W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

May 8, 2023 – 12:26 PM JST

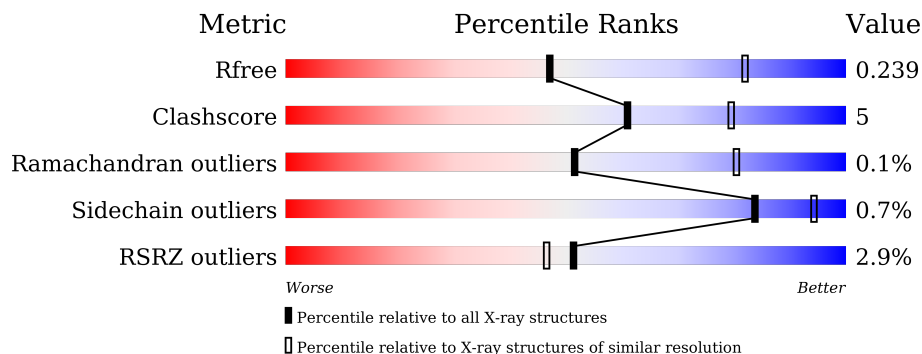|		
PDB ID	:	8IF2
Title	:	Crystal structure of the receptor binding domain of SARS-CoV-2 Omicron BQ.1.1 variant spike protein in complex with its receptor ACE2
Authors	:	Kimura, K.; Suzuki, T.; Hashiguchi, T.
Deposited on	:	2023-02-17
Resolution	:	2.78 Å(reported)

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 2.78 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	Percentile Ranks	Value
Rfree		0.239
Clashscore		5
Ramachandran outliers		0.1%
Sidechain outliers		0.7%
RSRZ outliers		2.9%

Worse   *Better*

▌Percentile relative to all X-ray structures

❘Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 <=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	608	4% / 84% / 13% / ..
2	B	224	83% / 5% / 11%
3	J	3	100%
3	N	3	67% / 33%
3	O	3	33% / 67%
4	K	7	43% / 43% / 14%

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Mol	Chain	Length	Quality of chain
5	L	2	50% 50%

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
3	BMA	N	3	-	-	-	X

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 6713 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 Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total 4857	C 3108	N 804	O 916	S 29	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	618	GLY	-	expression tag	UNP Q9BYF1
A	619	THR	-	expression tag	UNP Q9BYF1
A	620	LYS	-	expression tag	UNP Q9BYF1
A	621	HIS	-	expression tag	UNP Q9BYF1
A	622	HIS	-	expression tag	UNP Q9BYF1
A	623	HIS	-	expression tag	UNP Q9BYF1
A	624	HIS	-	expression tag	UNP Q9BYF1
A	625	HIS	-	expression tag	UNP Q9BYF1
A	626	HIS	-	expression tag	UNP Q9BYF1

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	199	Total 1583	C 1023	N 264	O 288	S 8	0	0	0

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	339	ASP	GLY	variant	UNP P0DTC2
B	346	THR	ARG	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	444	THR	LYS	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	VAL	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	537	GLY	-	expression tag	UNP P0DTC2
B	538	THR	-	expression tag	UNP P0DTC2
B	539	LYS	-	expression tag	UNP P0DTC2
B	540	HIS	-	expression tag	UNP P0DTC2
B	541	HIS	-	expression tag	UNP P0DTC2
B	542	HIS	-	expression tag	UNP P0DTC2
B	543	HIS	-	expression tag	UNP P0DTC2
B	544	HIS	-	expression tag	UNP P0DTC2
B	545	HIS	-	expression tag	UNP P0DTC2

- 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.
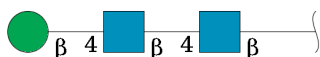
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	J	3	Total 39	C 22	N 2	O 15	0	0	0
3	N	3	Total 39	C 22	N 2	O 15	0	0	0
3	O	3	Total 39	C 22	N 2	O 15	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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.
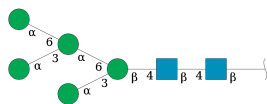
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	K	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	13	Total	O	0	0
			13	13		
8	B	17	Total	O	0	0
			17	17		

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.
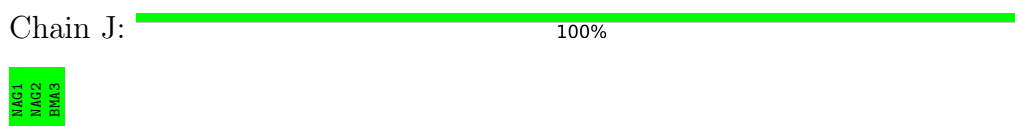
• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:
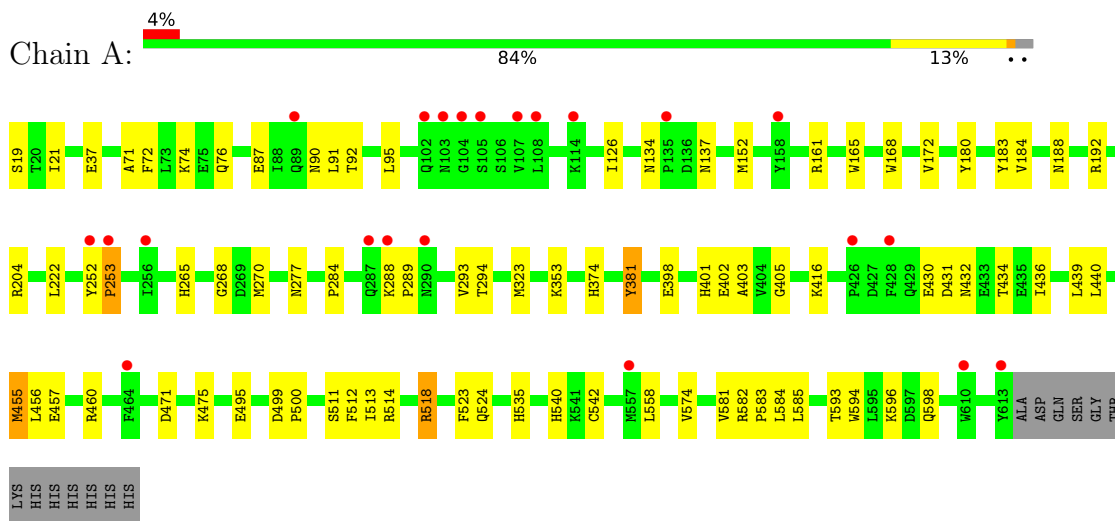
• Molecule 2: Spike protein S1
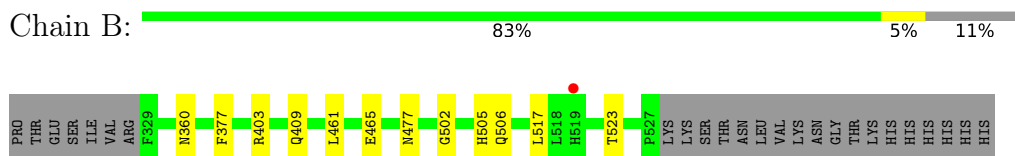
Chain B:

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

Chain J:

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

Chain N:
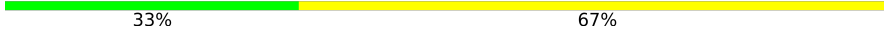
NAG1 NAG2 BMA3

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

Chain O: 33%   67%

NAG1 NAG2 BMA3

• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 K: 43%   43%   14%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6 MAN7

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 50%   50%

NAG1 NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α, β, γ	120.05Å 120.05Å 167.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.17 – 2.78 49.17 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.17-2.78) 99.8 (49.17-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.200 , 0.245 0.198 , 0.239	Depositor DCC
R_{free} test set	1733 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	72.3	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 38.7	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6713	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, MAN, BMA, ZN

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	0.25	0/4994	0.44	0/6785
2	B	0.26	0/1632	0.49	0/2225
All	All	0.25	0/6626	0.45	0/9010

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	4857	0	4628	52	0
2	B	1583	0	1504	7	0
3	J	39	0	34	0	0
3	N	39	0	34	0	0
3	O	39	0	34	1	0
4	K	83	0	70	1	0
5	L	28	0	25	0	0
6	A	1	0	0	0	0
7	A	14	0	13	1	0
8	A	13	0	0	0	0
8	B	17	0	0	0	0
All	All	6713	0	6342	59	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 5.

The worst 5 of 59 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:A:289:PRO:HB3	1:A:434:THR:HG22	1.66	0.77
1:A:284:PRO:HD3	1:A:440:LEU:HD22	1.77	0.66
2:B:409:GLN:HE22	4:K:6:MAN:H2	1.65	0.60
1:A:457:GLU:HG2	1:A:513:ILE:HB	1.81	0.60
1:A:436:ILE:HG13	7:A:702:NAG:H81	1.84	0.59

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	593/608 (98%)	572 (96%)	20 (3%)	1 (0%)	47	76
2	B	197/224 (88%)	193 (98%)	4 (2%)	0	100	100
All	All	790/832 (95%)	765 (97%)	24 (3%)	1 (0%)	51	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	PRO

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	526/537 (98%)	522 (99%)	4 (1%)	81	93
2	B	171/195 (88%)	170 (99%)	1 (1%)	86	95
All	All	697/732 (95%)	692 (99%)	5 (1%)	84	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	381	TYR
1	A	401	HIS
1	A	455	MET
1	A	518	ARG
2	B	377	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

18 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	J	1	3,1	14,14,15	0.53	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|>2$	Counts	RMSZ	#$\|Z\|>2$
3	NAG	J	2	3	14,14,15	0.39	0	17,19,21	0.42	0
3	BMA	J	3	3	11,11,12	0.92	0	15,15,17	0.93	0
4	NAG	K	1	4,1	14,14,15	0.35	0	17,19,21	0.56	0
4	NAG	K	2	4	14,14,15	0.26	0	17,19,21	0.41	0
4	BMA	K	3	4	11,11,12	0.54	0	15,15,17	0.89	0
4	MAN	K	4	4	11,11,12	0.77	0	15,15,17	0.98	2 (13%)
4	MAN	K	5	4	11,11,12	0.81	1 (9%)	15,15,17	1.12	2 (13%)
4	MAN	K	6	4	11,11,12	0.75	0	15,15,17	1.32	2 (13%)
4	MAN	K	7	4	11,11,12	0.66	0	15,15,17	0.93	1 (6%)
5	NAG	L	1	5,1	14,14,15	0.35	0	17,19,21	0.68	1 (5%)
5	NAG	L	2	5	14,14,15	0.49	0	17,19,21	0.49	0
3	NAG	N	1	3,1	14,14,15	0.39	0	17,19,21	0.57	0
3	NAG	N	2	3	14,14,15	0.20	0	17,19,21	0.47	0
3	BMA	N	3	3	11,11,12	0.85	1 (9%)	15,15,17	0.78	0
3	NAG	O	1	3,2	14,14,15	0.33	0	17,19,21	0.54	0
3	NAG	O	2	3	14,14,15	0.38	0	17,19,21	0.43	0
3	BMA	O	3	3	11,11,12	0.62	0	15,15,17	0.71	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	J	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	4/6/23/26	0/1/1/1
3	BMA	J	3	3	-	0/2/19/22	0/1/1/1
4	NAG	K	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	BMA	K	3	4	-	0/2/19/22	0/1/1/1
4	MAN	K	4	4	-	2/2/19/22	0/1/1/1
4	MAN	K	5	4	-	2/2/19/22	0/1/1/1
4	MAN	K	6	4	-	2/2/19/22	1/1/1/1
4	MAN	K	7	4	-	0/2/19/22	0/1/1/1
5	NAG	L	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	L	2	5	-	2/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	BMA	N	3	3	-	2/2/19/22	0/1/1/1

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	5	MAN	C1-C2	2.10	1.57	1.52
3	N	3	BMA	C1-C2	2.08	1.56	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	6	MAN	C1-O5-C5	3.72	117.23	112.19
4	K	5	MAN	C1-O5-C5	2.66	115.80	112.19
4	K	4	MAN	O2-C2-C3	-2.20	105.72	110.14
5	L	1	NAG	C1-O5-C5	2.18	115.14	112.19
4	K	7	MAN	O2-C2-C3	-2.17	105.79	110.14

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	1	NAG	O5-C5-C6-O6
4	K	5	MAN	C4-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
4	K	5	MAN	O5-C5-C6-O6
3	N	3	BMA	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	6	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	2	NAG	1	0
4	K	6	MAN	1	0
3	O	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.

Oligosaccharide Chain J

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain N

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain O

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain K

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain L
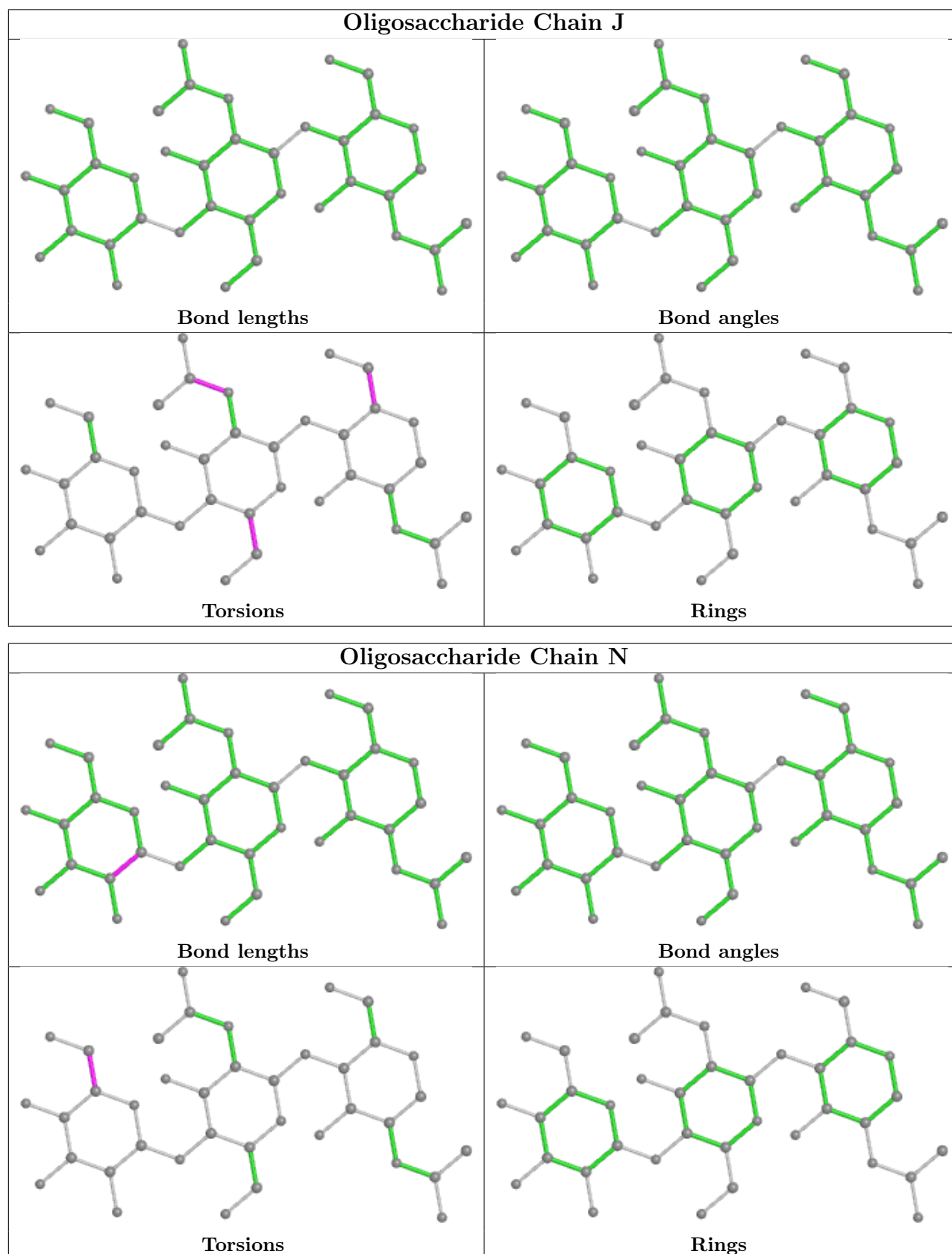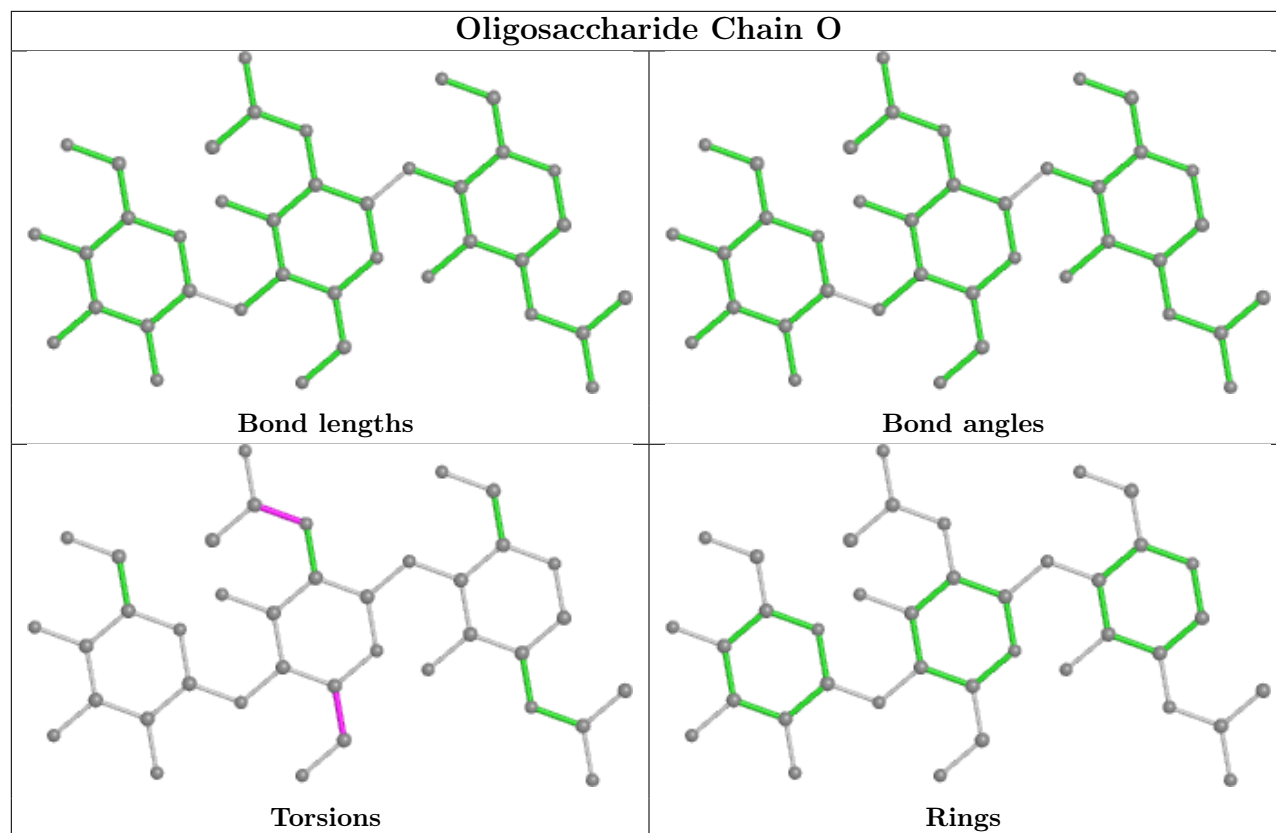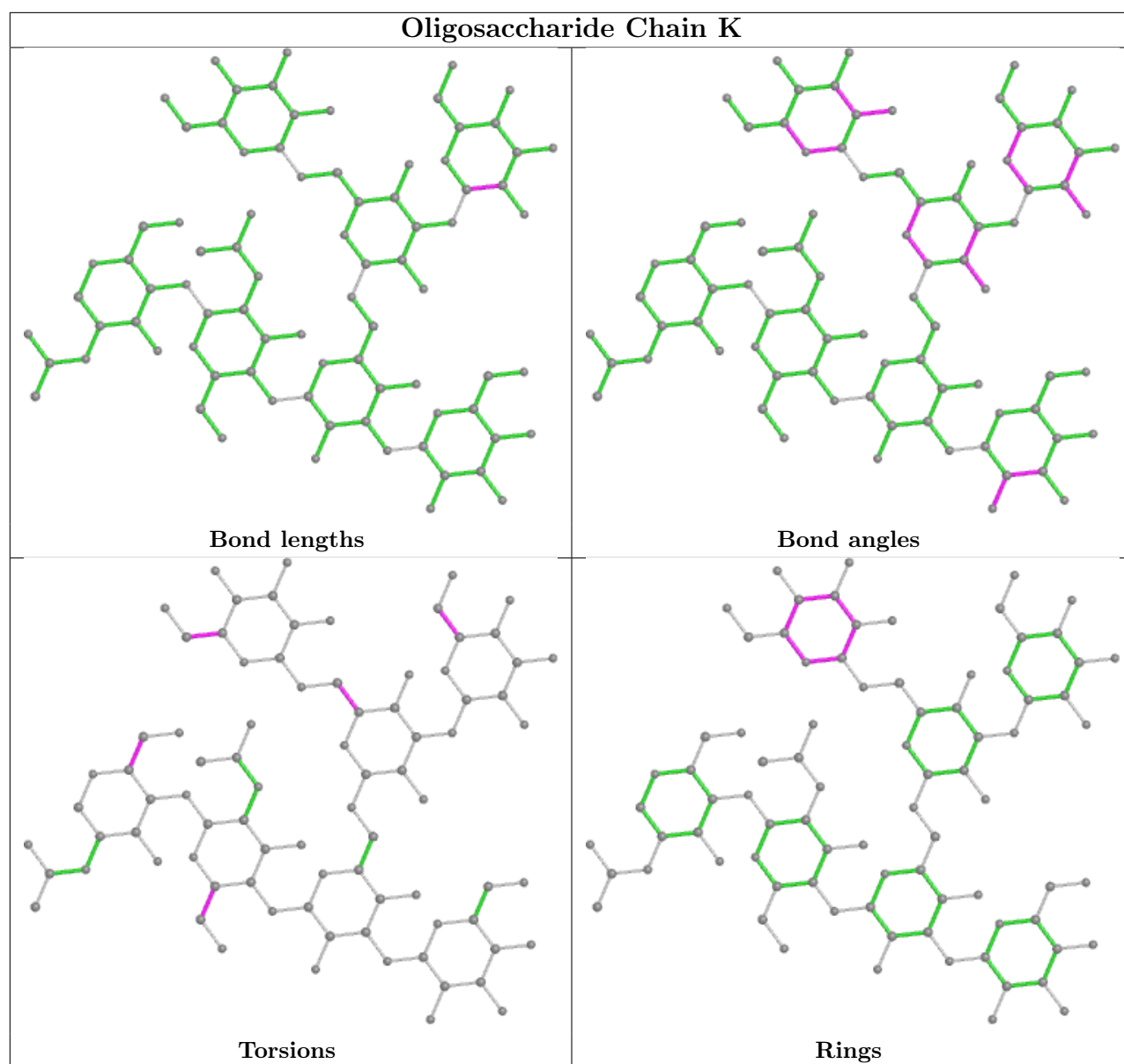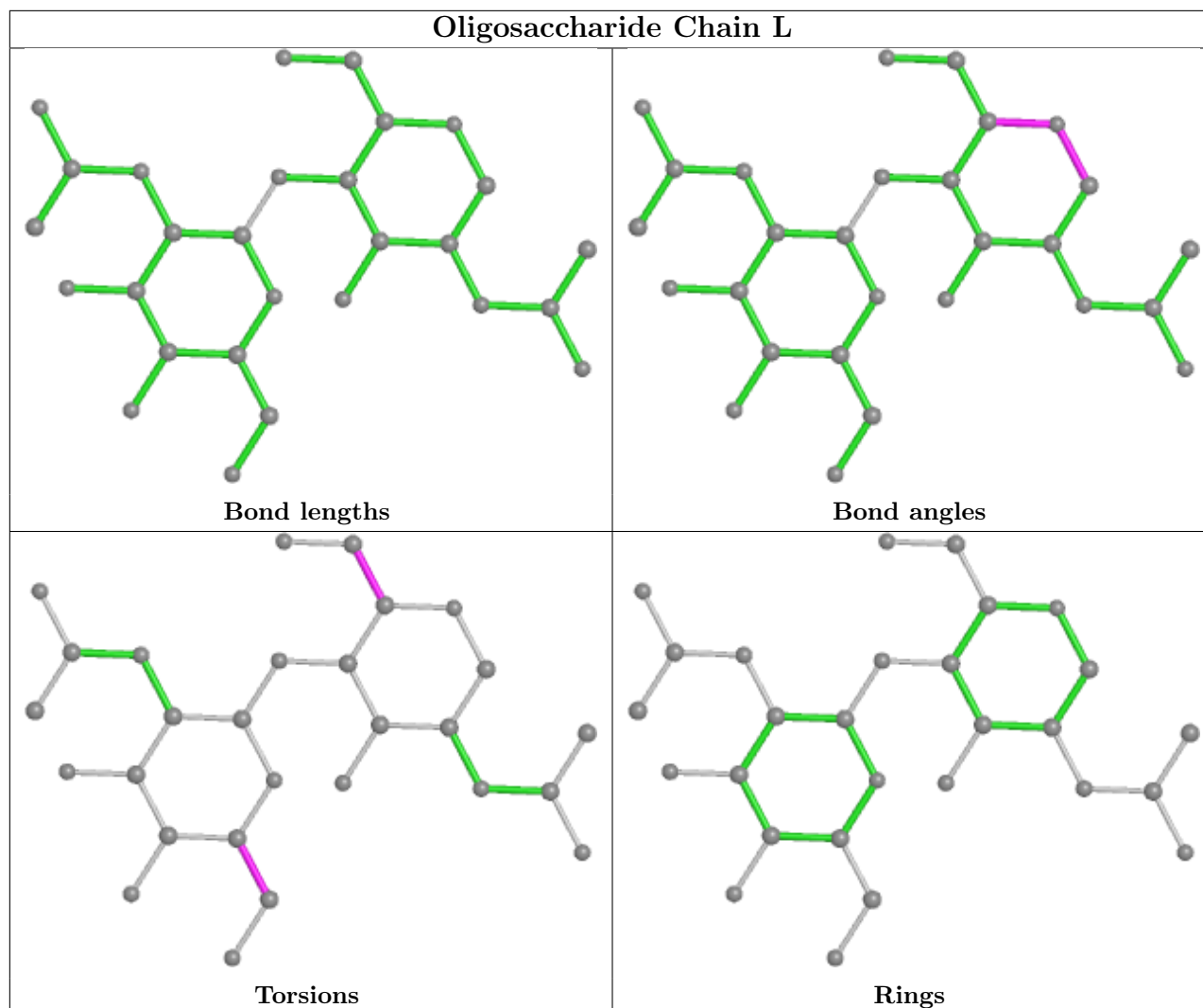
5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\| > 2$
7	NAG	A	702	1	14,14,15	0.41	0	17,19,21	0.38	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	A	702	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	702	NAG	O5-C5-C6-O6
7	A	702	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	702	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 then 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.

Ligand NAG A 702

Bond lengths

Bond angles

Torsions

Rings
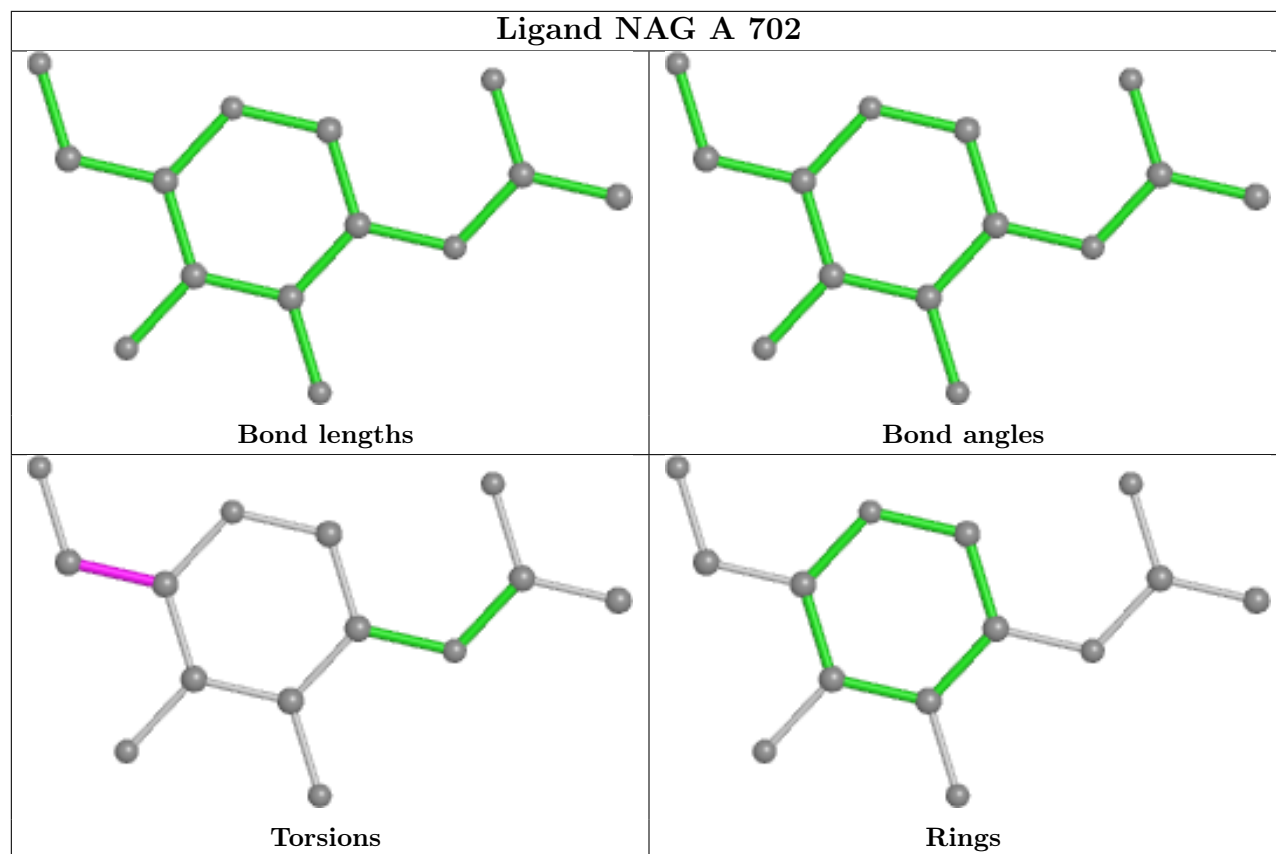
5.7 Other polymers ⓘ

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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(Å²)	Q<0.9
1	A	595/608 (97%)	0.17	22 (3%)	41	36	44, 86, 130, 167	0
2	B	199/224 (88%)	-0.09	1 (0%)	91	90	40, 60, 102, 137	0
All	All	794/832 (95%)	0.11	23 (2%)	51	46	40, 79, 128, 167	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	104	GLY	8.2
1	A	613	TYR	6.1
1	A	103	ASN	4.4
1	A	253	PRO	3.5
1	A	89	GLN	3.3

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

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

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(Å²)	Q<0.9
4	MAN	K	4	11/12	0.69	0.29	121,155,162,162	0
4	BMA	K	3	11/12	0.73	0.27	110,134,144,148	0
3	BMA	J	3	11/12	0.76	0.22	106,127,138,150	0
4	MAN	K	5	11/12	0.76	0.37	128,155,159,160	0
3	BMA	O	3	11/12	0.77	0.17	69,95,107,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BMA	N	3	11/12	0.77	0.47	135,167,174,175	0
5	NAG	L	2	14/15	0.81	0.44	101,133,149,150	0
3	NAG	N	2	14/15	0.82	0.34	108,145,164,169	0
4	MAN	K	6	11/12	0.84	0.27	124,131,135,159	0
3	NAG	O	2	14/15	0.84	0.24	52,86,120,134	0
4	MAN	K	7	11/12	0.85	0.25	127,139,148,150	0
3	NAG	N	1	14/15	0.88	0.27	96,112,134,151	0
3	NAG	J	2	14/15	0.90	0.15	66,104,118,133	0
4	NAG	K	1	14/15	0.91	0.18	99,118,122,124	0
4	NAG	K	2	14/15	0.91	0.24	115,129,138,144	0
5	NAG	L	1	14/15	0.92	0.16	67,85,119,126	0
3	NAG	J	1	14/15	0.95	0.14	47,64,75,79	0
3	NAG	O	1	14/15	0.97	0.13	47,61,80,88	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.
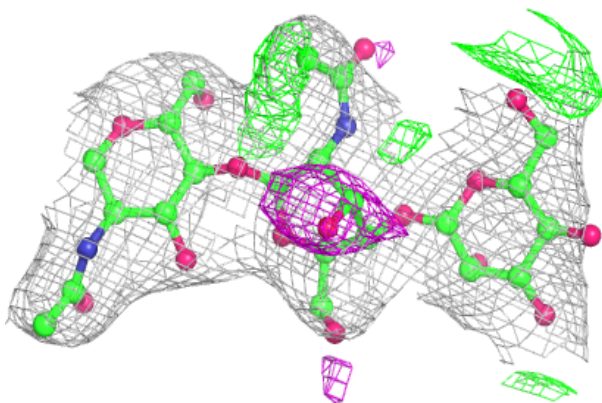
Electron density around Chain J:

$2\text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray
$\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative)
and green (positive)
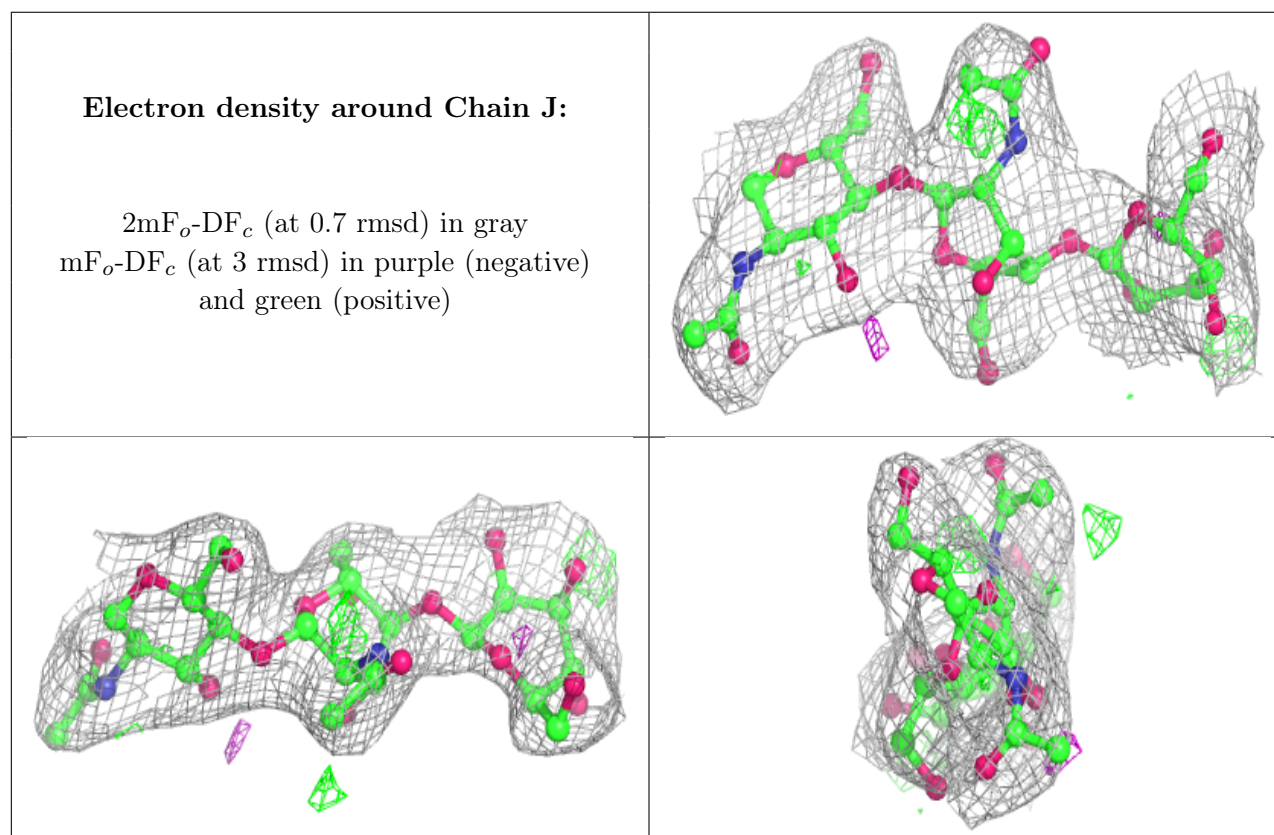
Electron density around Chain N:

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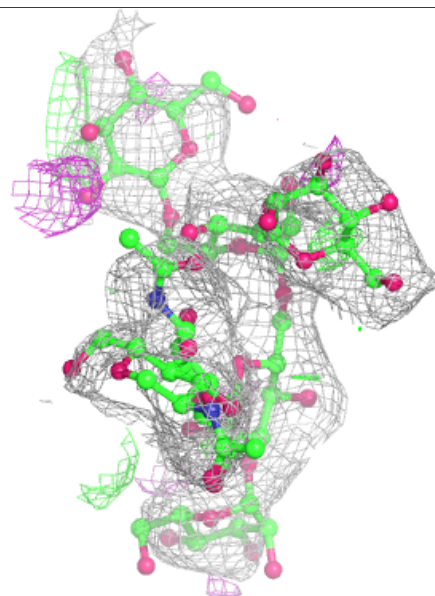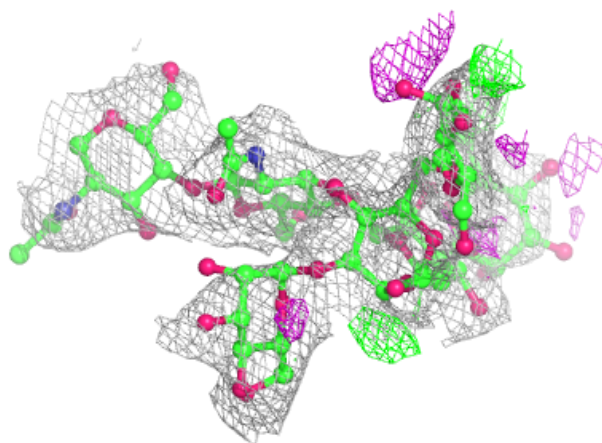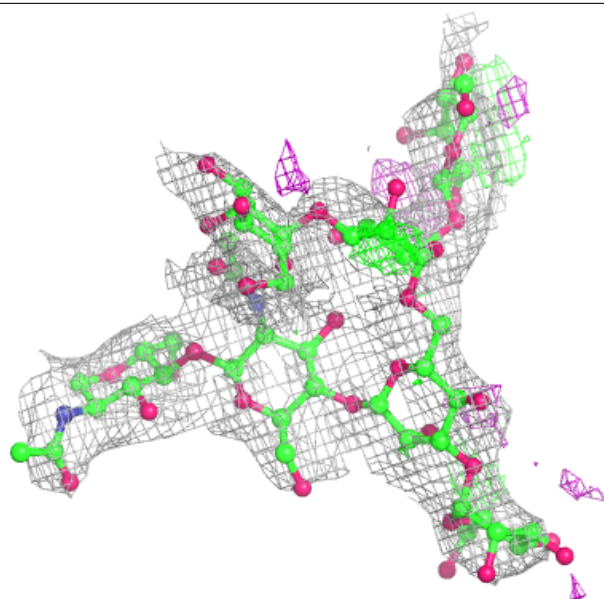mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
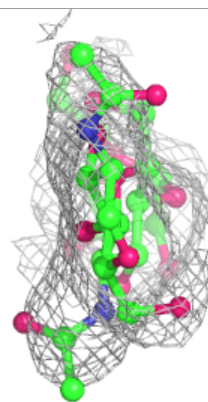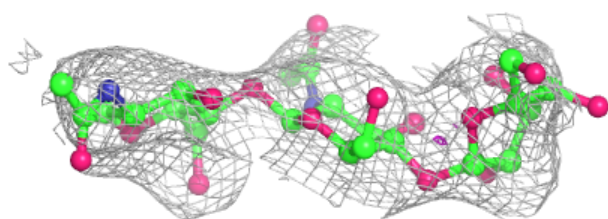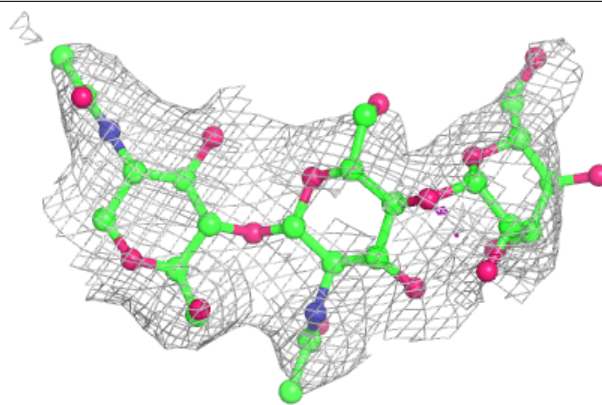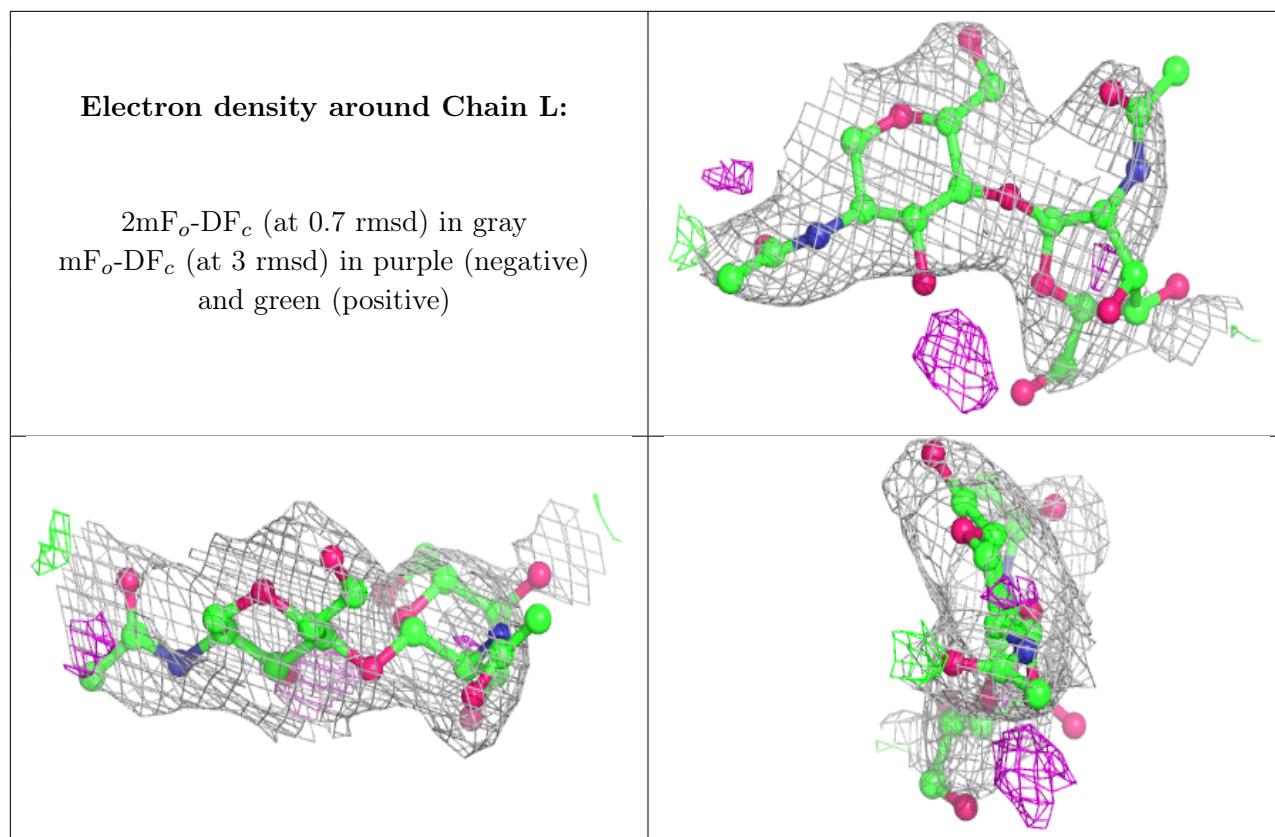

Electron density around Chain O:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
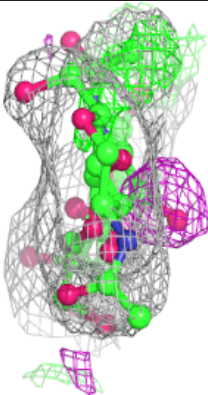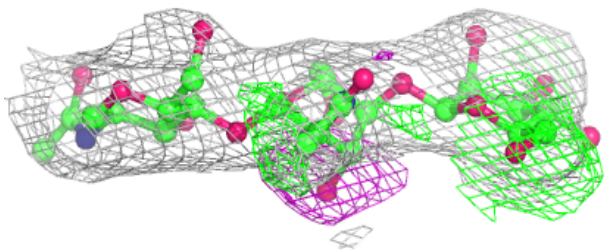
Electron density around Chain K:

$2mF_o$-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 L:

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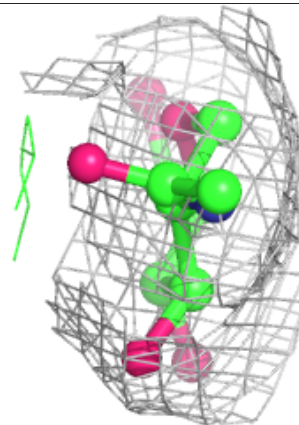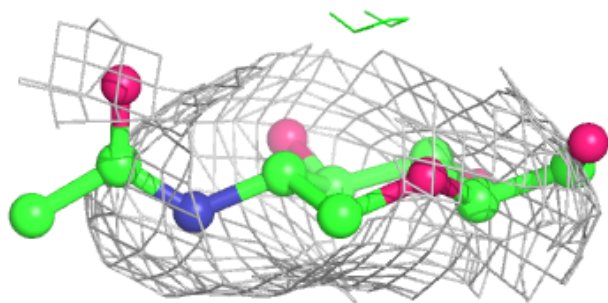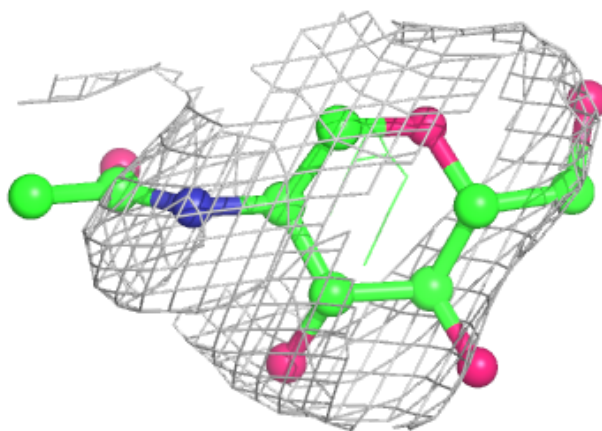and green (positive)

6.4 Ligands ⓘ

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.
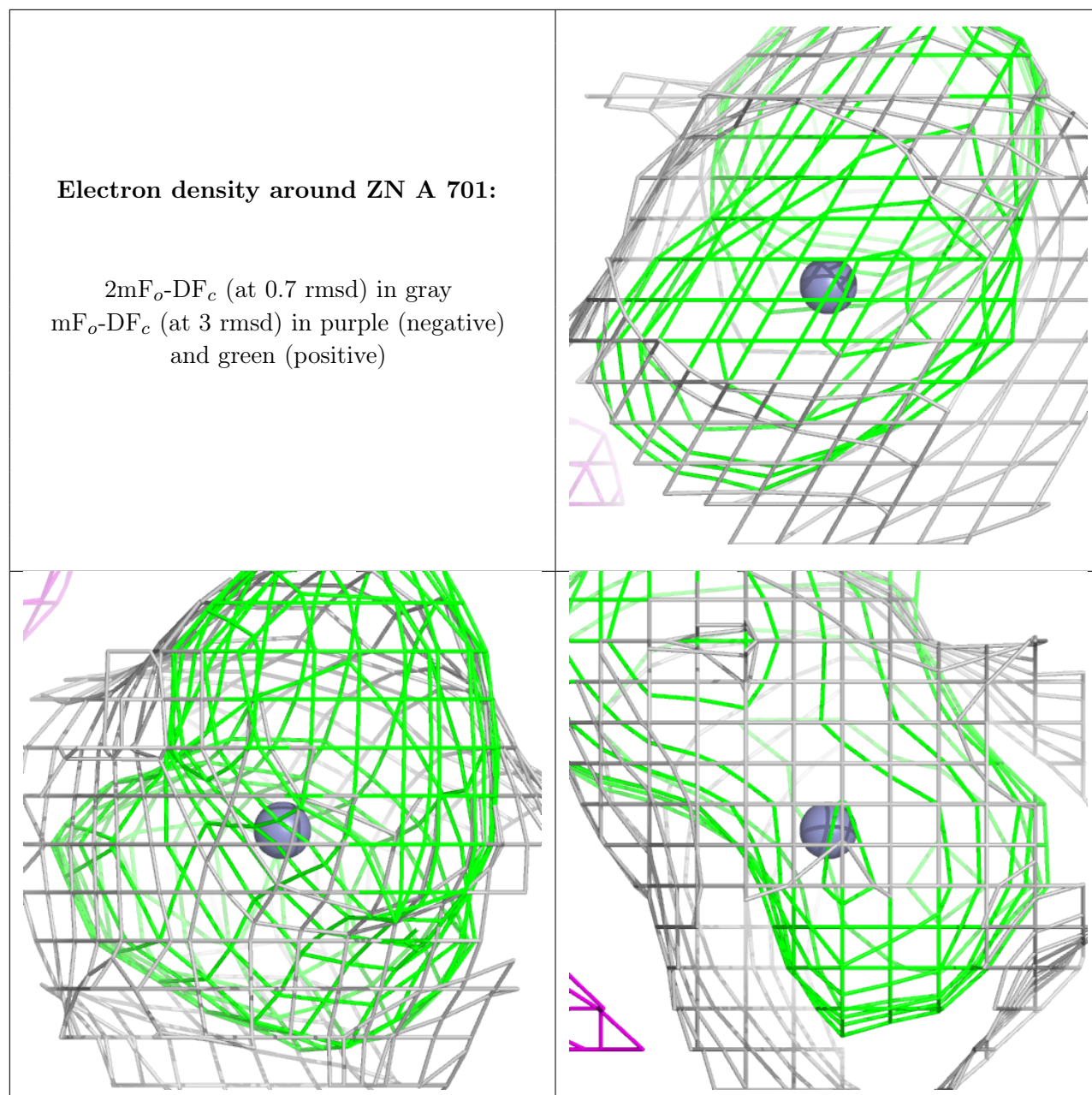
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	A	702	14/15	0.76	0.28	130,143,151,152	0
6	ZN	A	701	1/1	0.98	0.29	64,64,64,64	0

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 NAG A 702:

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 ZN A 701:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.