



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 19, 2024 – 11:05 AM EDT

PDB ID : 5HU8
Title : The crystal structure of hemagglutinin from A/Sichuan/26221/2014 (H5N6) influenza virus
Authors : Yang, H.; Carney, P.J.; Guo, Z.; Chang, J.C.; Stevens, J.
Deposited on : 2016-01-27
Resolution : 2.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

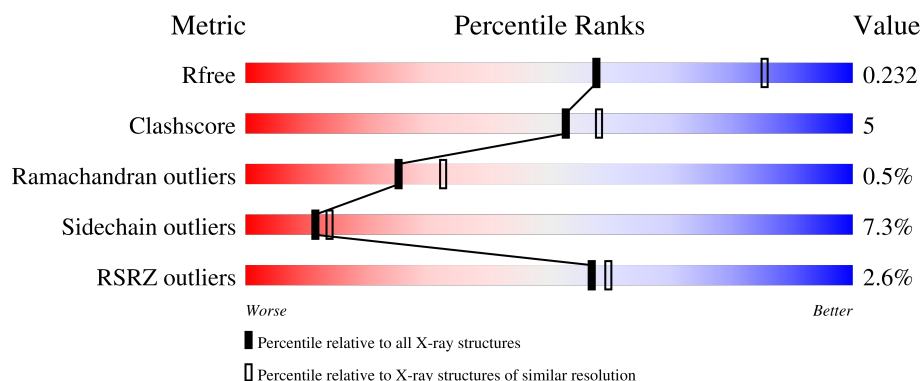
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 Å.

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




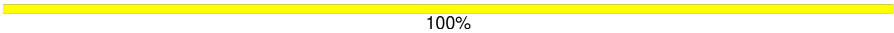
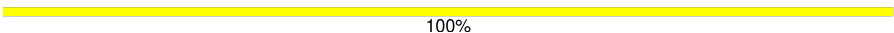

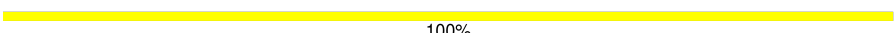

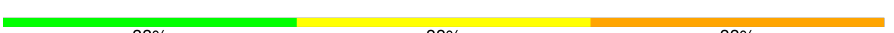
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1096 (2.46-2.46)
Clashscore	180529	1178 (2.46-2.46)
Ramachandran outliers	177936	1170 (2.46-2.46)
Sidechain outliers	177891	1170 (2.46-2.46)
RSRZ outliers	164620	1096 (2.46-2.46)

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	334	<div> <div>0%</div> <div>81% 13% . .</div> </div>
1	C	334	<div> <div>2%</div> <div>80% 13% . .</div> </div>
1	E	334	<div> <div>0%</div> <div>84% 10% . .</div> </div>
2	B	181	<div> <div>0%</div> <div>71% 17% . 10%</div> </div>
2	D	181	<div> <div>6%</div> <div>71% 16% . 10%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	181	 6% 70% 17% 10%
3	G	2	 100%
3	I	2	 100%
3	K	2	 50% 50%
4	H	3	 100%
4	J	3	 67% 33%
4	L	3	 33% 33% 33%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12524 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 HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2537	1605	440	477	15			
1	C	320	Total	C	N	O	S	0	0	0
			2537	1605	440	477	15			
1	E	320	Total	C	N	O	S	0	0	0
			2537	1605	440	477	15			

- Molecule 2 is a protein called hemagglutinin HA2.

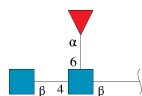
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	162	Total	C	N	O	S	0	0	0
			1329	823	234	264	8			
2	D	162	Total	C	N	O	S	0	0	0
			1329	823	234	264	8			
2	F	162	Total	C	N	O	S	0	0	0
			1329	823	234	264	8			

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



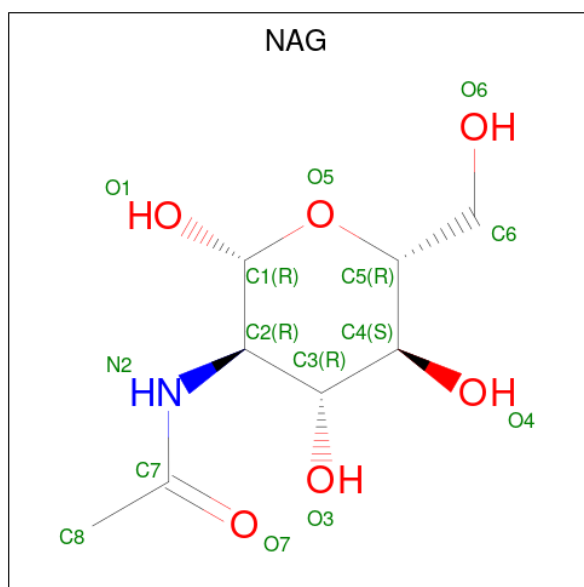
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	I	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	K	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 4 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
4	H	3	Total	C	N	O	0	0	0
			38	22	2	14			
4	J	3	Total	C	N	O	0	0	0
			38	22	2	14			
4	L	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

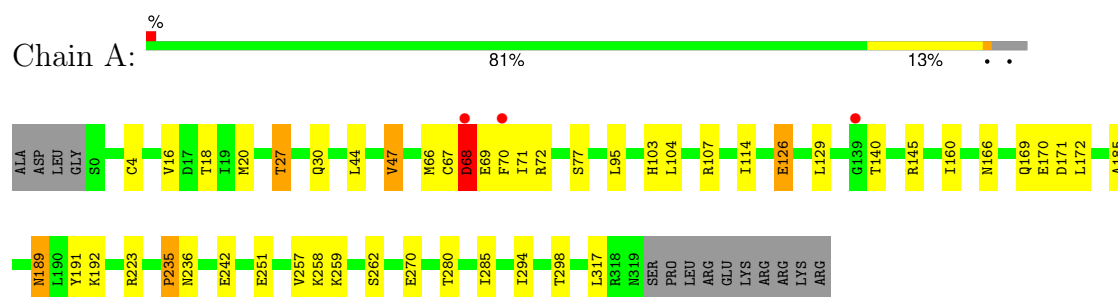
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	177	Total 177	O 177	0	0
6	C	154	Total 154	O 154	0	0
6	E	148	Total 148	O 148	0	0
6	B	76	Total 76	O 76	0	0
6	D	71	Total 71	O 71	0	0
6	F	72	Total 72	O 72	0	0

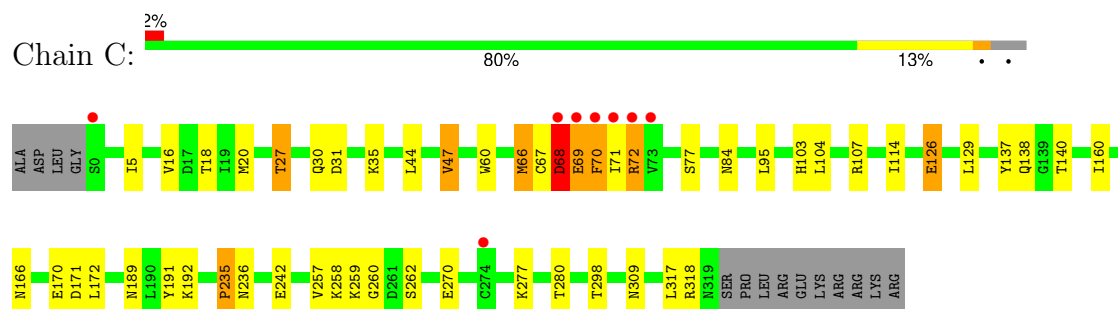
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

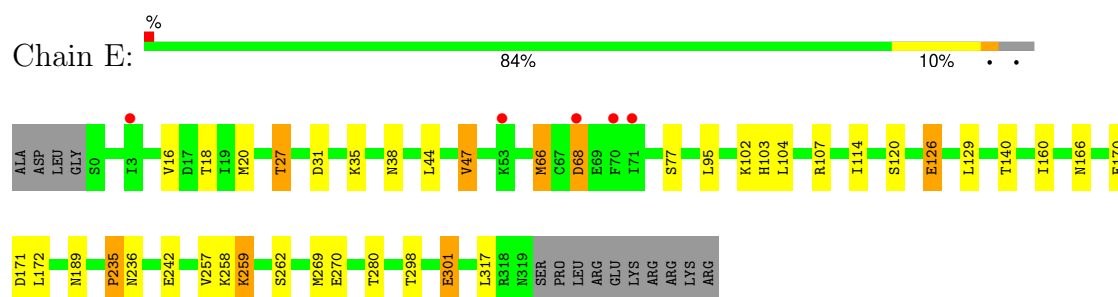
• Molecule 1: hemagglutinin HA1



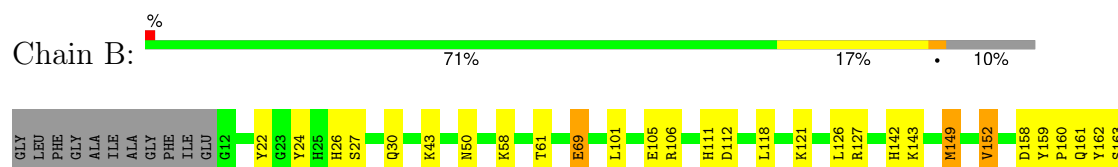
• Molecule 1: hemagglutinin HA1

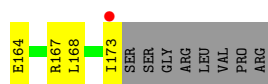


• Molecule 1: hemagglutinin HA1



• Molecule 2: hemagglutinin HA2

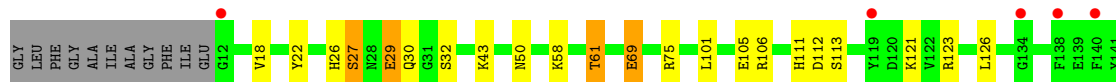




- Molecule 2: hemagglutinin HA2



- Molecule 2: hemagglutinin HA2



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



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



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



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



MAG1
MAG2
FUC3

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

Chain J:  67% 33%

MAG1
MAG2
FUC3

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

Chain L:  33% 33% 33%

MAG1
MAG2
FUC3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.50Å 104.42Å 215.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.45 49.39 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.39-2.45) 99.6 (49.39-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.191 , 0.227 0.197 , 0.232	Depositor DCC
R_{free} test set	3763 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12524	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: FUC, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.76	1/2599 (0.0%)	0.86	3/3534 (0.1%)
1	C	0.69	1/2599 (0.0%)	0.82	2/3534 (0.1%)
1	E	0.69	1/2599 (0.0%)	0.85	2/3534 (0.1%)
2	B	0.74	1/1354 (0.1%)	0.79	0/1819
2	D	0.70	1/1354 (0.1%)	0.77	0/1819
2	F	0.69	1/1354 (0.1%)	0.77	0/1819
All	All	0.71	6/11859 (0.1%)	0.82	7/16059 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	3
All	All	0	4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	69	GLU	CD-OE1	8.68	1.35	1.25
2	F	69	GLU	CD-OE1	7.01	1.33	1.25
1	C	60	TRP	CB-CG	-6.31	1.38	1.50
1	E	301	GLU	CD-OE1	5.44	1.31	1.25
1	A	236	ASN	N-CA	5.36	1.57	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	PRO	C-N-CA	-6.52	105.41	121.70
1	E	235	PRO	C-N-CA	-6.03	106.62	121.70
1	C	235	PRO	C-N-CA	-5.48	108.01	121.70
1	A	259	LYS	N-CA-C	5.45	125.72	111.00
1	E	259	LYS	N-CA-C	5.11	124.80	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	72	ARG	Peptide
1	C	309	ASN	Peptide
1	C	68	ASP	Peptide
1	C	72	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2537	0	2484	22	1
1	C	2537	0	2484	29	1
1	E	2537	0	2484	21	1
2	B	1329	0	1242	17	0
2	D	1329	0	1242	17	0
2	F	1329	0	1242	19	1
3	G	24	0	22	0	0
3	I	24	0	22	0	0
3	K	24	0	22	0	0
4	H	38	0	34	0	0
4	J	38	0	34	1	0
4	L	38	0	34	1	0
5	A	14	0	13	0	0
5	C	14	0	13	0	0
5	E	14	0	13	0	0
6	A	177	0	0	2	0
6	B	76	0	0	5	0
6	C	154	0	0	6	0
6	D	71	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	148	0	0	3	0
6	F	72	0	0	6	0
All	All	12524	0	11385	113	2

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 5.

The worst 5 of 113 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:ASN:HB3	6:C:623:HOH:O	1.58	1.03
1:E:18:THR:HG21	6:E:589:HOH:O	1.58	1.02
1:C:66:MET:HE2	6:C:638:HOH:O	1.75	0.85
2:B:105:GLU:HG3	6:B:266:HOH:O	1.81	0.80
1:C:137:TYR:O	1:C:140:THR:HG22	1.83	0.78

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:SER:OG	2:F:165:GLU:OE1[2_564]	1.81	0.39
1:A:251:GLU:OE2	1:C:138:GLN:OE1[3_444]	2.19	0.01

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	318/334 (95%)	299 (94%)	17 (5%)	2 (1%)	22 28
1	C	318/334 (95%)	298 (94%)	17 (5%)	3 (1%)	14 18
1	E	318/334 (95%)	299 (94%)	18 (6%)	1 (0%)	37 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	160/181 (88%)	152 (95%)	8 (5%)	0	100	100
2	D	160/181 (88%)	151 (94%)	8 (5%)	1 (1%)	22	28
2	F	160/181 (88%)	152 (95%)	8 (5%)	0	100	100
All	All	1434/1545 (93%)	1351 (94%)	76 (5%)	7 (0%)	25	32

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	68	ASP
1	C	70	PHE
1	A	68	ASP
1	A	70	PHE
1	C	69	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	285/298 (96%)	271 (95%)	14 (5%)	21	30
1	C	285/298 (96%)	271 (95%)	14 (5%)	21	30
1	E	285/298 (96%)	272 (95%)	13 (5%)	23	33
2	B	142/155 (92%)	126 (89%)	16 (11%)	4	4
2	D	142/155 (92%)	124 (87%)	18 (13%)	3	2
2	F	142/155 (92%)	123 (87%)	19 (13%)	3	2
All	All	1281/1359 (94%)	1187 (93%)	94 (7%)	11	14

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	27	SER
2	D	161	GLN
2	D	30	GLN
2	D	116	LYS

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Mol	Chain	Res	Type
2	F	18	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	142	HIS
2	D	125	GLN
2	D	111	HIS
2	D	142	HIS
1	C	220	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

18 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
3	NAG	K	1	1,3	14,14,15	0.94	1 (7%)	17,19,21	1.78	3 (17%)
4	NAG	H	1	1,4	14,14,15	0.87	1 (7%)	17,19,21	1.43	2 (11%)
4	NAG	J	2	4	14,14,15	0.76	0	17,19,21	1.92	3 (17%)
4	NAG	L	2	4	14,14,15	0.94	1 (7%)	17,19,21	2.11	4 (23%)
3	NAG	G	1	1,3	14,14,15	0.61	0	17,19,21	1.72	6 (35%)
3	NAG	I	1	1,3	14,14,15	0.90	0	17,19,21	1.21	2 (11%)
4	FUC	L	3	4	10,10,11	0.71	0	14,14,16	0.93	0
4	NAG	L	1	1,4	14,14,15	0.89	1 (7%)	17,19,21	1.69	4 (23%)
5	NAG	A	406	1	14,14,15	1.36	2 (14%)	17,19,21	2.53	5 (29%)
4	NAG	J	1	1,4	14,14,15	0.64	0	17,19,21	1.69	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FUC	H	3	4	10,10,11	0.87	0	14,14,16	1.22	1 (7%)
4	NAG	H	2	4	14,14,15	0.74	0	17,19,21	1.67	5 (29%)
5	NAG	C	406	1	14,14,15	0.71	0	17,19,21	1.55	3 (17%)
3	FUC	K	2	3	10,10,11	0.67	0	14,14,16	0.76	0
5	NAG	E	406	1	14,14,15	0.94	0	17,19,21	1.84	4 (23%)
3	FUC	G	2	3	10,10,11	0.71	0	14,14,16	1.46	3 (21%)
4	FUC	J	3	4	10,10,11	0.82	0	14,14,16	1.28	2 (14%)
3	FUC	I	2	3	10,10,11	0.79	0	14,14,16	2.16	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
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	1/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	I	2	3	-	-	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
4	FUC	L	3	4	-	-	0/1/1/1
4	NAG	L	1	1,4	-	2/6/23/26	0/1/1/1
5	NAG	A	406	1	-	0/6/23/26	0/1/1/1
4	FUC	H	3	4	-	-	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
5	NAG	C	406	1	-	0/6/23/26	0/1/1/1
5	NAG	E	406	1	-	2/6/23/26	0/1/1/1
3	FUC	K	2	3	-	-	0/1/1/1
3	FUC	G	2	3	-	-	0/1/1/1
4	FUC	J	3	4	-	-	0/1/1/1
4	NAG	J	1	1,4	-	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)
5	A	406	NAG	C1-C2	2.95	1.56	1.52
5	A	406	NAG	C2-N2	2.83	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1	NAG	C1-C2	2.80	1.56	1.52
4	L	2	NAG	C4-C5	2.28	1.57	1.53
4	L	1	NAG	O5-C1	-2.17	1.40	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	406	NAG	C2-N2-C7	5.29	129.99	122.90
4	J	2	NAG	C1-O5-C5	4.91	118.77	112.19
4	L	2	NAG	C3-C4-C5	4.83	118.98	110.23
5	A	406	NAG	O7-C7-C8	-4.65	113.78	122.05
4	L	2	NAG	O5-C1-C2	-4.56	104.24	111.29

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	1	NAG	O5-C5-C6-O6
5	E	406	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
5	E	406	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1	NAG	1	0
4	J	1	NAG	1	0

5.5 Carbohydrates

15 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
3	NAG	G	1	1,3	14,14,15	0.61	0	17,19,21	1.72	6 (35%)
3	FUC	G	2	3	10,10,11	0.71	0	14,14,16	1.46	3 (21%)
4	NAG	H	1	1,4	14,14,15	0.87	1 (7%)	17,19,21	1.43	2 (11%)
4	NAG	H	2	4	14,14,15	0.74	0	17,19,21	1.67	5 (29%)
4	FUC	H	3	4	10,10,11	0.87	0	14,14,16	1.22	1 (7%)
3	NAG	I	1	1,3	14,14,15	0.90	0	17,19,21	1.21	2 (11%)
3	FUC	I	2	3	10,10,11	0.79	0	14,14,16	2.16	5 (35%)
4	NAG	J	1	1,4	14,14,15	0.64	0	17,19,21	1.69	4 (23%)
4	NAG	J	2	4	14,14,15	0.76	0	17,19,21	1.92	3 (17%)
4	FUC	J	3	4	10,10,11	0.82	0	14,14,16	1.28	2 (14%)
3	NAG	K	1	1,3	14,14,15	0.94	1 (7%)	17,19,21	1.78	3 (17%)
3	FUC	K	2	3	10,10,11	0.67	0	14,14,16	0.76	0
4	NAG	L	1	1,4	14,14,15	0.89	1 (7%)	17,19,21	1.69	4 (23%)
4	NAG	L	2	4	14,14,15	0.94	1 (7%)	17,19,21	2.11	4 (23%)
4	FUC	L	3	4	10,10,11	0.71	0	14,14,16	0.93	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
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	G	2	3	-	-	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	FUC	H	3	4	-	-	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	I	2	3	-	-	0/1/1/1
4	NAG	J	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	FUC	J	3	4	-	-	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	K	2	3	-	-	0/1/1/1
4	NAG	L	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	1/6/23/26	0/1/1/1
4	FUC	L	3	4	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1	NAG	C1-C2	2.80	1.56	1.52
4	L	2	NAG	C4-C5	2.28	1.57	1.53
4	L	1	NAG	O5-C1	-2.17	1.40	1.43
4	H	1	NAG	O5-C1	-2.17	1.40	1.43

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	2	NAG	C1-O5-C5	4.91	118.77	112.19
4	L	2	NAG	C3-C4-C5	4.83	118.98	110.23
4	L	2	NAG	O5-C1-C2	-4.56	104.24	111.29
3	I	2	FUC	O5-C5-C4	3.99	116.74	109.55
3	K	1	NAG	O5-C5-C6	3.87	115.19	107.66

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

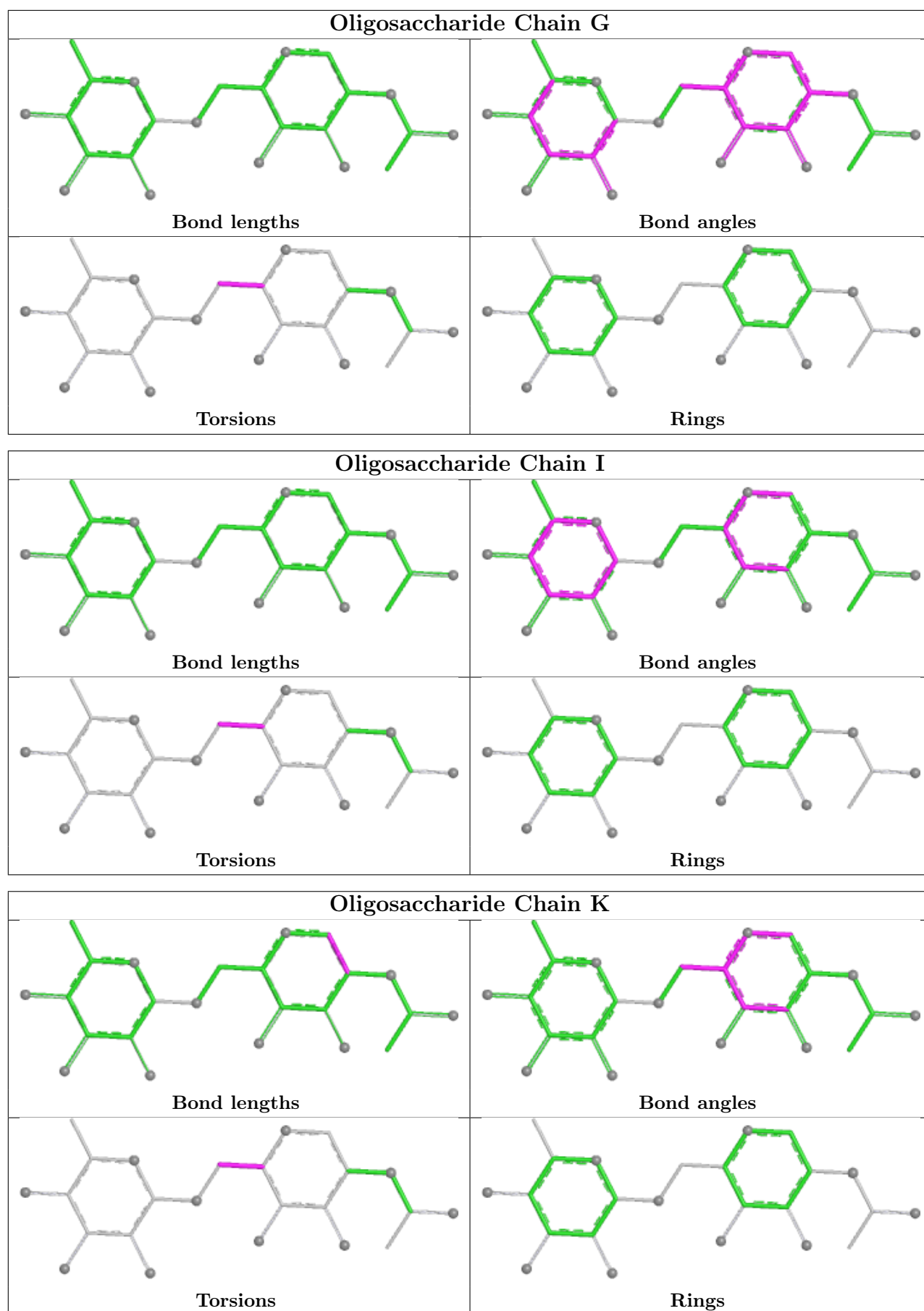
Mol	Chain	Res	Type	Atoms
3	K	1	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6

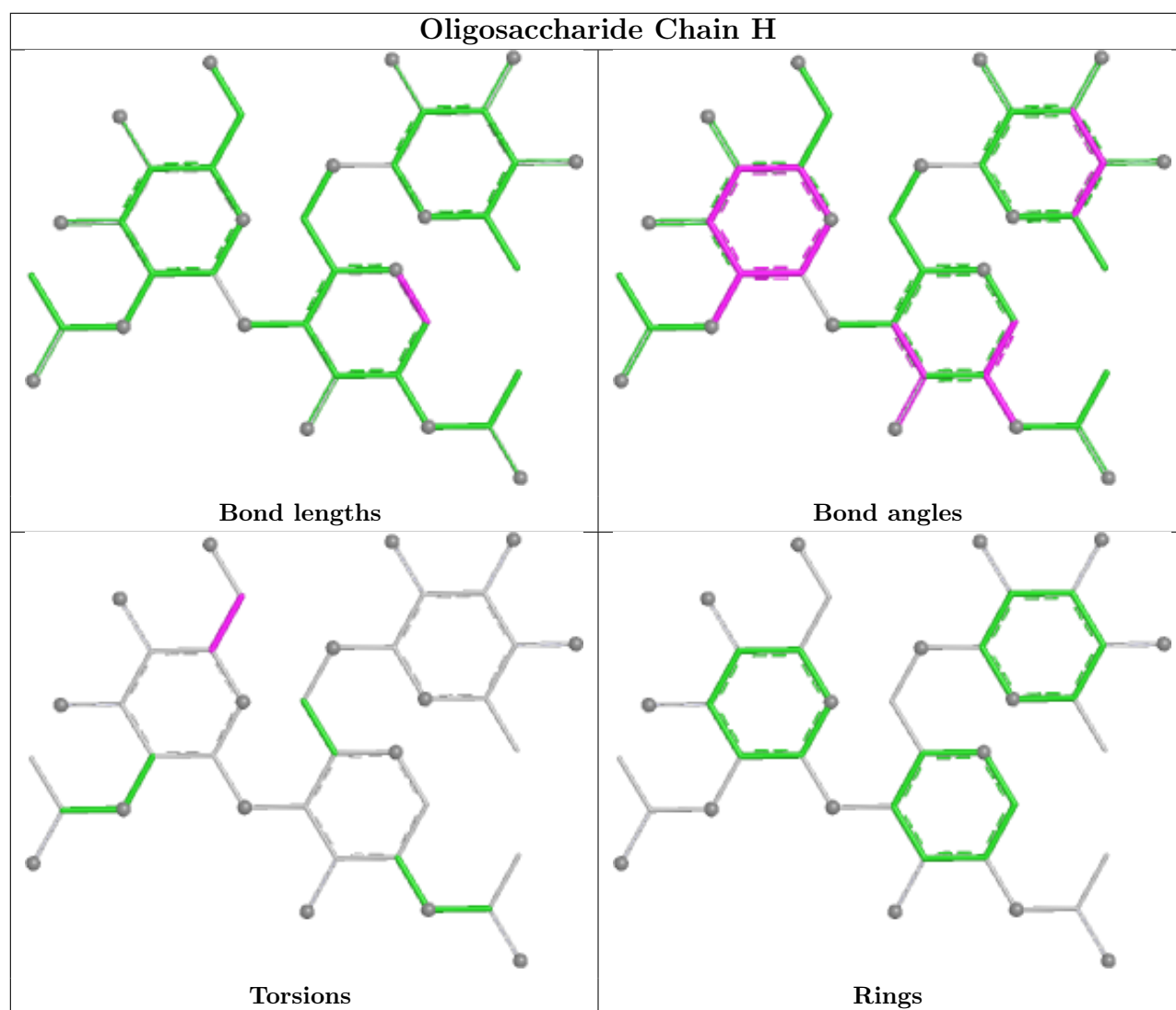
There are no ring outliers.

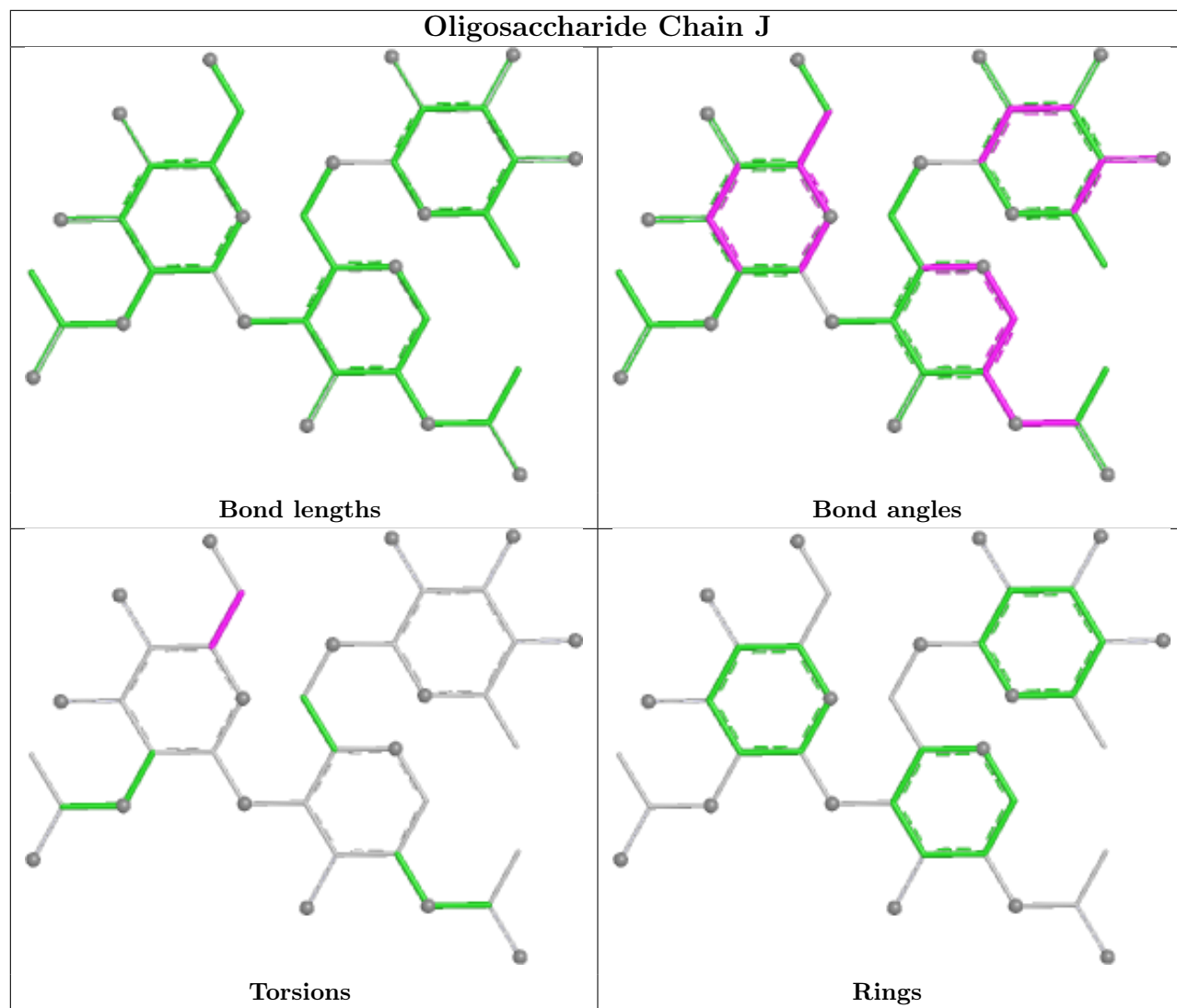
2 monomers are involved in 2 short contacts:

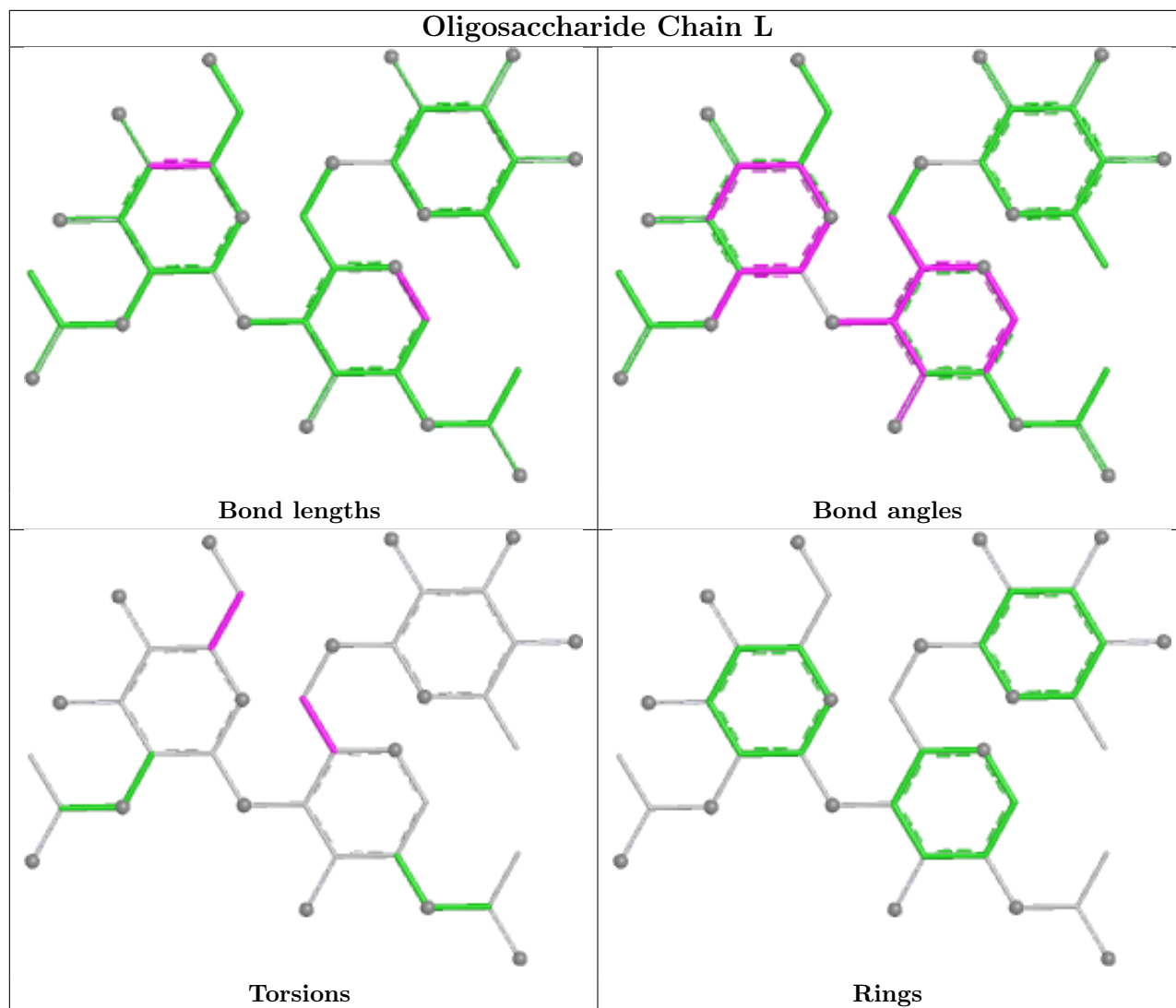
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1	NAG	1	0
4	J	1	NAG	1	0

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









5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
5	NAG	A	406	1	14,14,15	1.36	2 (14%)	17,19,21	2.53	5 (29%)
5	NAG	E	406	1	14,14,15	0.94	0	17,19,21	1.84	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	406	1	14,14,15	0.71	0	17,19,21	1.55	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	406	1	-	0/6/23/26	0/1/1/1
5	NAG	E	406	1	-	2/6/23/26	0/1/1/1
5	NAG	C	406	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	406	NAG	C1-C2	2.95	1.56	1.52
5	A	406	NAG	C2-N2	2.83	1.50	1.46

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	406	NAG	C2-N2-C7	5.29	129.99	122.90
5	A	406	NAG	O7-C7-C8	-4.65	113.78	122.05
5	A	406	NAG	O7-C7-N2	4.14	129.30	121.98
5	E	406	NAG	C4-C3-C2	3.79	116.58	111.02
5	C	406	NAG	O4-C4-C5	3.55	118.07	109.32

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	406	NAG	O5-C5-C6-O6
5	E	406	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

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	320/334 (95%)	-0.43	3 (0%) 81 81	26, 42, 74, 131	0
1	C	320/334 (95%)	-0.23	8 (2%) 58 61	32, 50, 79, 163	0
1	E	320/334 (95%)	-0.16	5 (1%) 70 72	28, 51, 81, 169	0
2	B	162/181 (89%)	0.05	1 (0%) 85 87	29, 63, 96, 120	0
2	D	162/181 (89%)	0.38	10 (6%) 28 28	28, 74, 122, 159	0
2	F	162/181 (89%)	0.45	11 (6%) 25 25	31, 76, 111, 139	0
All	All	1446/1545 (93%)	-0.08	38 (2%) 57 60	26, 52, 101, 169	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	173	ILE	6.7
2	B	173	ILE	5.9
1	E	70	PHE	5.1
1	C	68	ASP	4.8
1	C	71	ILE	4.7

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, 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
4	NAG	J	2	14/15	0.49	0.14	83,113,124,128	0
5	NAG	E	406	14/15	0.52	0.20	89,112,132,136	0
3	NAG	K	1	14/15	0.64	0.15	100,108,130,146	0
3	NAG	I	1	14/15	0.64	0.14	103,119,137,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	A	406	14/15	0.67	0.16	91,104,109,114	0
5	NAG	C	406	14/15	0.67	0.13	89,102,105,107	0
4	NAG	L	2	14/15	0.68	0.13	82,104,116,118	0
3	FUC	G	2	10/11	0.68	0.13	95,113,116,116	0
3	FUC	I	2	10/11	0.69	0.14	142,156,169,172	0
4	NAG	H	2	14/15	0.69	0.11	88,101,114,123	0
4	FUC	J	3	10/11	0.70	0.13	117,128,140,143	0
3	FUC	K	2	10/11	0.71	0.15	121,147,156,161	0
4	FUC	L	3	10/11	0.74	0.14	103,128,131,141	0
4	FUC	H	3	10/11	0.75	0.14	91,110,116,119	0
3	NAG	G	1	14/15	0.77	0.12	97,106,113,117	0
4	NAG	J	1	14/15	0.86	0.09	74,80,101,111	0
4	NAG	H	1	14/15	0.91	0.08	45,59,91,108	0
4	NAG	L	1	14/15	0.93	0.09	58,64,88,117	0

6.3 Carbohydrates

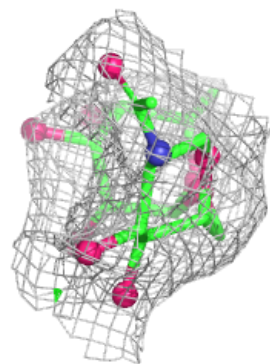
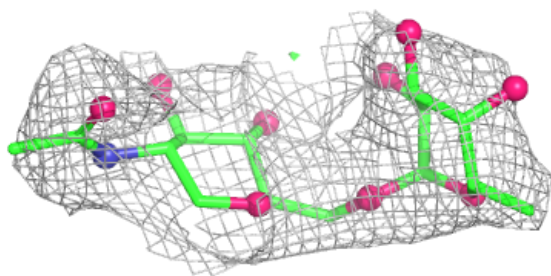
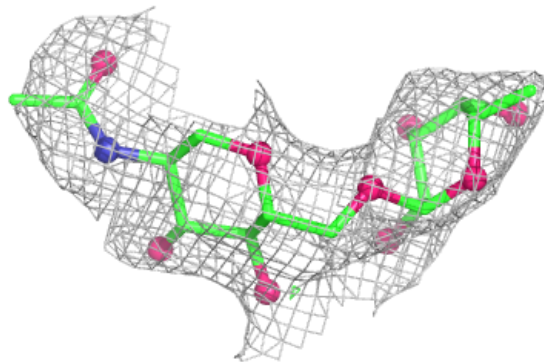
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	J	2	14/15	0.49	0.14	83,113,124,128	0
3	NAG	K	1	14/15	0.64	0.15	100,108,130,146	0
3	NAG	I	1	14/15	0.64	0.14	103,119,137,146	0
3	FUC	G	2	10/11	0.68	0.13	95,113,116,116	0
4	NAG	L	2	14/15	0.68	0.13	82,104,116,118	0
3	FUC	I	2	10/11	0.69	0.14	142,156,169,172	0
4	NAG	H	2	14/15	0.69	0.11	88,101,114,123	0
4	FUC	J	3	10/11	0.70	0.13	117,128,140,143	0
3	FUC	K	2	10/11	0.71	0.15	121,147,156,161	0
4	FUC	L	3	10/11	0.74	0.14	103,128,131,141	0
4	FUC	H	3	10/11	0.75	0.14	91,110,116,119	0
3	NAG	G	1	14/15	0.77	0.12	97,106,113,117	0
4	NAG	J	1	14/15	0.86	0.09	74,80,101,111	0
4	NAG	H	1	14/15	0.91	0.08	45,59,91,108	0
4	NAG	L	1	14/15	0.93	0.09	58,64,88,117	0

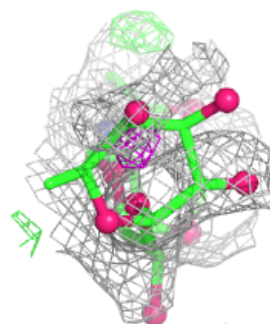
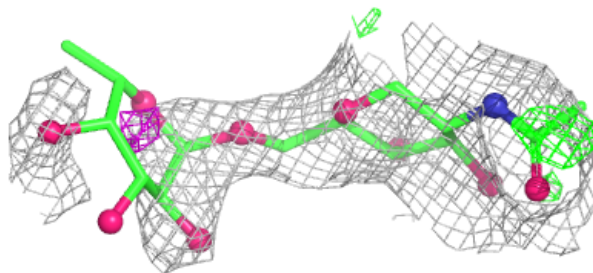
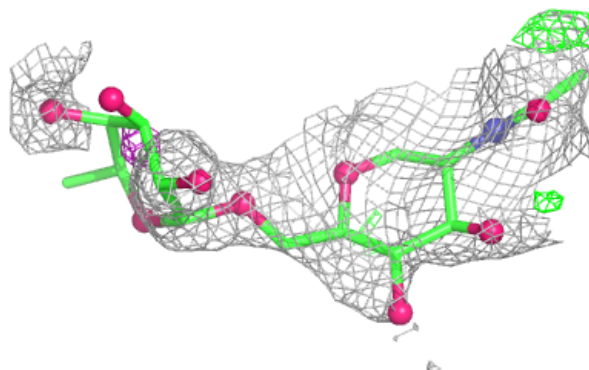
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

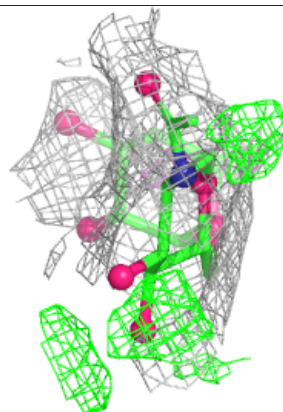
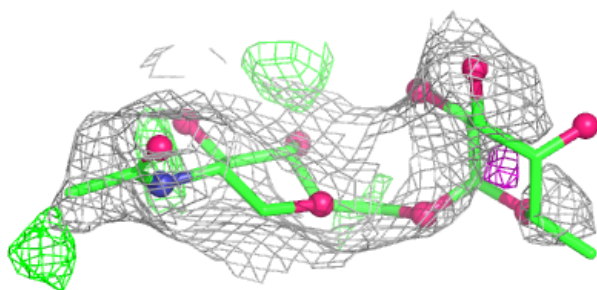
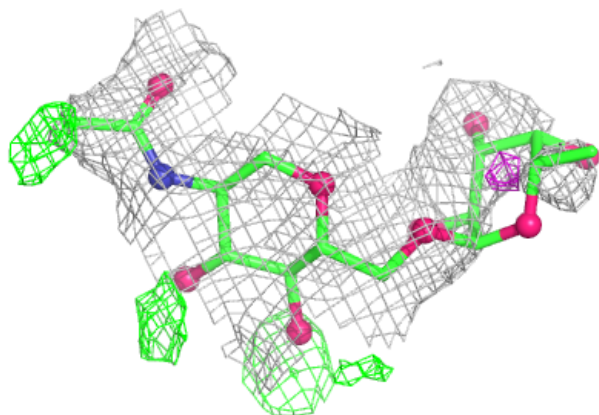
**Electron density around Chain I:**

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



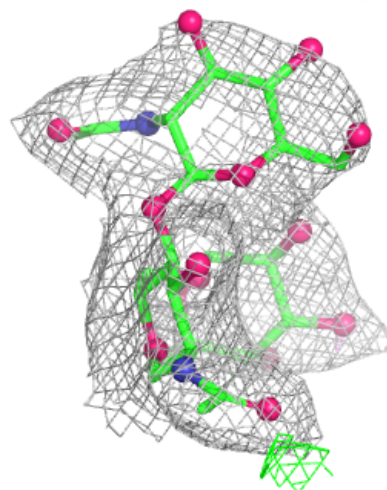
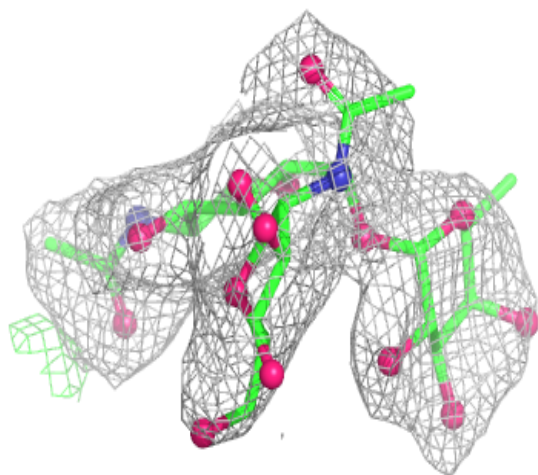
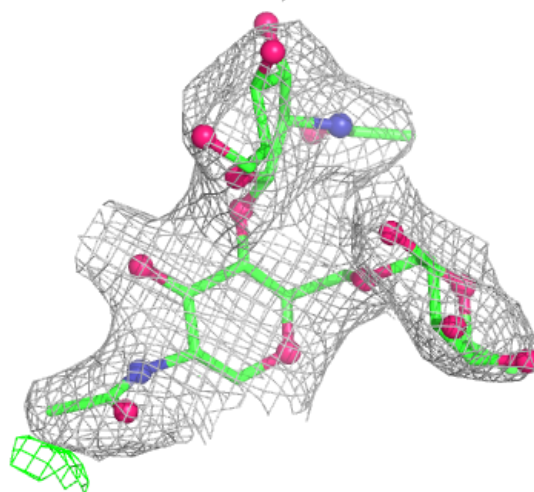
Electron density around Chain K:

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



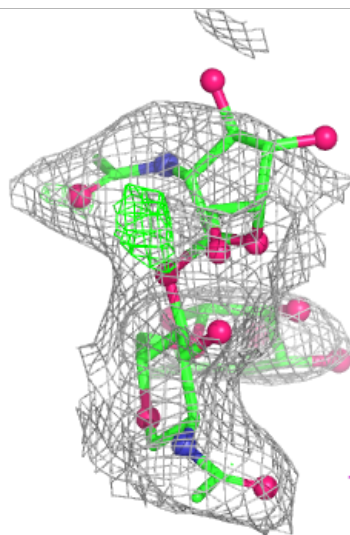
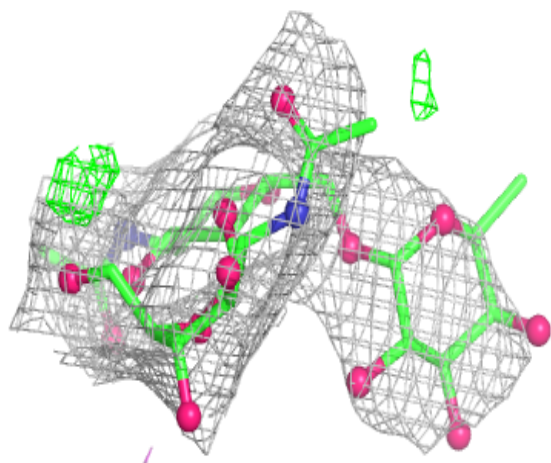
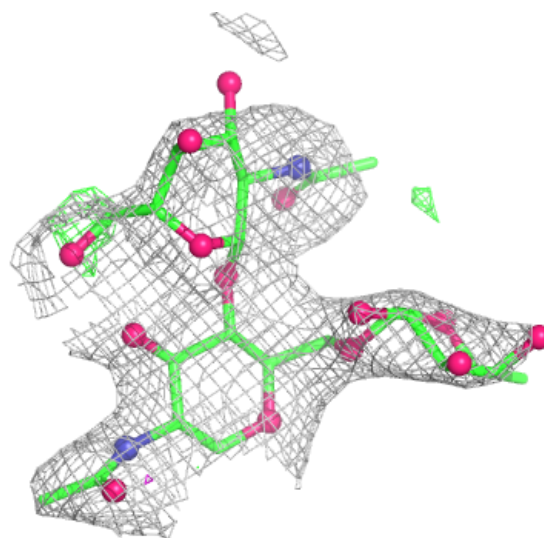
Electron density around Chain H:

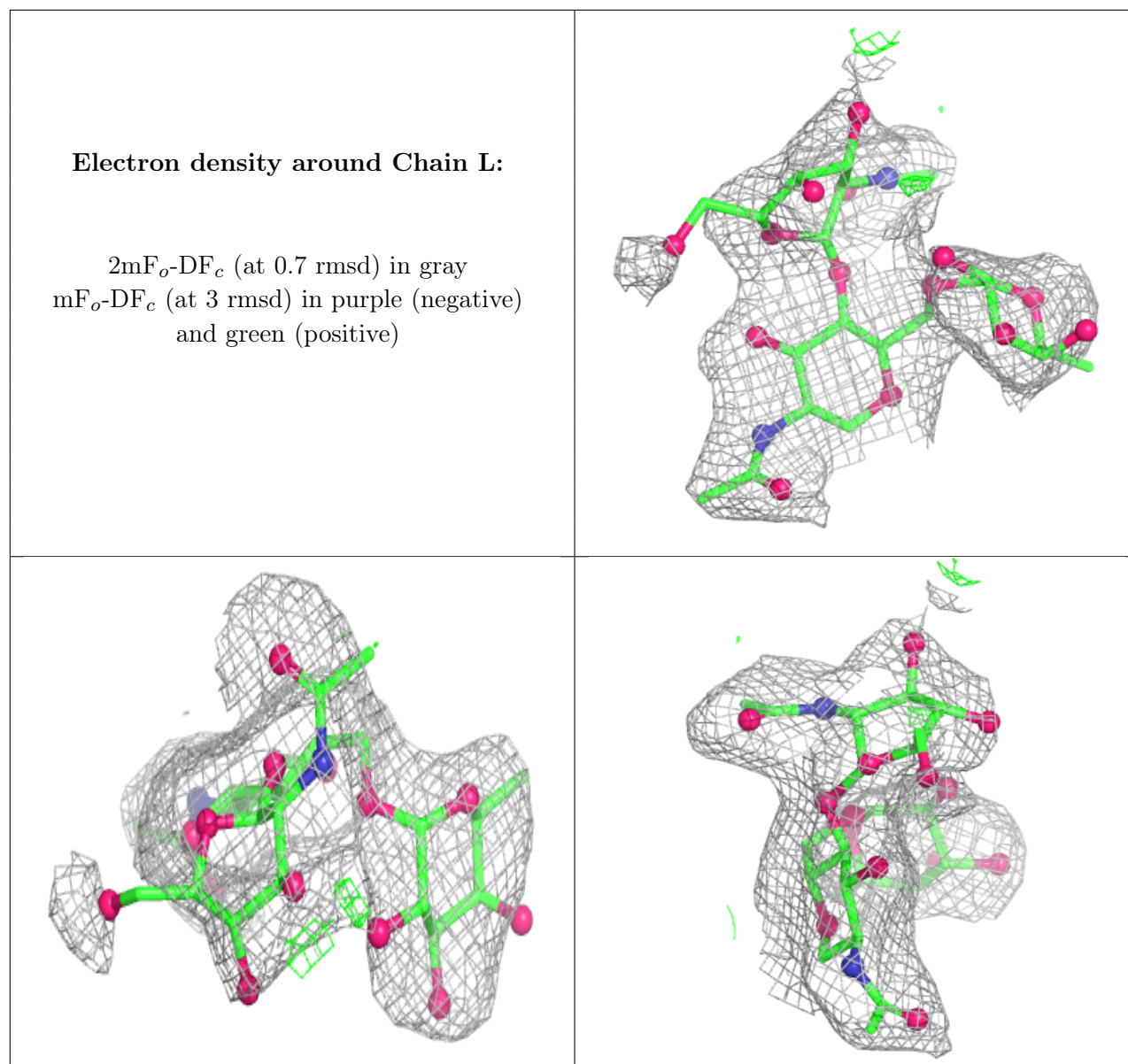
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain J:

$2mF_o-DF_c$ (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
5	NAG	E	406	14/15	0.52	0.20	89,112,132,136	0
5	NAG	C	406	14/15	0.67	0.13	89,102,105,107	0
5	NAG	A	406	14/15	0.67	0.16	91,104,109,114	0

6.5 Other polymers [i](#)

There are no such residues in this entry.