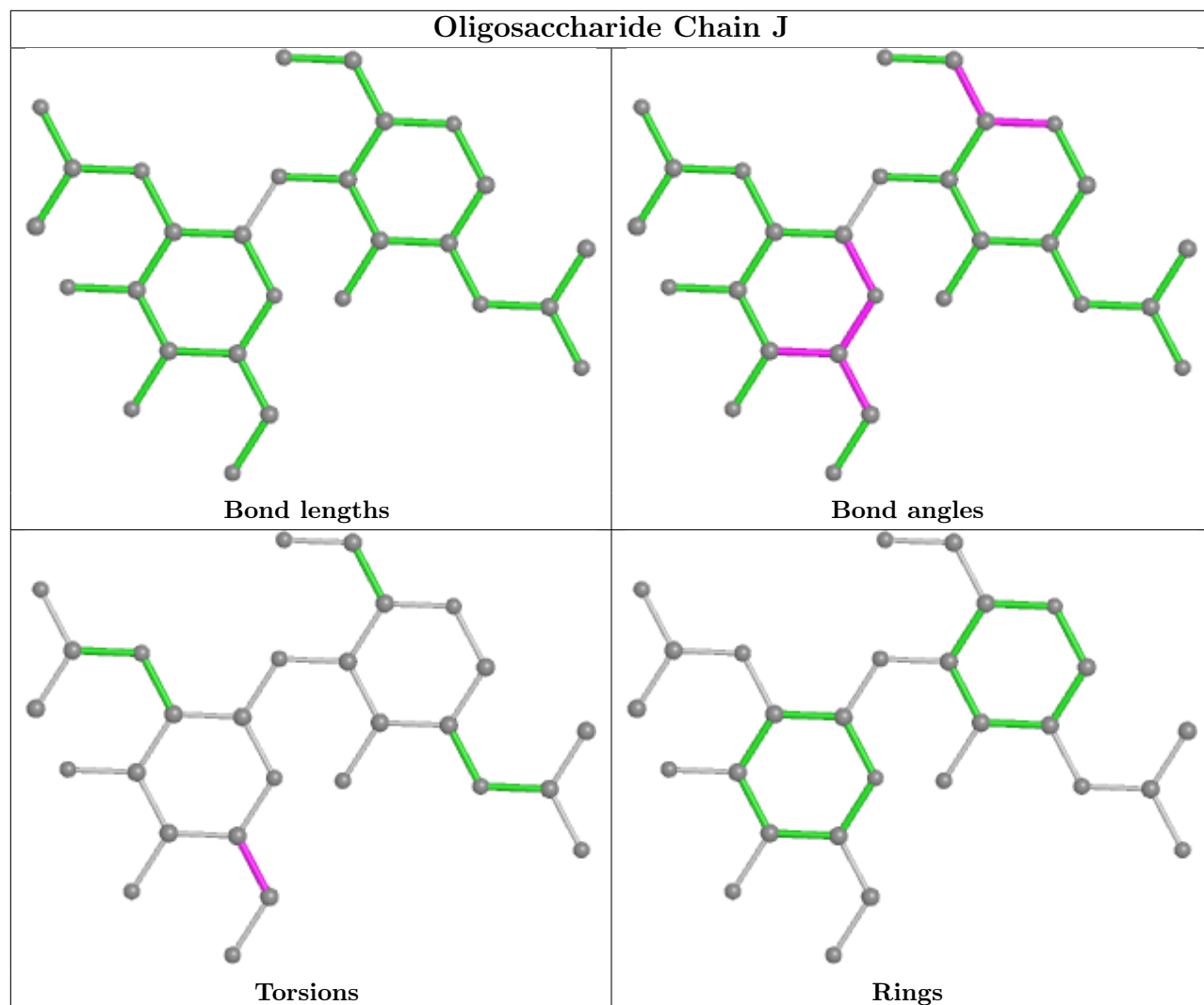
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

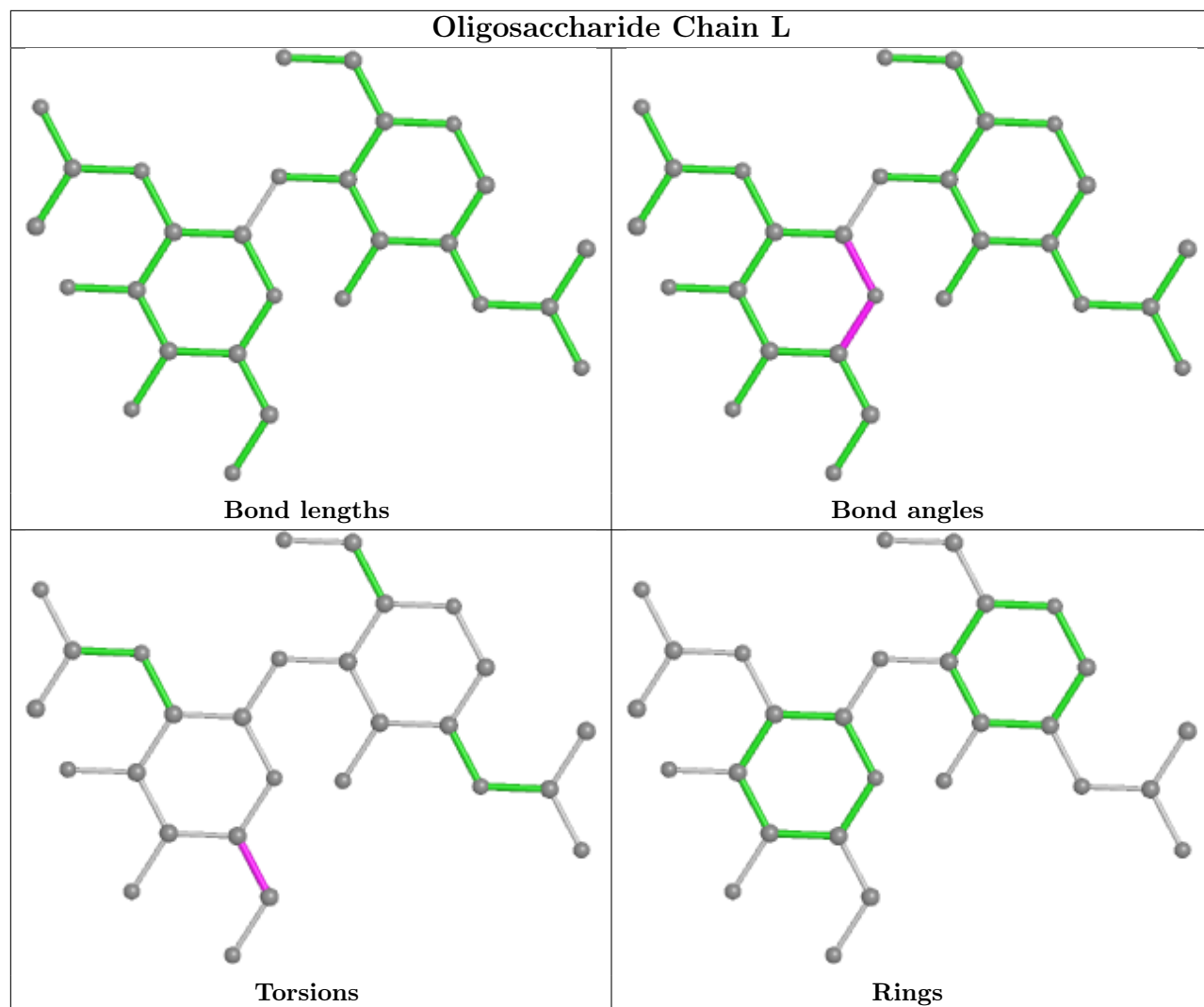


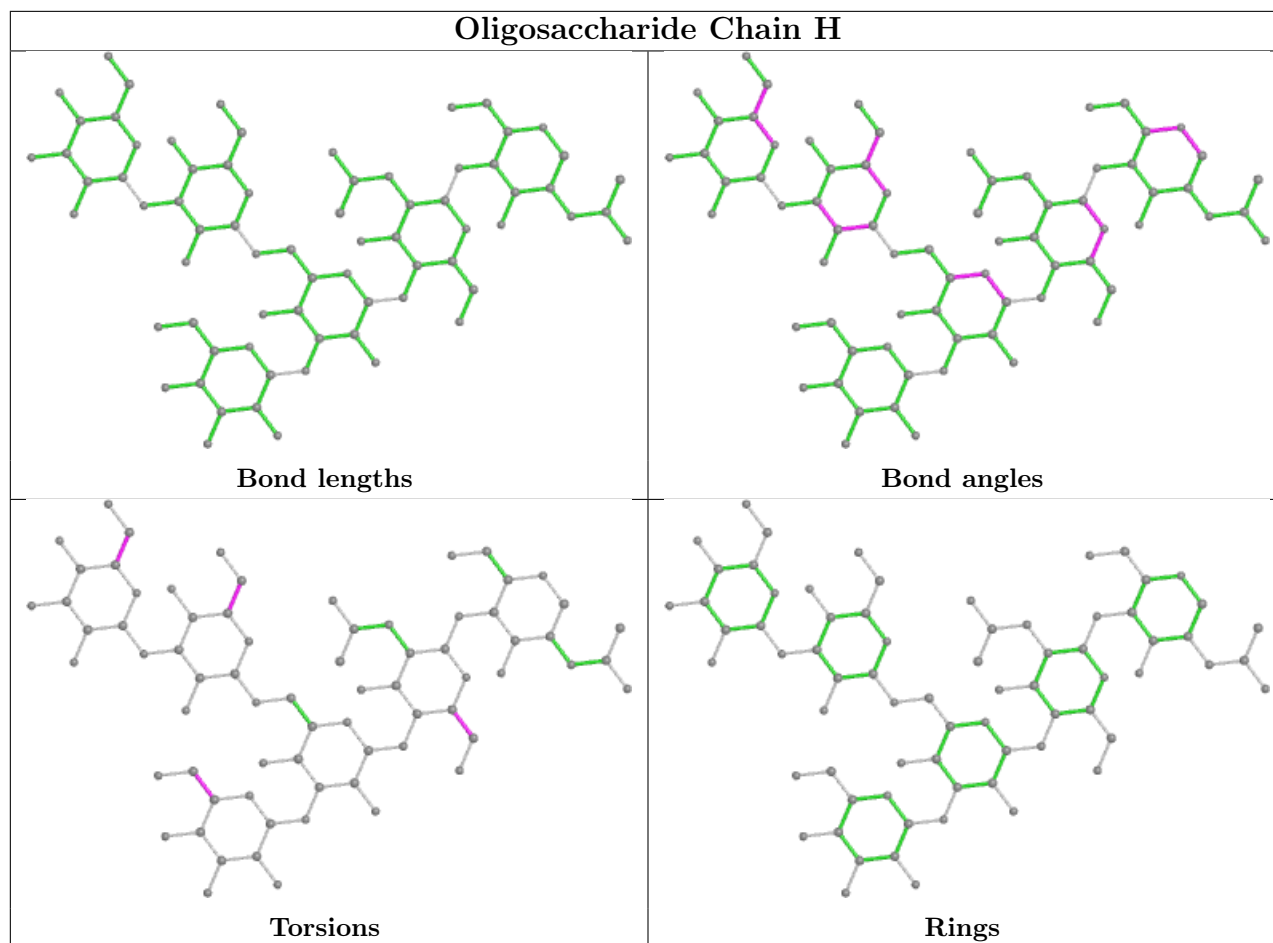












5.6 Ligand geometry [i](#)

50 ligands 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
7	NAG	D	705	1	14,14,15	0.29	0	17,19,21	0.78	0
6	MAN	C	705	1	11,11,12	0.40	0	15,15,17	0.68	0
7	NAG	C	708	1	14,14,15	0.35	0	17,19,21	0.77	0
9	FRU	A	714	-	11,12,12	0.62	0	10,18,18	0.83	0
6	MAN	D	703	1	11,11,12	0.27	0	15,15,17	0.81	1 (6%)
7	NAG	B	708	1	14,14,15	0.40	0	17,19,21	0.91	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	A	705	1	14,14,15	0.27	0	17,19,21	0.91	1 (5%)
6	MAN	C	704	1	11,11,12	0.35	0	15,15,17	0.80	0
7	NAG	A	709	1	14,14,15	0.40	0	17,19,21	0.77	0
7	NAG	D	707	1	14,14,15	0.25	0	17,19,21	0.61	0
8	BTB	B	709	-	13,13,13	0.94	1 (7%)	7,16,16	0.45	0
6	MAN	A	703	1	11,11,12	0.42	0	15,15,17	0.75	0
7	NAG	A	704	1	14,14,15	0.20	0	17,19,21	1.07	2 (11%)
7	NAG	A	708	1	14,14,15	0.28	0	17,19,21	1.12	1 (5%)
8	BTB	C	713	-	13,13,13	1.02	1 (7%)	7,16,16	0.29	0
8	BTB	D	711	-	13,13,13	0.97	1 (7%)	7,16,16	0.33	0
6	MAN	A	701	1	11,11,12	0.33	0	15,15,17	1.14	2 (13%)
7	NAG	C	709	1	14,14,15	0.38	0	17,19,21	0.80	0
6	MAN	C	703	1	11,11,12	0.35	0	15,15,17	1.00	0
7	NAG	A	707	1	14,14,15	0.39	0	17,19,21	0.75	0
7	NAG	C	710	1	14,14,15	0.32	0	17,19,21	0.89	1 (5%)
9	FRU	C	714	-	11,12,12	0.65	0	10,18,18	0.70	0
8	BTB	A	713	-	13,13,13	0.95	1 (7%)	7,16,16	0.32	0
6	MAN	D	704	1	11,11,12	0.36	0	15,15,17	0.82	0
7	NAG	D	706	1	14,14,15	0.45	0	17,19,21	1.19	1 (5%)
9	FRU	B	710	-	11,12,12	0.78	0	10,18,18	1.01	1 (10%)
7	NAG	A	710	1	14,14,15	0.38	0	17,19,21	1.40	2 (11%)
10	PEG	D	701	-	6,6,6	0.24	0	5,5,5	0.18	0
7	NAG	D	710	1	14,14,15	0.32	0	17,19,21	0.68	0
7	NAG	A	706	1	14,14,15	0.33	0	17,19,21	0.90	0
7	NAG	B	703	1	14,14,15	0.41	0	17,19,21	1.43	3 (17%)
7	NAG	B	706	1	14,14,15	0.28	0	17,19,21	0.93	1 (5%)
7	NAG	C	706	1	14,14,15	0.26	0	17,19,21	0.66	0
7	NAG	D	709	1	14,14,15	0.66	1 (7%)	17,19,21	1.15	2 (11%)
6	MAN	C	701	1	11,11,12	0.29	0	15,15,17	0.73	0
6	MAN	D	702	1	11,11,12	0.31	0	15,15,17	0.75	0
7	NAG	B	705	1	14,14,15	0.44	0	17,19,21	0.93	1 (5%)
7	NAG	B	707	1	14,14,15	0.49	0	17,19,21	1.78	5 (29%)
7	NAG	C	707	1	14,14,15	0.48	0	17,19,21	1.29	3 (17%)
7	NAG	B	704	1	14,14,15	0.23	0	17,19,21	0.94	0
7	NAG	D	708	1	14,14,15	0.28	0	17,19,21	0.72	0
9	FRU	D	712	-	11,12,12	0.80	1 (9%)	10,18,18	0.90	0
6	MAN	B	702	1	11,11,12	0.29	0	15,15,17	0.82	0
7	NAG	C	712	1	14,14,15	0.22	0	17,19,21	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	A	702	1	11,11,12	0.26	0	15,15,17	0.82	0
7	NAG	A	712	1	14,14,15	0.31	0	17,19,21	1.03	2 (11%)
7	NAG	C	711	1	14,14,15	0.58	0	17,19,21	1.58	3 (17%)
6	MAN	B	701	1	11,11,12	0.32	0	15,15,17	0.88	0
6	MAN	C	702	1	11,11,12	0.35	0	15,15,17	0.87	0
7	NAG	A	711	1	14,14,15	0.37	0	17,19,21	0.89	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
7	NAG	D	705	1	-	0/6/23/26	0/1/1/1
6	MAN	C	705	1	-	0/2/19/22	0/1/1/1
7	NAG	C	708	1	-	1/6/23/26	0/1/1/1
9	FRU	A	714	-	-	3/5/24/24	0/1/1/1
6	MAN	D	703	1	-	0/2/19/22	0/1/1/1
7	NAG	B	708	1	-	0/6/23/26	0/1/1/1
7	NAG	A	705	1	-	0/6/23/26	0/1/1/1
6	MAN	C	704	1	-	0/2/19/22	0/1/1/1
7	NAG	A	709	1	-	0/6/23/26	0/1/1/1
7	NAG	D	707	1	-	0/6/23/26	0/1/1/1
8	BTB	B	709	-	-	1/21/21/21	-
6	MAN	A	703	1	-	1/2/19/22	0/1/1/1
7	NAG	A	704	1	-	1/6/23/26	0/1/1/1
7	NAG	A	708	1	-	0/6/23/26	0/1/1/1
8	BTB	C	713	-	-	0/21/21/21	-
8	BTB	D	711	-	-	1/21/21/21	-
6	MAN	A	701	1	-	2/2/19/22	0/1/1/1
7	NAG	C	709	1	-	0/6/23/26	0/1/1/1
6	MAN	C	703	1	-	2/2/19/22	0/1/1/1
7	NAG	A	707	1	-	0/6/23/26	0/1/1/1
7	NAG	C	710	1	-	0/6/23/26	0/1/1/1
9	FRU	C	714	-	-	5/5/24/24	0/1/1/1
8	BTB	A	713	-	-	1/21/21/21	-
6	MAN	D	704	1	-	2/2/19/22	0/1/1/1
7	NAG	D	706	1	-	1/6/23/26	0/1/1/1
9	FRU	B	710	-	-	5/5/24/24	0/1/1/1
7	NAG	A	710	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PEG	D	701	-	-	4/4/4/4	-
7	NAG	D	710	1	-	0/6/23/26	0/1/1/1
7	NAG	A	706	1	-	0/6/23/26	0/1/1/1
7	NAG	B	703	1	-	0/6/23/26	0/1/1/1
7	NAG	B	706	1	-	0/6/23/26	0/1/1/1
7	NAG	C	706	1	-	1/6/23/26	0/1/1/1
7	NAG	D	709	1	-	4/6/23/26	0/1/1/1
6	MAN	C	701	1	-	1/2/19/22	0/1/1/1
6	MAN	D	702	1	-	0/2/19/22	0/1/1/1
7	NAG	B	705	1	-	0/6/23/26	0/1/1/1
7	NAG	B	707	1	-	3/6/23/26	0/1/1/1
7	NAG	C	707	1	-	1/6/23/26	0/1/1/1
7	NAG	B	704	1	-	0/6/23/26	0/1/1/1
7	NAG	D	708	1	-	0/6/23/26	0/1/1/1
9	FRU	D	712	-	-	4/5/24/24	0/1/1/1
6	MAN	B	702	1	-	0/2/19/22	0/1/1/1
7	NAG	C	712	1	-	0/6/23/26	0/1/1/1
6	MAN	A	702	1	-	0/2/19/22	0/1/1/1
7	NAG	A	712	1	-	4/6/23/26	0/1/1/1
7	NAG	C	711	1	-	4/6/23/26	0/1/1/1
6	MAN	B	701	1	-	0/2/19/22	0/1/1/1
6	MAN	C	702	1	-	1/2/19/22	0/1/1/1
7	NAG	A	711	1	-	0/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	712	FRU	O2-C2	2.41	1.44	1.40
8	C	713	BTB	C2-N	2.39	1.53	1.48
7	D	709	NAG	O7-C7	2.21	1.28	1.23
8	D	711	BTB	C2-N	2.18	1.52	1.48
8	B	709	BTB	C5-N	2.02	1.50	1.48

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	711	NAG	C2-N2-C7	-4.83	116.03	122.90
7	B	707	NAG	C2-N2-C7	-4.75	116.14	122.90
7	A	710	NAG	C1-C2-N2	-3.61	104.33	110.49
6	A	701	MAN	C1-O5-C5	3.58	117.04	112.19
7	C	710	NAG	C1-O5-C5	3.31	116.68	112.19

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

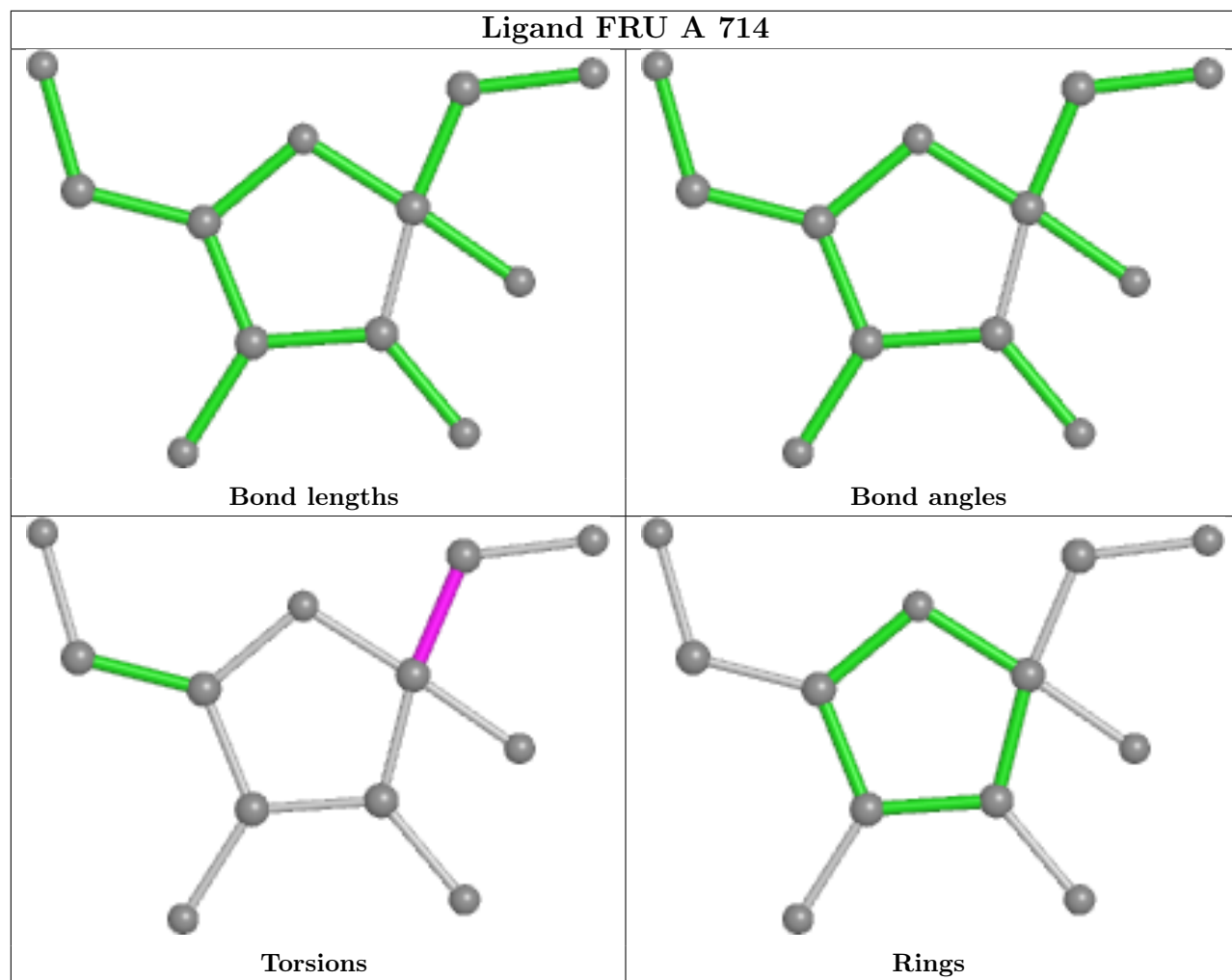
Mol	Chain	Res	Type	Atoms
7	A	710	NAG	C8-C7-N2-C2
7	A	710	NAG	O7-C7-N2-C2
7	B	707	NAG	C8-C7-N2-C2
7	B	707	NAG	O7-C7-N2-C2
7	C	711	NAG	C8-C7-N2-C2

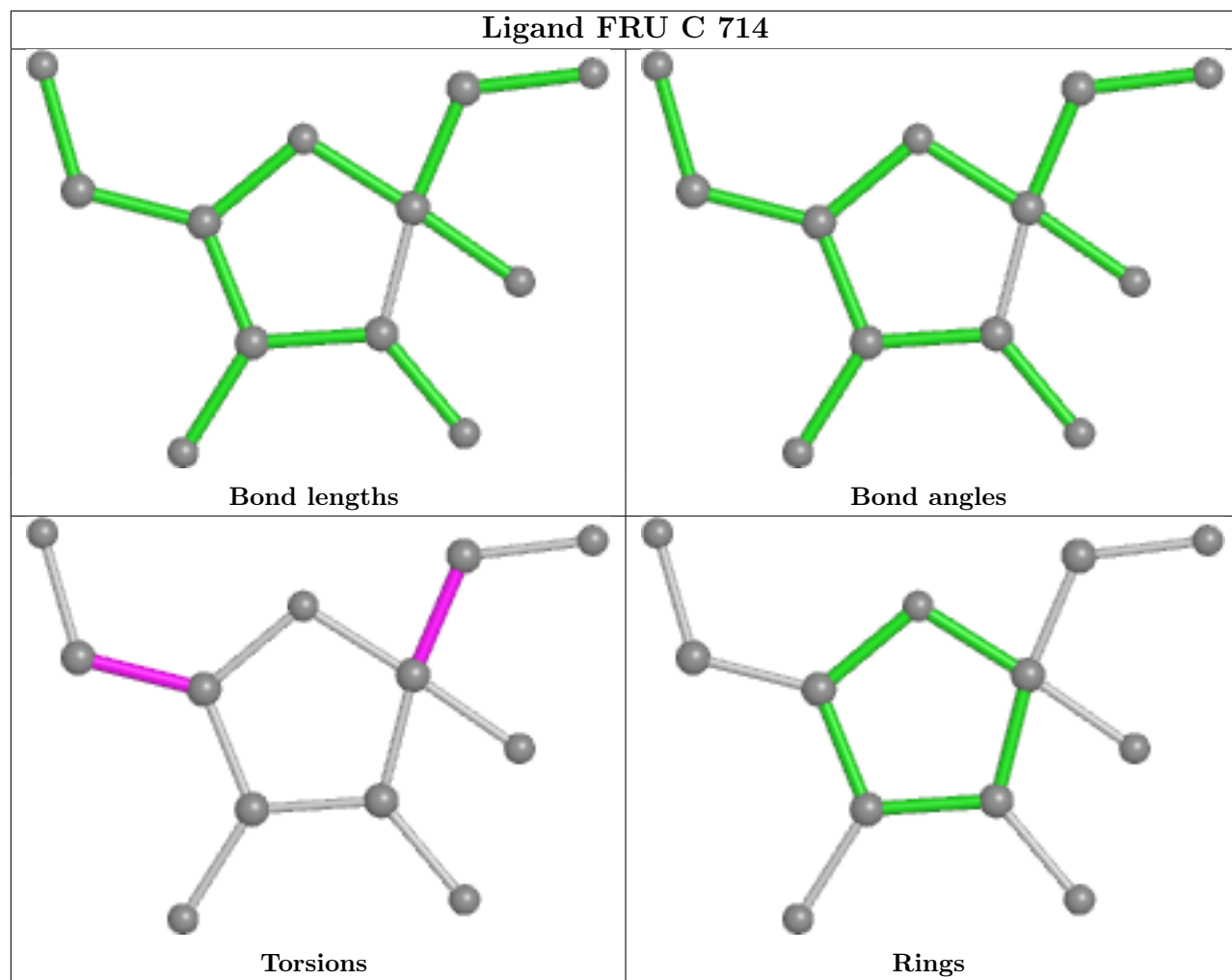
There are no ring outliers.

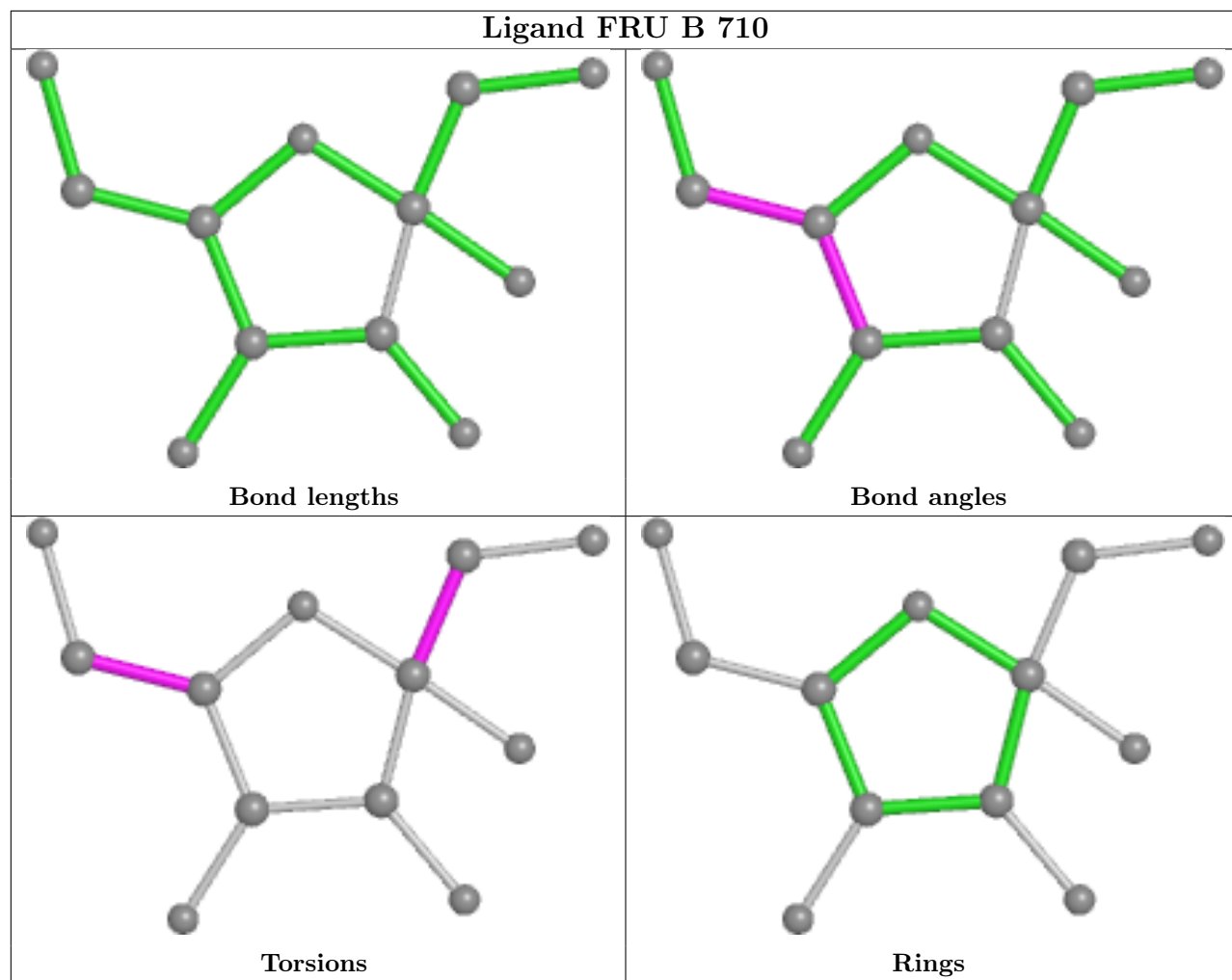
16 monomers are involved in 21 short contacts:

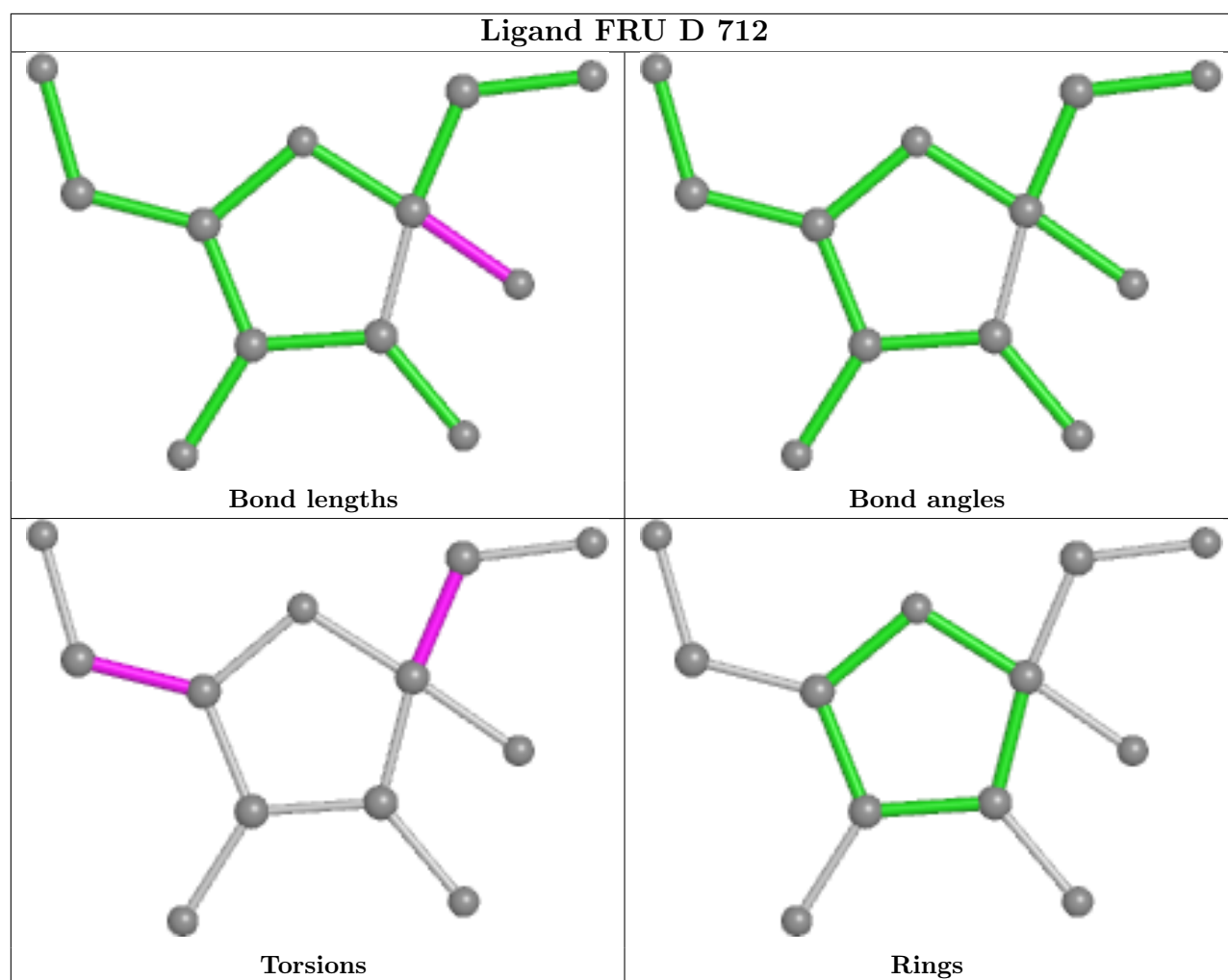
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	705	NAG	1	0
8	B	709	BTB	1	0
7	A	708	NAG	1	0
8	D	711	BTB	1	0
6	A	701	MAN	1	0
6	C	703	MAN	1	0
7	A	710	NAG	1	0
10	D	701	PEG	1	0
7	B	703	NAG	3	0
7	D	709	NAG	1	0
7	B	707	NAG	1	0
7	B	704	NAG	1	0
6	A	702	MAN	1	0
7	A	712	NAG	4	0
7	C	711	NAG	1	0
6	B	701	MAN	1	0

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, 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	526/675 (77%)	0.05	16 (3%) 50 48	13, 21, 41, 60	0
1	B	526/675 (77%)	0.31	41 (7%) 13 13	12, 23, 50, 78	0
1	C	524/675 (77%)	0.28	24 (4%) 32 31	15, 27, 47, 69	0
1	D	524/675 (77%)	0.66	60 (11%) 4 4	14, 27, 58, 81	0
All	All	2100/2700 (77%)	0.33	141 (6%) 17 17	12, 24, 51, 81	0

The worst 5 of 141 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	555	CYS	7.7
1	C	143	CYS	7.7
1	D	436	ASN	7.2
1	B	555	CYS	6.5
1	D	531	ALA	6.3

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	F	3	11/12	0.54	0.45	81,86,88,88	0
3	BMA	K	3	11/12	0.57	0.41	61,63,65,65	0

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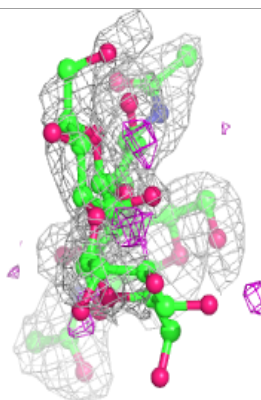
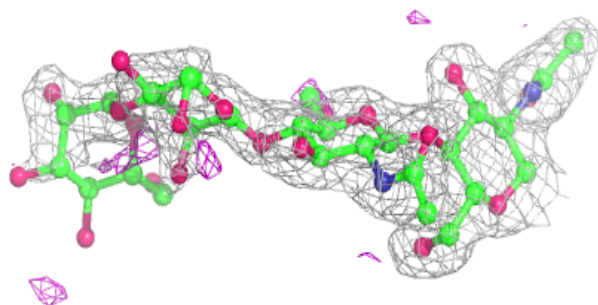
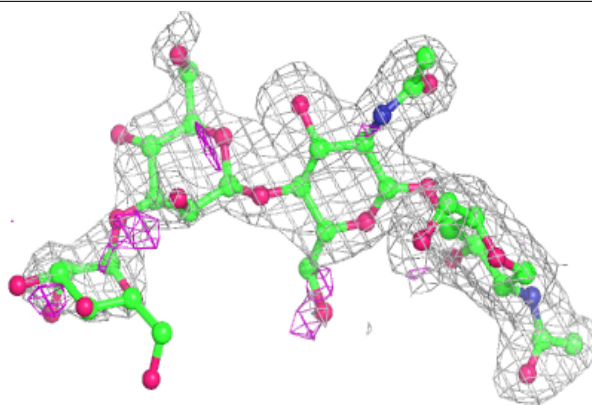
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MAN	H	5	11/12	0.60	0.37	53,63,68,68	0
5	MAN	H	4	11/12	0.64	0.27	77,81,84,84	0
4	NAG	L	2	14/15	0.65	0.43	75,83,87,90	0
4	NAG	I	2	14/15	0.68	0.34	58,64,72,73	0
4	NAG	J	2	14/15	0.70	0.21	49,52,54,57	0
3	NAG	K	2	14/15	0.70	0.27	47,51,57,59	0
4	NAG	G	2	14/15	0.73	0.45	67,77,79,81	0
2	MAN	E	4	11/12	0.74	0.52	88,92,95,97	0
2	BMA	E	3	11/12	0.77	0.38	66,69,73,76	0
5	BMA	H	3	11/12	0.77	0.23	63,69,72,74	0
5	MAN	H	6	11/12	0.80	0.28	75,78,79,80	0
2	NAG	E	2	14/15	0.81	0.22	38,41,49,51	0
3	NAG	F	2	14/15	0.82	0.23	42,50,59,60	0
4	NAG	J	1	14/15	0.85	0.18	45,47,51,52	0
5	NAG	H	2	14/15	0.85	0.20	41,43,50,54	0
4	NAG	L	1	14/15	0.89	0.10	36,39,47,51	0
5	NAG	H	1	14/15	0.92	0.18	34,38,41,42	0
2	NAG	E	1	14/15	0.92	0.11	28,32,34,35	0
3	NAG	F	1	14/15	0.93	0.09	22,26,29,30	0
3	NAG	K	1	14/15	0.93	0.12	25,28,30,34	0
4	NAG	I	1	14/15	0.94	0.10	23,26,32,34	0
4	NAG	G	1	14/15	0.94	0.10	28,29,37,40	0

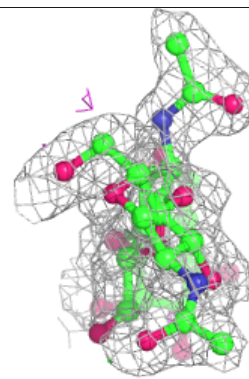
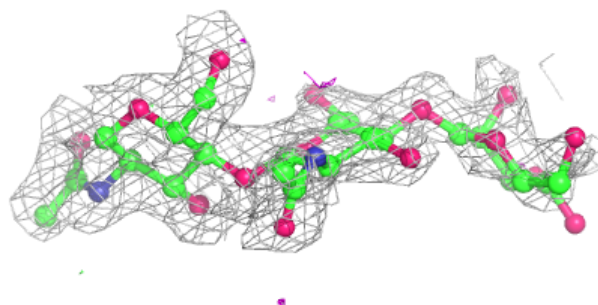
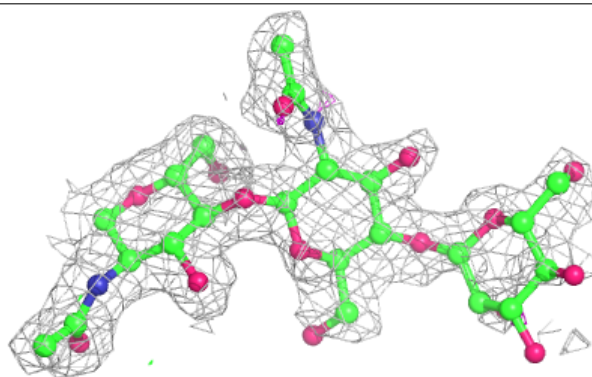
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

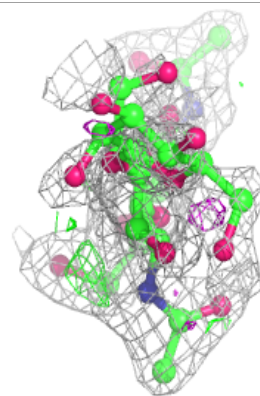
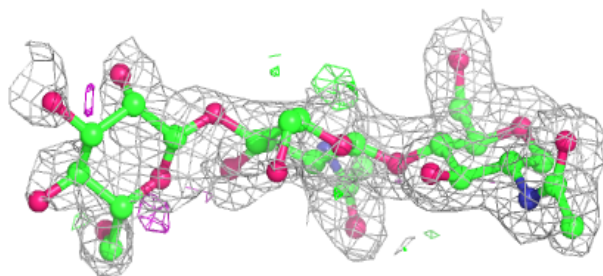
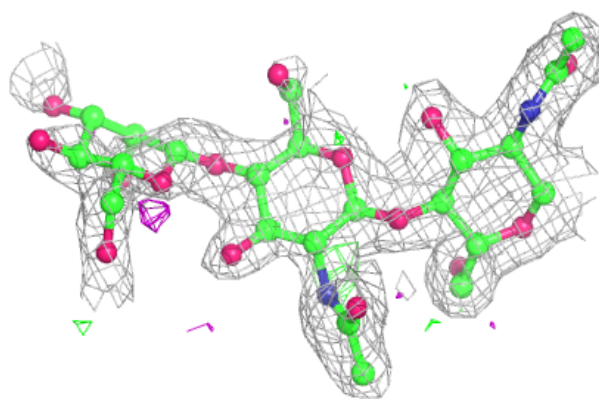
**Electron density around Chain F:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

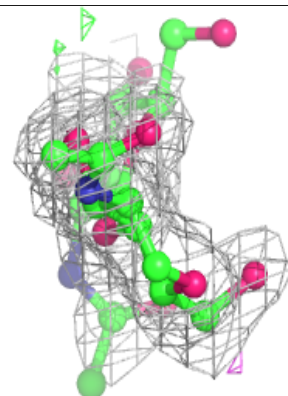
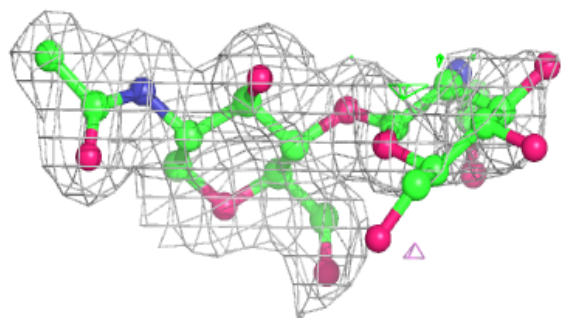
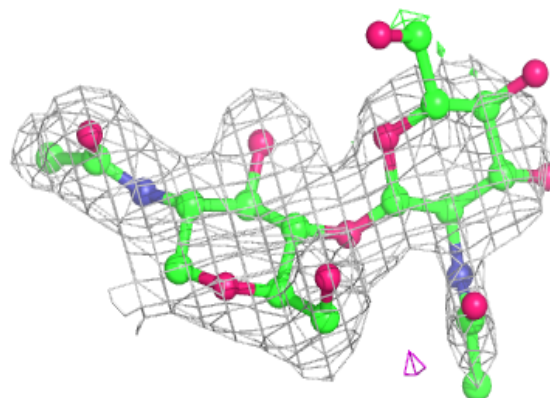


Electron density around Chain K:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

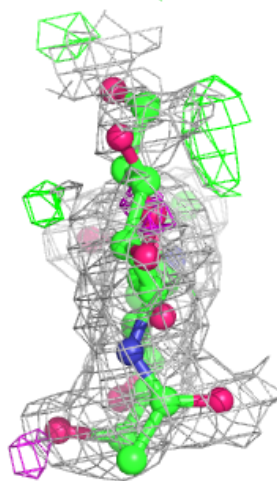
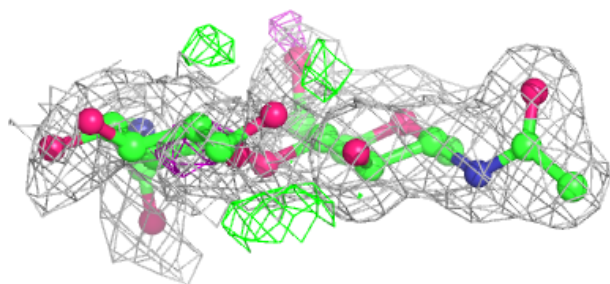
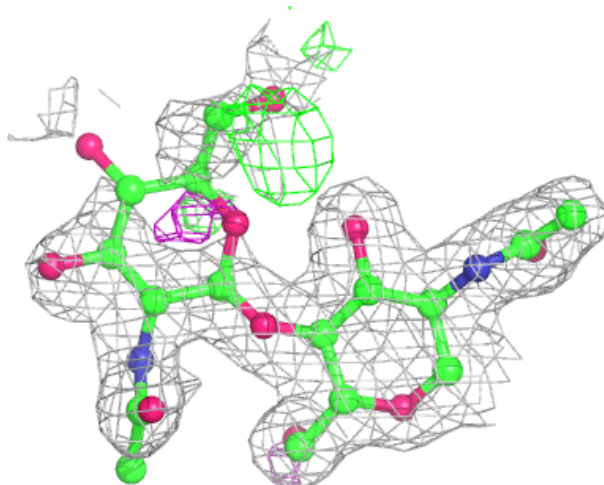
**Electron density around Chain G:**

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



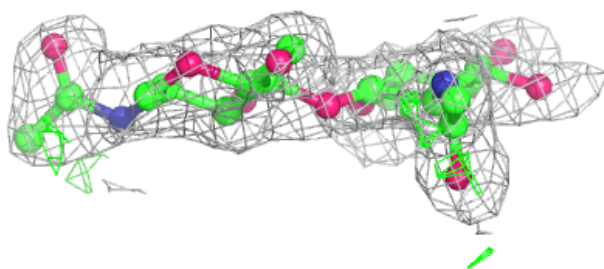
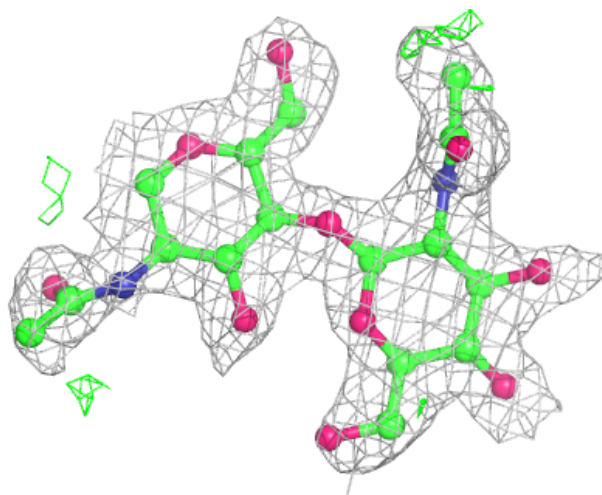
Electron density around Chain I:

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



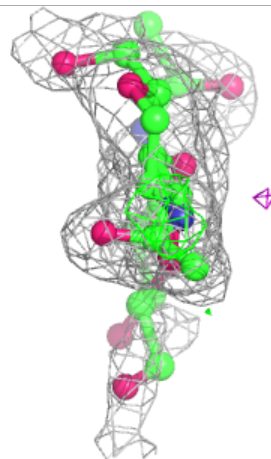
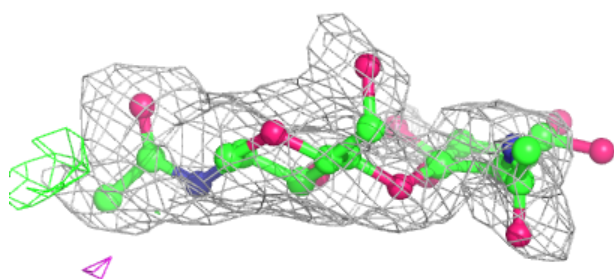
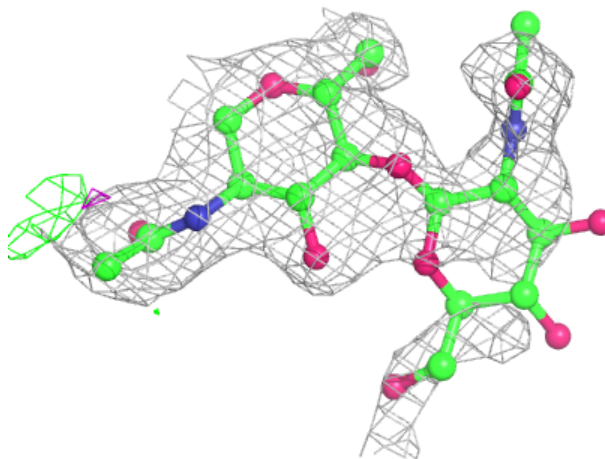
Electron density around Chain J:

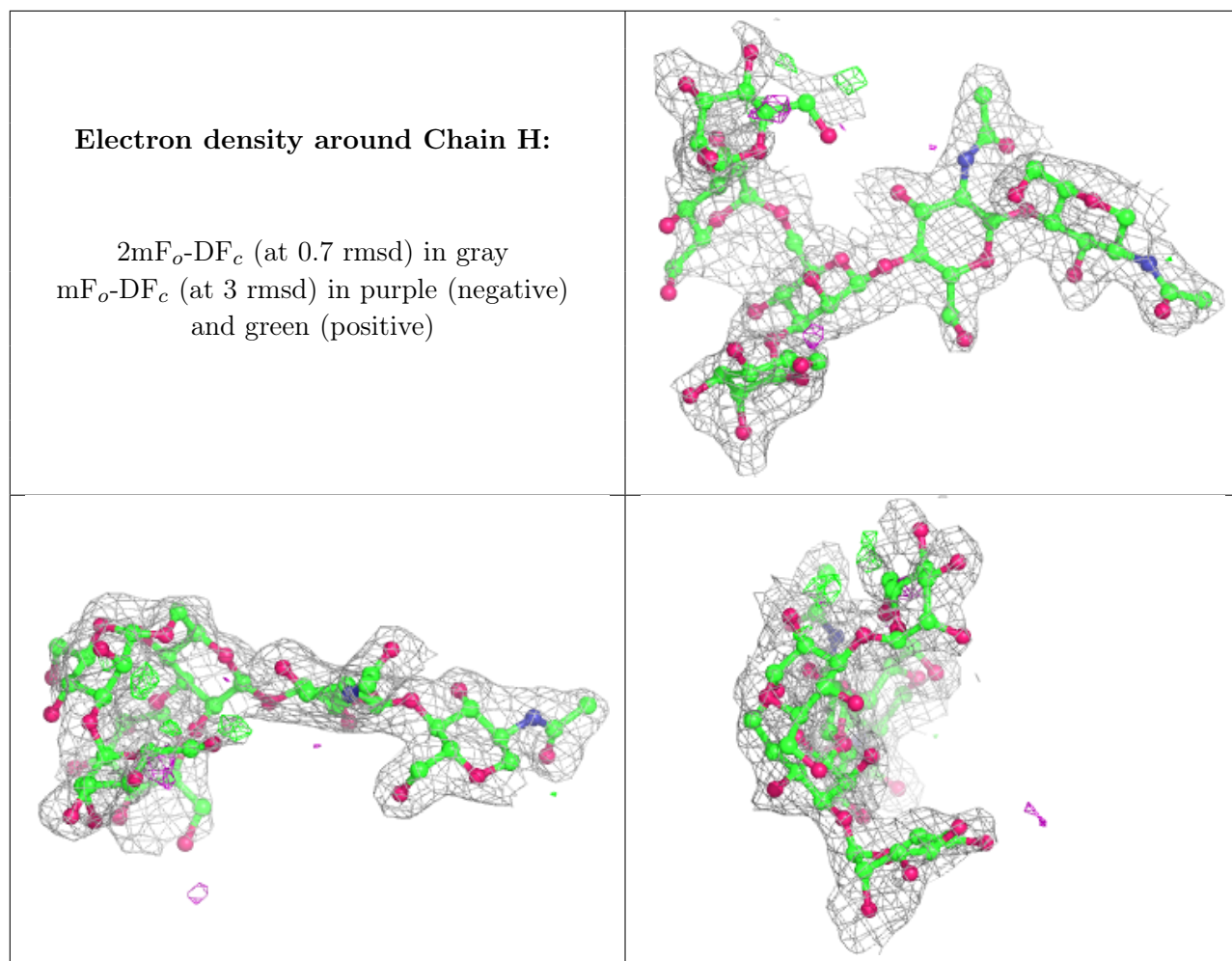
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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	MAN	C	703	11/12	0.56	0.27	53,55,57,58	0
7	NAG	A	712	14/15	0.58	0.29	47,52,56,57	0
6	MAN	A	703	11/12	0.61	0.33	44,47,49,51	0
7	NAG	D	709	14/15	0.65	0.32	76,82,84,85	0
6	MAN	D	702	11/12	0.66	0.43	74,78,80,81	0
6	MAN	D	704	11/12	0.66	0.34	64,68,71,72	0
7	NAG	C	708	14/15	0.67	0.24	49,53,54,58	0
6	MAN	B	702	11/12	0.68	0.39	59,65,67,67	0
7	NAG	B	707	14/15	0.71	0.35	40,42,45,46	0
7	NAG	B	708	14/15	0.71	0.36	38,40,43,43	0

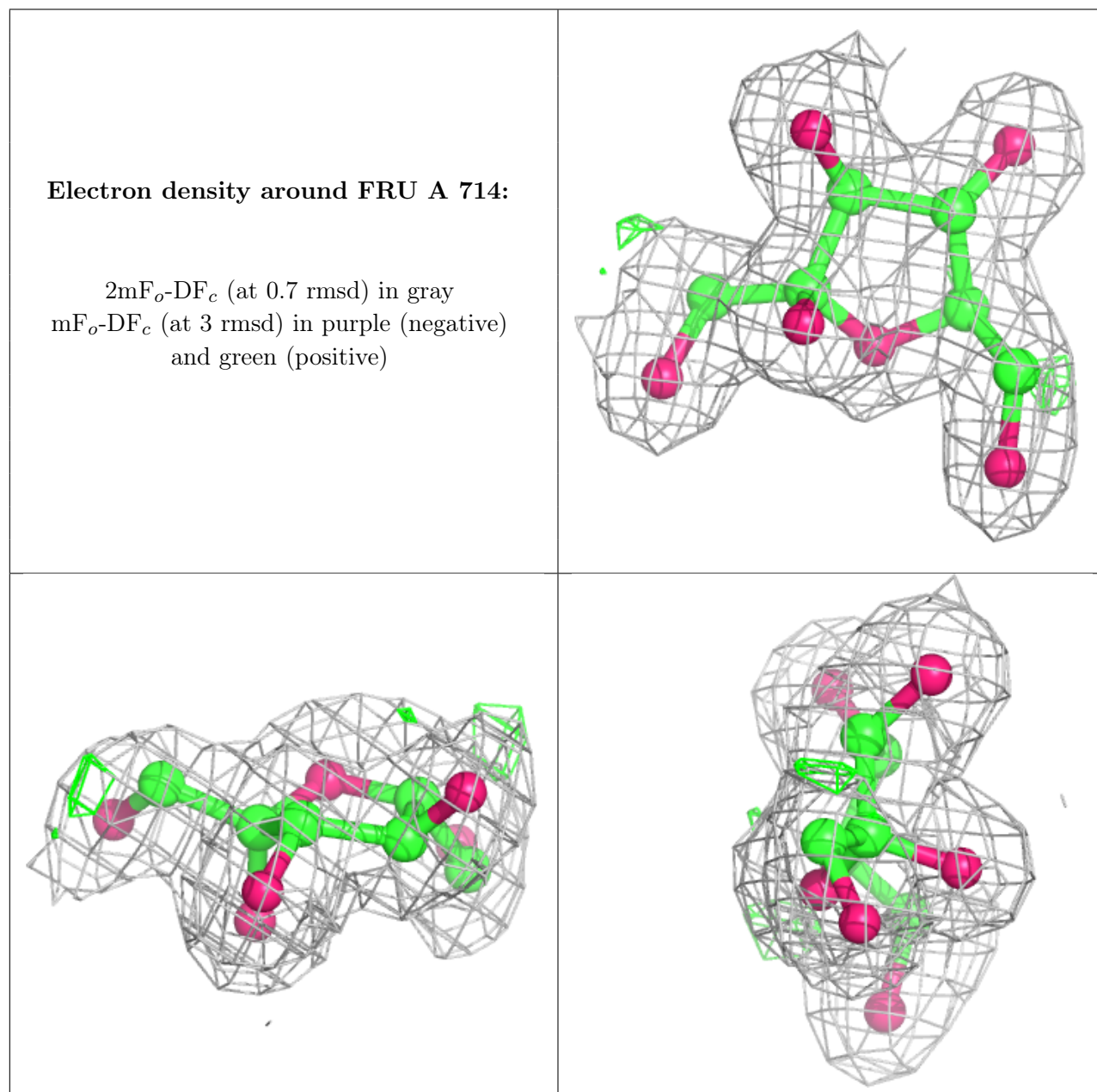
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	C	711	14/15	0.72	0.25	48,55,60,60	0
6	MAN	C	702	11/12	0.73	0.48	74,82,84,86	0
6	MAN	D	703	11/12	0.75	0.38	66,73,75,76	0
6	MAN	C	705	11/12	0.76	0.20	47,49,52,53	0
6	MAN	A	702	11/12	0.76	0.33	59,67,70,73	0
7	NAG	B	704	14/15	0.77	0.31	41,47,50,50	0
7	NAG	A	709	14/15	0.77	0.25	39,41,46,48	0
7	NAG	B	706	14/15	0.78	0.29	53,56,58,59	0
6	MAN	C	704	11/12	0.79	0.28	50,54,60,63	0
6	MAN	C	701	11/12	0.80	0.37	71,74,76,78	0
7	NAG	A	708	14/15	0.81	0.14	32,37,41,44	0
7	NAG	C	707	14/15	0.82	0.20	38,41,42,44	0
7	NAG	A	710	14/15	0.82	0.24	39,46,51,53	0
6	MAN	B	701	11/12	0.82	0.38	66,75,77,79	0
7	NAG	D	706	14/15	0.82	0.19	45,47,49,49	0
6	MAN	A	701	11/12	0.82	0.35	60,65,68,68	0
7	NAG	A	704	14/15	0.83	0.21	31,36,40,40	0
10	PEG	D	701	7/7	0.83	0.21	34,42,47,48	0
7	NAG	A	705	14/15	0.84	0.24	51,58,60,62	0
7	NAG	C	706	14/15	0.84	0.22	53,55,63,63	0
7	NAG	A	706	14/15	0.85	0.17	36,42,42,45	0
7	NAG	C	709	14/15	0.85	0.20	39,44,48,49	0
8	BTB	C	713	14/14	0.85	0.14	30,36,38,41	0
7	NAG	B	703	14/15	0.85	0.19	43,48,50,51	0
7	NAG	A	711	14/15	0.87	0.17	31,36,41,42	0
8	BTB	A	713	14/14	0.88	0.11	30,35,42,44	0
7	NAG	D	707	14/15	0.88	0.25	37,42,44,44	0
7	NAG	D	710	14/15	0.88	0.16	52,55,58,62	0
7	NAG	C	712	14/15	0.89	0.14	37,39,45,47	0
7	NAG	D	705	14/15	0.89	0.12	39,40,50,52	0
7	NAG	A	707	14/15	0.89	0.11	21,24,29,31	0
7	NAG	D	708	14/15	0.90	0.15	35,40,44,45	0
7	NAG	C	710	14/15	0.90	0.12	39,41,44,45	0
8	BTB	B	709	14/14	0.91	0.12	24,28,33,35	0
9	FRU	A	714	12/12	0.92	0.12	19,23,24,26	0
7	NAG	B	705	14/15	0.93	0.09	20,22,26,27	0
8	BTB	D	711	14/14	0.93	0.11	23,27,34,34	0
9	FRU	D	712	12/12	0.94	0.11	18,19,21,23	0
9	FRU	C	714	12/12	0.95	0.10	21,23,25,26	0
9	FRU	B	710	12/12	0.96	0.12	17,19,22,26	0

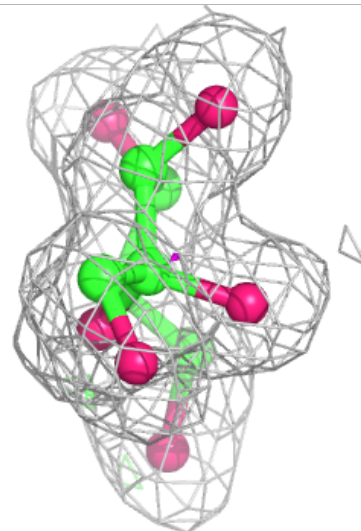
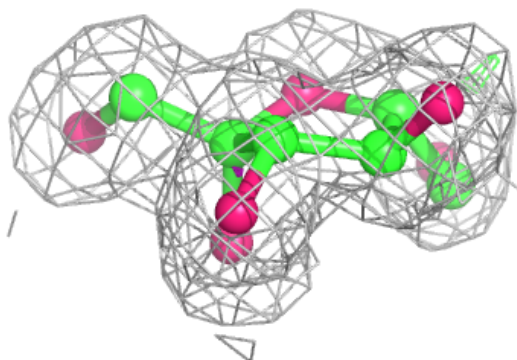
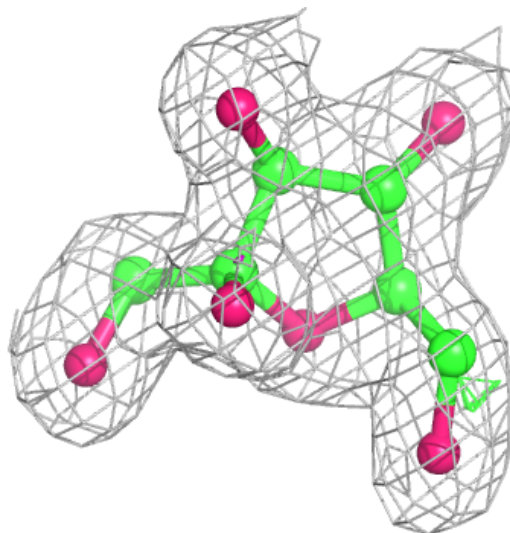
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

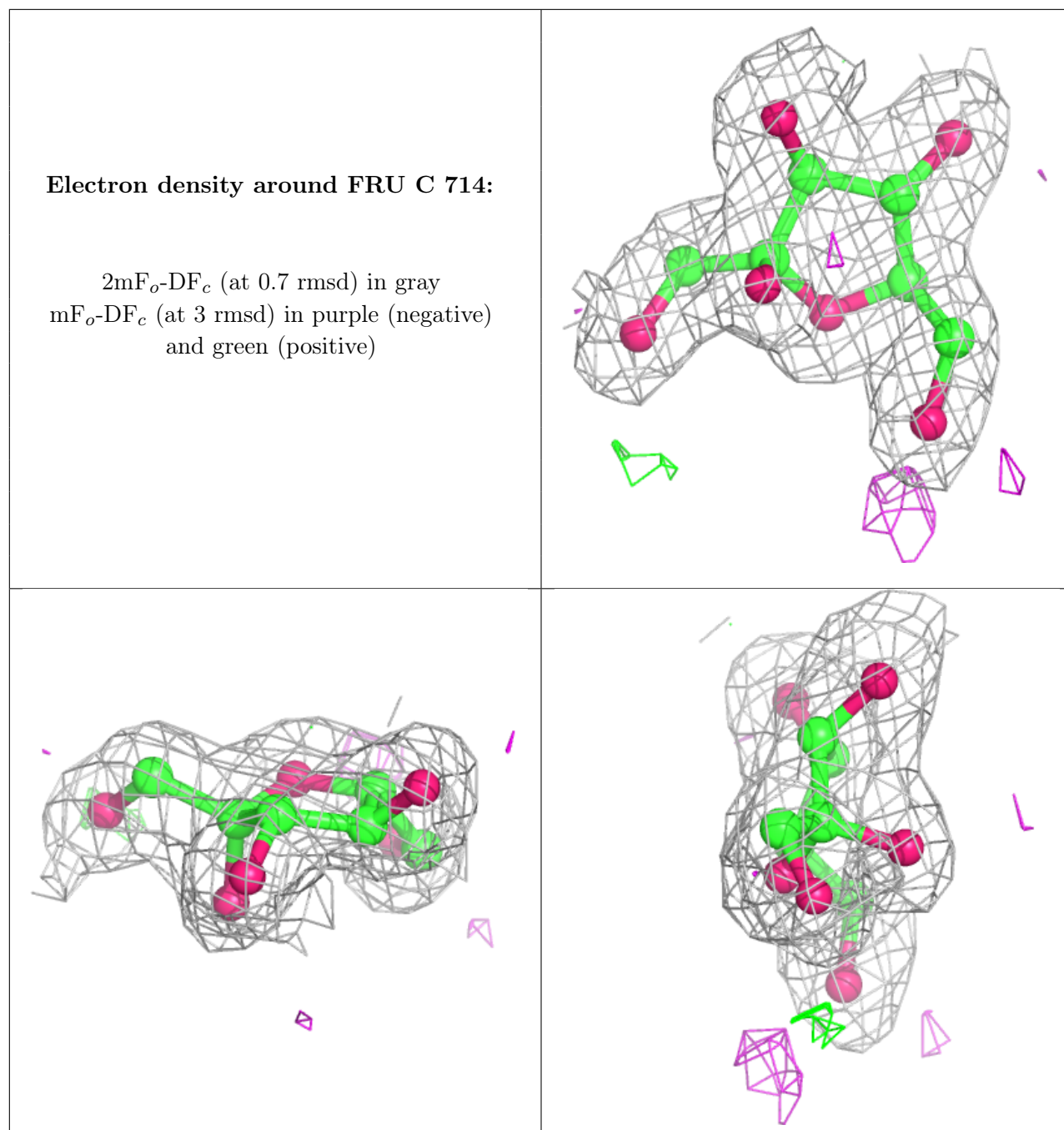
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

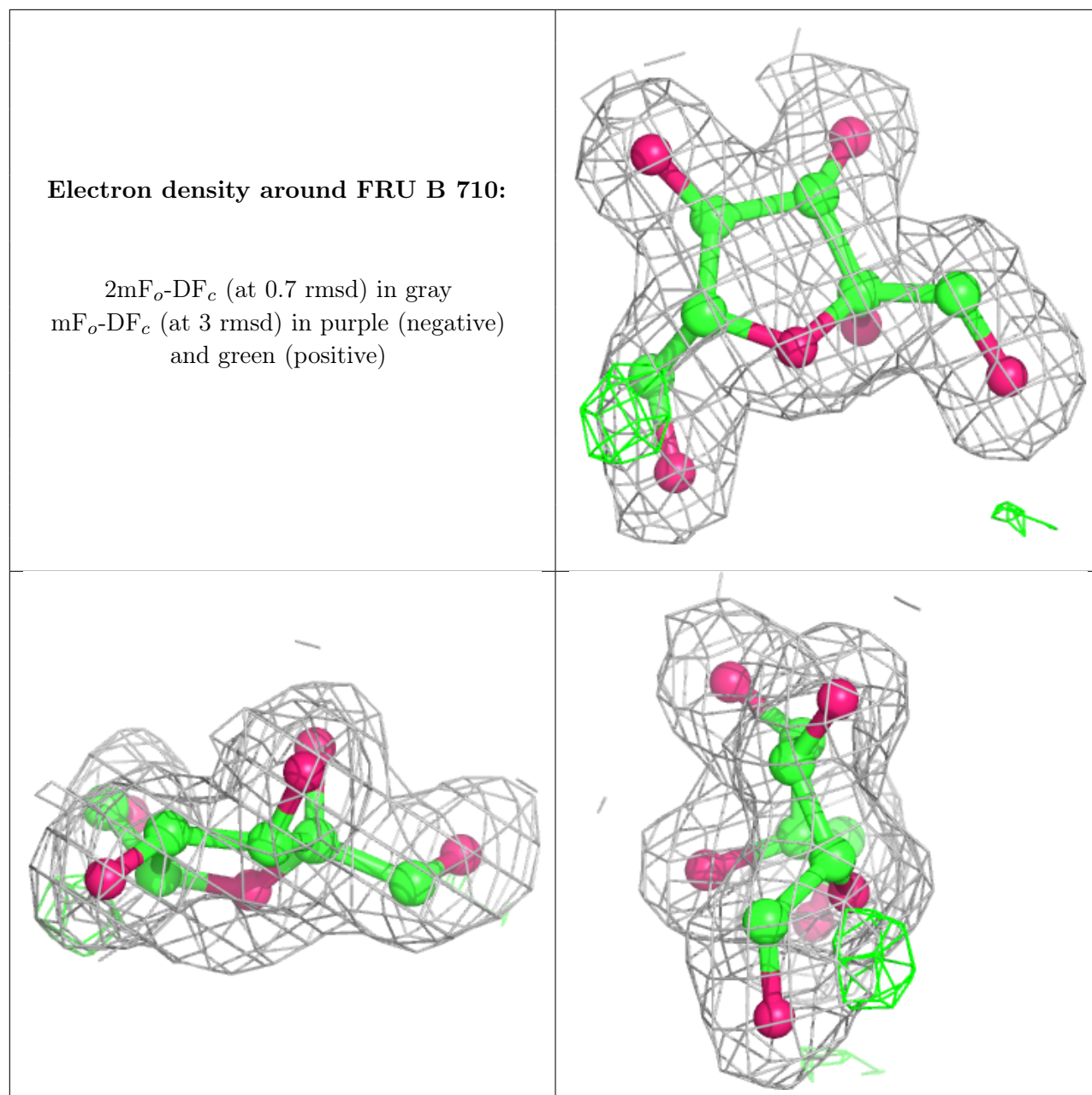


Electron density around FRU D 712:

$2mF_o-DF_c$ (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.