



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 16, 2024 – 01:08 PM JST

PDB ID : 8WDR
Title : Crystal structure of BQ.1.1 RBD complexed with human ACE2
Authors : Li, W.; Xie, Y.
Deposited on : 2023-09-16
Resolution : 3.47 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

<https://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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

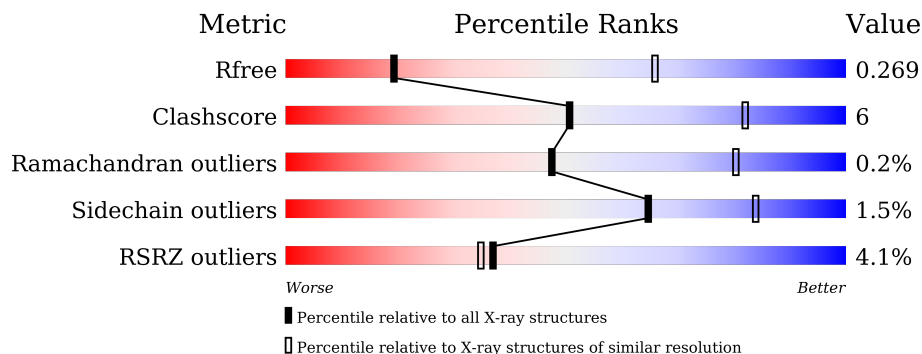
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.47 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.




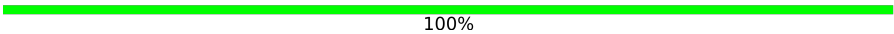
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

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	805	 9% 65% 9% 26%
1	C	805	 2% 62% 12% 26%
2	B	247	 7% 63% 15% 21%
2	D	247	 9% 68% 11% 21%
3	E	2	 100%
3	G	2	 100%

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Mol	Chain	Length	Quality of chain
3	H	2	 50% 50%
4	F	3	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	A	903	-	-	-	X
6	NAG	B	601	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13055 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	596	4862	3111	805	917	29	0	0	0
1	C	596	4857	3110	801	917	29	0	1	0

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	195	1558	1004	261	285	8	0	1	0
2	D	195	1555	1003	260	284	8	0	1	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	301	MET	-	initiating methionine	UNP P0DTC2
B	302	HIS	-	expression tag	UNP P0DTC2
B	303	SER	-	expression tag	UNP P0DTC2
B	304	SER	-	expression tag	UNP P0DTC2
B	305	ALA	-	expression tag	UNP P0DTC2
B	306	LEU	-	expression tag	UNP P0DTC2
B	307	LEU	-	expression tag	UNP P0DTC2
B	308	CYS	-	expression tag	UNP P0DTC2
B	309	CYS	-	expression tag	UNP P0DTC2
B	310	LEU	-	expression tag	UNP P0DTC2
B	311	VAL	-	expression tag	UNP P0DTC2
B	312	LEU	-	expression tag	UNP P0DTC2
B	313	LEU	-	expression tag	UNP P0DTC2
B	314	THR	-	expression tag	UNP P0DTC2
B	315	GLY	-	expression tag	UNP P0DTC2
B	316	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	317	ARG	-	expression tag	UNP P0DTC2
B	318	ALA	-	expression tag	UNP P0DTC2
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
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	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
B	546	HIS	-	expression tag	UNP P0DTC2
B	547	HIS	-	expression tag	UNP P0DTC2
D	301	MET	-	initiating methionine	UNP P0DTC2
D	302	HIS	-	expression tag	UNP P0DTC2
D	303	SER	-	expression tag	UNP P0DTC2
D	304	SER	-	expression tag	UNP P0DTC2
D	305	ALA	-	expression tag	UNP P0DTC2
D	306	LEU	-	expression tag	UNP P0DTC2
D	307	LEU	-	expression tag	UNP P0DTC2
D	308	CYS	-	expression tag	UNP P0DTC2
D	309	CYS	-	expression tag	UNP P0DTC2
D	310	LEU	-	expression tag	UNP P0DTC2
D	311	VAL	-	expression tag	UNP P0DTC2
D	312	LEU	-	expression tag	UNP P0DTC2
D	313	LEU	-	expression tag	UNP P0DTC2
D	314	THR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	315	GLY	-	expression tag	UNP P0DTC2
D	316	VAL	-	expression tag	UNP P0DTC2
D	317	ARG	-	expression tag	UNP P0DTC2
D	318	ALA	-	expression tag	UNP P0DTC2
D	339	ASP	GLY	variant	UNP P0DTC2
D	346	THR	ARG	variant	UNP P0DTC2
D	371	PHE	SER	variant	UNP P0DTC2
D	373	PRO	SER	variant	UNP P0DTC2
D	375	PHE	SER	variant	UNP P0DTC2
D	376	ALA	THR	variant	UNP P0DTC2
D	405	ASN	ASP	variant	UNP P0DTC2
D	408	SER	ARG	variant	UNP P0DTC2
D	417	ASN	LYS	variant	UNP P0DTC2
D	440	LYS	ASN	variant	UNP P0DTC2
D	444	THR	LYS	variant	UNP P0DTC2
D	452	ARG	LEU	variant	UNP P0DTC2
D	460	LYS	ASN	variant	UNP P0DTC2
D	477	ASN	SER	variant	UNP P0DTC2
D	478	LYS	THR	variant	UNP P0DTC2
D	484	ALA	GLU	variant	UNP P0DTC2
D	486	VAL	PHE	variant	UNP P0DTC2
D	498	ARG	GLN	variant	UNP P0DTC2
D	501	TYR	ASN	variant	UNP P0DTC2
D	505	HIS	TYR	variant	UNP P0DTC2
D	542	HIS	-	expression tag	UNP P0DTC2
D	543	HIS	-	expression tag	UNP P0DTC2
D	544	HIS	-	expression tag	UNP P0DTC2
D	545	HIS	-	expression tag	UNP P0DTC2
D	546	HIS	-	expression tag	UNP P0DTC2
D	547	HIS	-	expression tag	UNP P0DTC2

- Molecule 3 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	
			Total	C	N				O
3	E	2	28	16	2	10	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 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
4	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	C	1	Total	Zn	0	0
			1	1		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

Chain H:  50% 50%

MAG1
MAG2

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

Chain F:  100%

MAG1
MAG2
BOM3

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	123.58Å 135.41Å 154.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 3.47 29.75 – 3.47	Depositor EDS
% Data completeness (in resolution range)	95.7 (29.75-3.47) 95.8 (29.75-3.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.47Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.211 , 0.269 0.213 , 0.269	Depositor DCC
R_{free} test set	1646 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	82.3	Xtrriage
Anisotropy	0.460	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13055	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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: NAG, ZN, BMA

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	0.24	0/4999	0.44	0/6792
1	C	0.32	4/4998 (0.1%)	0.50	5/6793 (0.1%)
2	B	0.27	0/1605	0.51	0/2187
2	D	0.26	0/1605	0.50	0/2187
All	All	0.28	4/13207 (0.0%)	0.48	5/17959 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	252	TYR	CD1-CE1	-7.14	1.28	1.39
1	C	252	TYR	CD2-CE2	6.06	1.48	1.39
1	C	255	TYR	CD2-CE2	-5.81	1.30	1.39
1	C	255	TYR	CB-CG	-5.51	1.43	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	255	TYR	CB-CG-CD2	-10.30	114.82	121.00
1	C	252	TYR	CB-CG-CD2	7.95	125.77	121.00
1	C	252	TYR	CB-CG-CD1	-5.90	117.46	121.00
1	C	255	TYR	CB-CG-CD1	5.51	124.31	121.00
1	C	252	TYR	CD1-CE1-CZ	5.08	124.37	119.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4862	0	4635	40	1
1	C	4857	0	4618	66	1
2	B	1558	0	1478	26	0
2	D	1555	0	1480	13	0
3	E	28	0	25	0	0
3	G	28	0	25	1	0
3	H	28	0	25	1	0
4	F	39	0	34	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	42	0	39	0	0
6	B	14	0	13	0	0
6	C	42	0	39	2	0
All	All	13055	0	12411	145	1

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 6.

The worst 5 of 145 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:252:TYR:HD1	1:C:255:TYR:HH	0.97	0.91
1:C:252:TYR:HB3	1:C:255:TYR:CE1	2.11	0.86
1:C:252:TYR:HD1	1:C:255:TYR:OH	1.69	0.75
1:C:157:ASP:OD1	1:C:158:TYR:N	2.22	0.72
2:B:359:SER:HA	2:B:524:VAL:HG22	1.73	0.69

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:ASN:ND2	1:C:254:SER:O[4_444]	2.15	0.05

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	594/805 (74%)	577 (97%)	16 (3%)	1 (0%)	47	80
1	C	595/805 (74%)	563 (95%)	31 (5%)	1 (0%)	47	80
2	B	194/247 (78%)	176 (91%)	17 (9%)	1 (0%)	29	66
2	D	194/247 (78%)	178 (92%)	16 (8%)	0	100	100
All	All	1577/2104 (75%)	1494 (95%)	80 (5%)	3 (0%)	47	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	338	ASN
2	B	344	ALA
1	C	54	ILE

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	526/711 (74%)	521 (99%)	5 (1%)	76	89
1	C	525/711 (74%)	516 (98%)	9 (2%)	60	82
2	B	168/216 (78%)	164 (98%)	4 (2%)	49	75
2	D	168/216 (78%)	165 (98%)	3 (2%)	59	81
All	All	1387/1854 (75%)	1366 (98%)	21 (2%)	65	84

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	385	TYR
1	C	602	SER
2	D	500	THR
2	D	377	PHE
1	C	597	ASP

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

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](#)

9 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	E	1	1,3	14,14,15	0.28	0	17,19,21	0.45	0
3	NAG	E	2	3	14,14,15	0.31	0	17,19,21	0.59	0
4	NAG	F	1	1,4	14,14,15	0.18	0	17,19,21	0.49	0
4	NAG	F	2	4	14,14,15	0.28	0	17,19,21	0.52	0
4	BMA	F	3	4	11,11,12	0.66	0	15,15,17	0.75	0
3	NAG	G	1	1,3	14,14,15	0.22	0	17,19,21	0.71	0
3	NAG	G	2	3	14,14,15	0.29	0	17,19,21	0.45	0
3	NAG	H	1	1,3	14,14,15	0.15	0	17,19,21	0.51	0
3	NAG	H	2	3	14,14,15	0.24	0	17,19,21	0.45	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	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

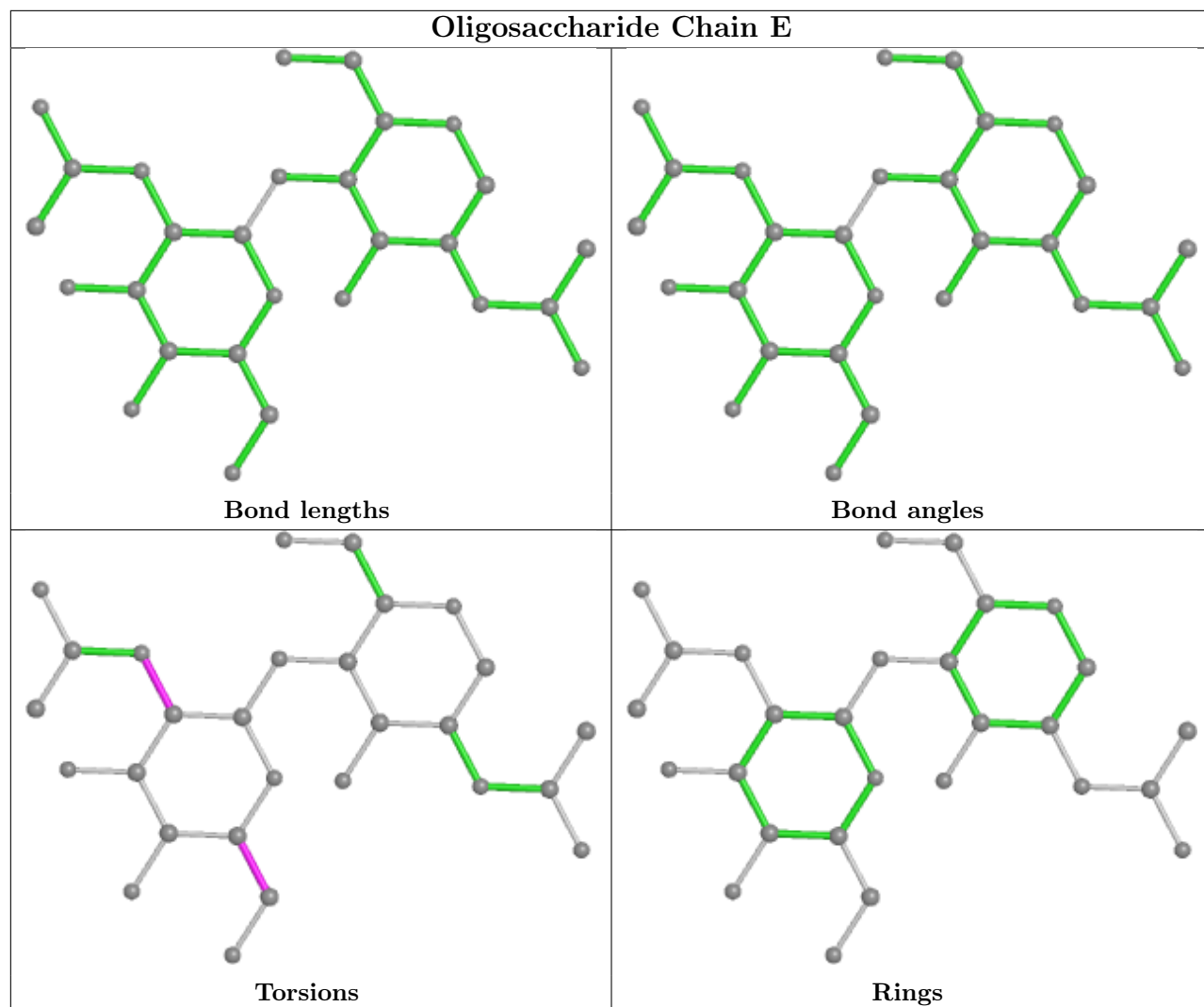
Mol	Chain	Res	Type	Atoms
4	F	3	BMA	O5-C5-C6-O6
4	F	3	BMA	C4-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6

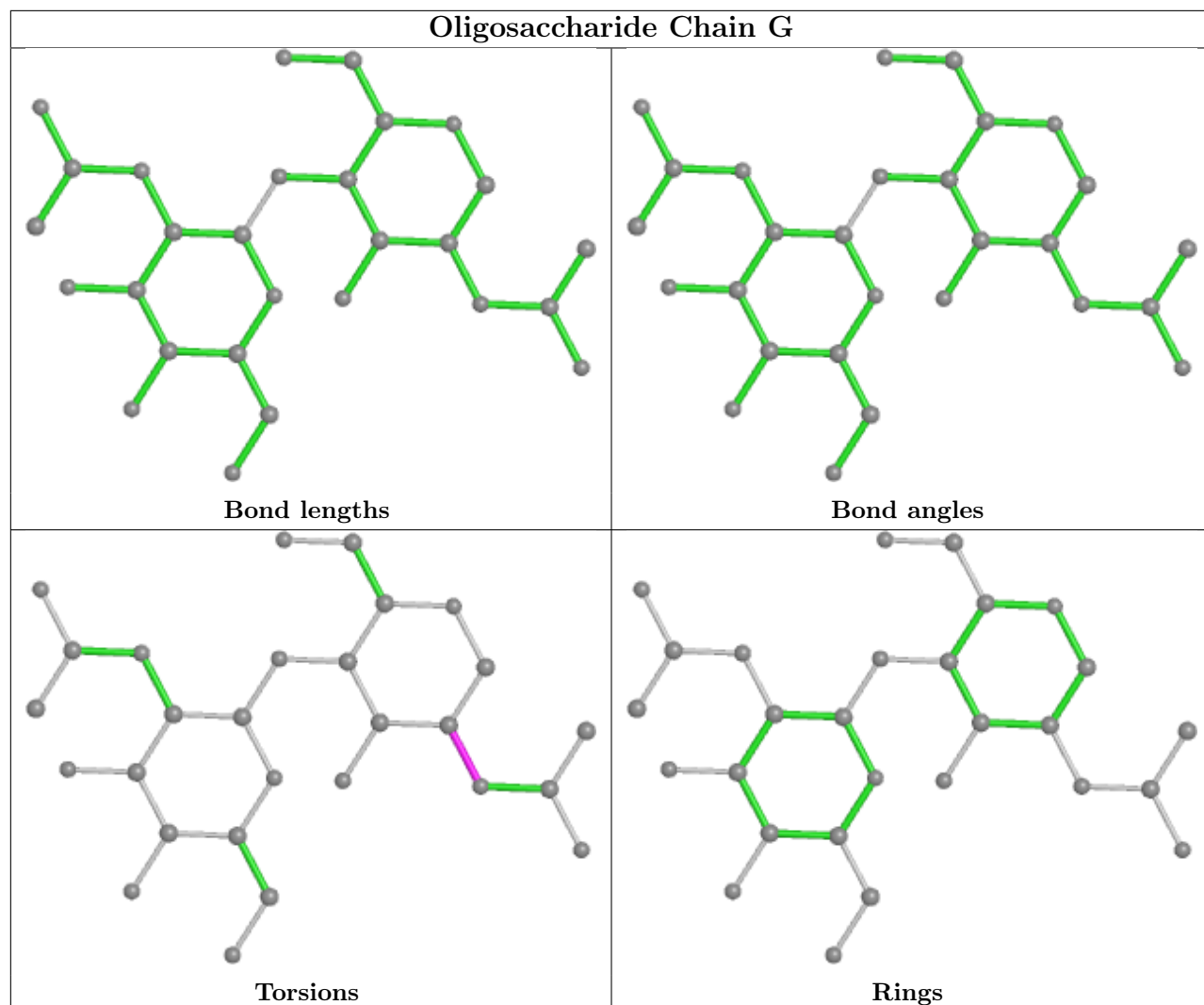
There are no ring outliers.

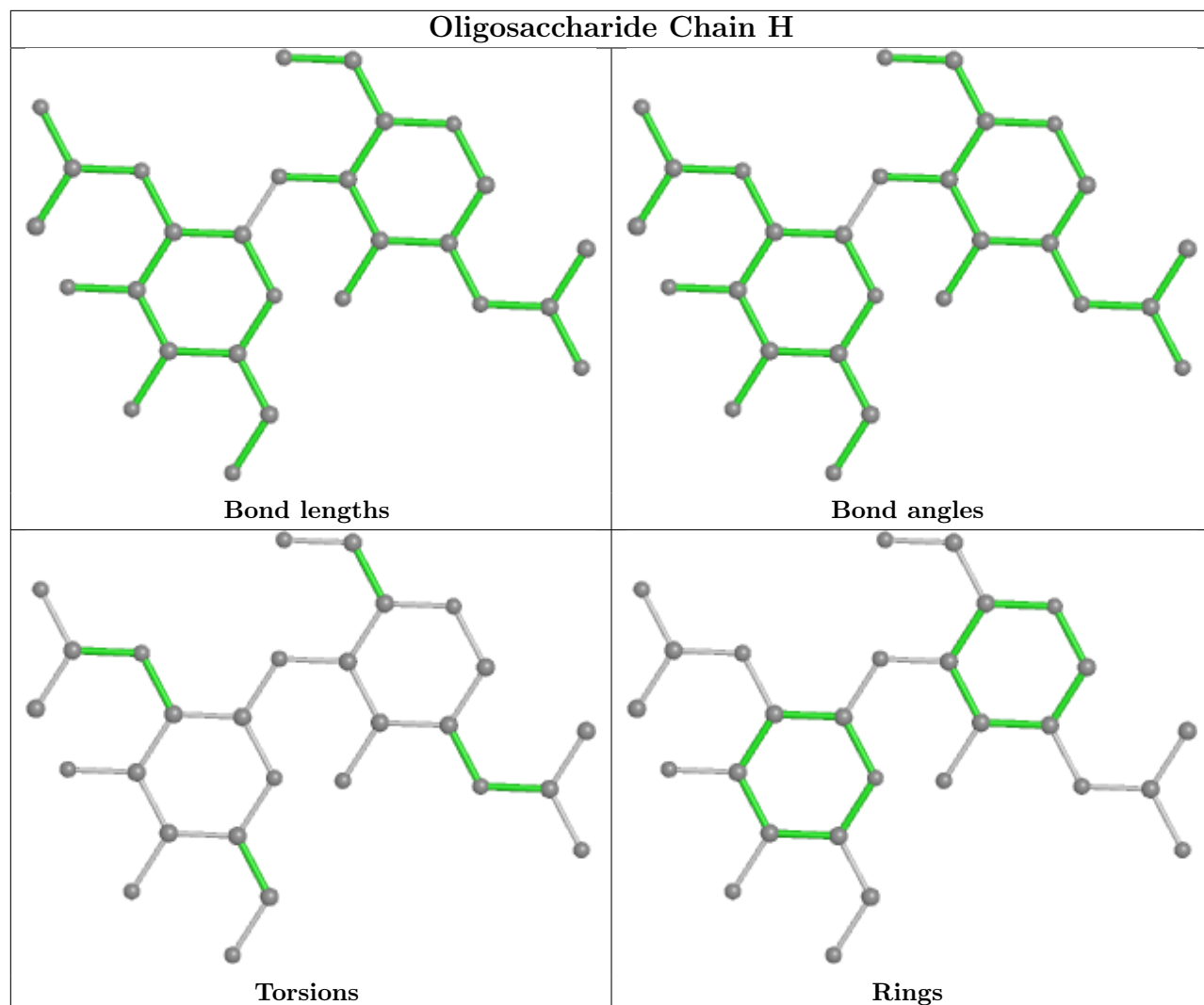
3 monomers are involved in 2 short contacts:

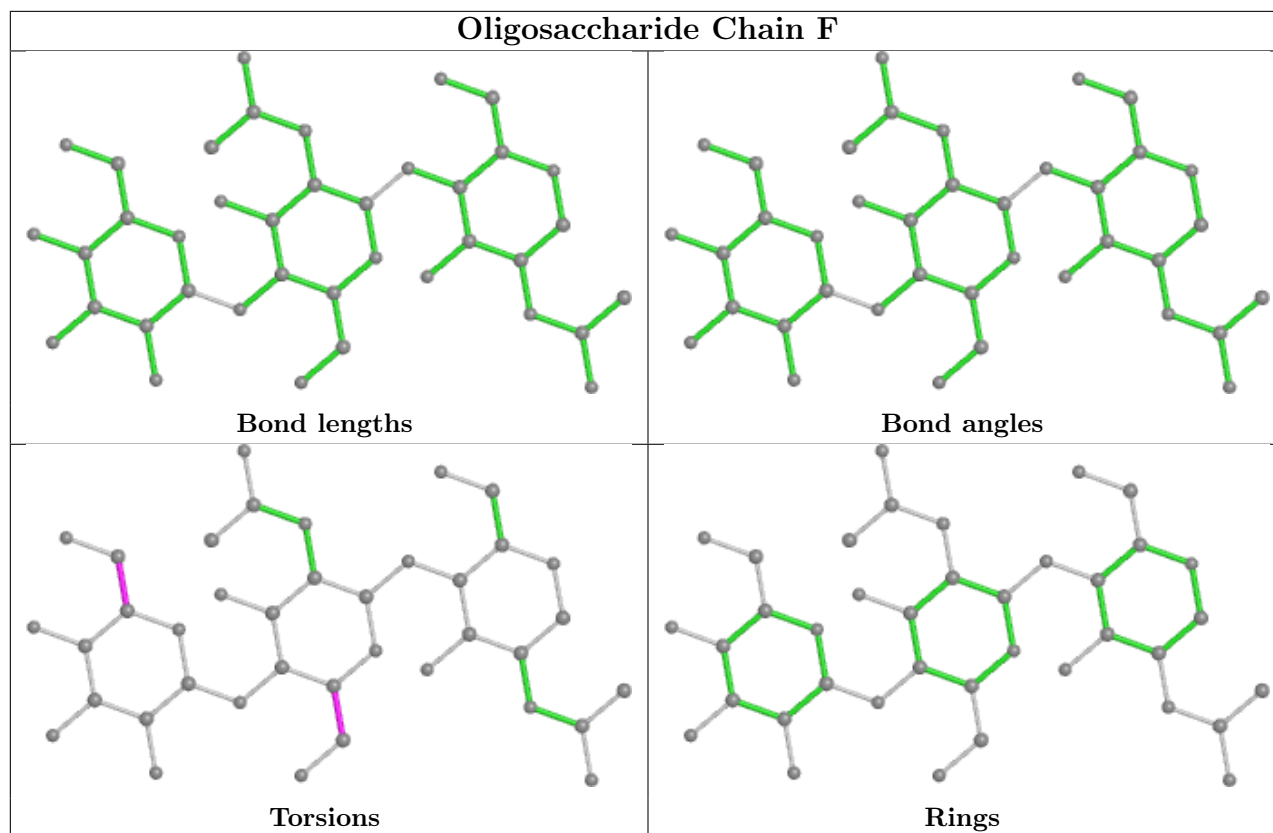
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2	NAG	1	0
3	G	1	NAG	1	0
3	H	1	NAG	1	0

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](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	$\# Z > 2$
6	NAG	A	902	1	14,14,15	0.33	0	17,19,21	0.45	0
6	NAG	C	903	1	14,14,15	0.71	1 (7%)	17,19,21	0.59	0
6	NAG	A	903	1	14,14,15	0.20	0	17,19,21	0.44	0
6	NAG	C	904	1	14,14,15	0.28	0	17,19,21	1.28	1 (5%)
6	NAG	A	904	1	14,14,15	0.33	0	17,19,21	0.44	0
6	NAG	C	902	1	14,14,15	0.58	0	17,19,21	0.54	0
6	NAG	B	601	2	14,14,15	0.15	0	17,19,21	0.34	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
6	NAG	A	902	1	-	2/6/23/26	0/1/1/1
6	NAG	C	903	1	-	2/6/23/26	0/1/1/1
6	NAG	A	903	1	-	3/6/23/26	0/1/1/1
6	NAG	C	904	1	-	5/6/23/26	0/1/1/1
6	NAG	A	904	1	-	0/6/23/26	0/1/1/1
6	NAG	C	902	1	-	2/6/23/26	0/1/1/1
6	NAG	B	601	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	903	NAG	C1-C2	2.40	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	904	NAG	C2-N2-C7	4.39	129.16	122.90

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	902	NAG	O5-C5-C6-O6
6	A	902	NAG	C4-C5-C6-O6
6	C	902	NAG	C1-C2-N2-C7
6	A	903	NAG	C4-C5-C6-O6
6	B	601	NAG	C8-C7-N2-C2

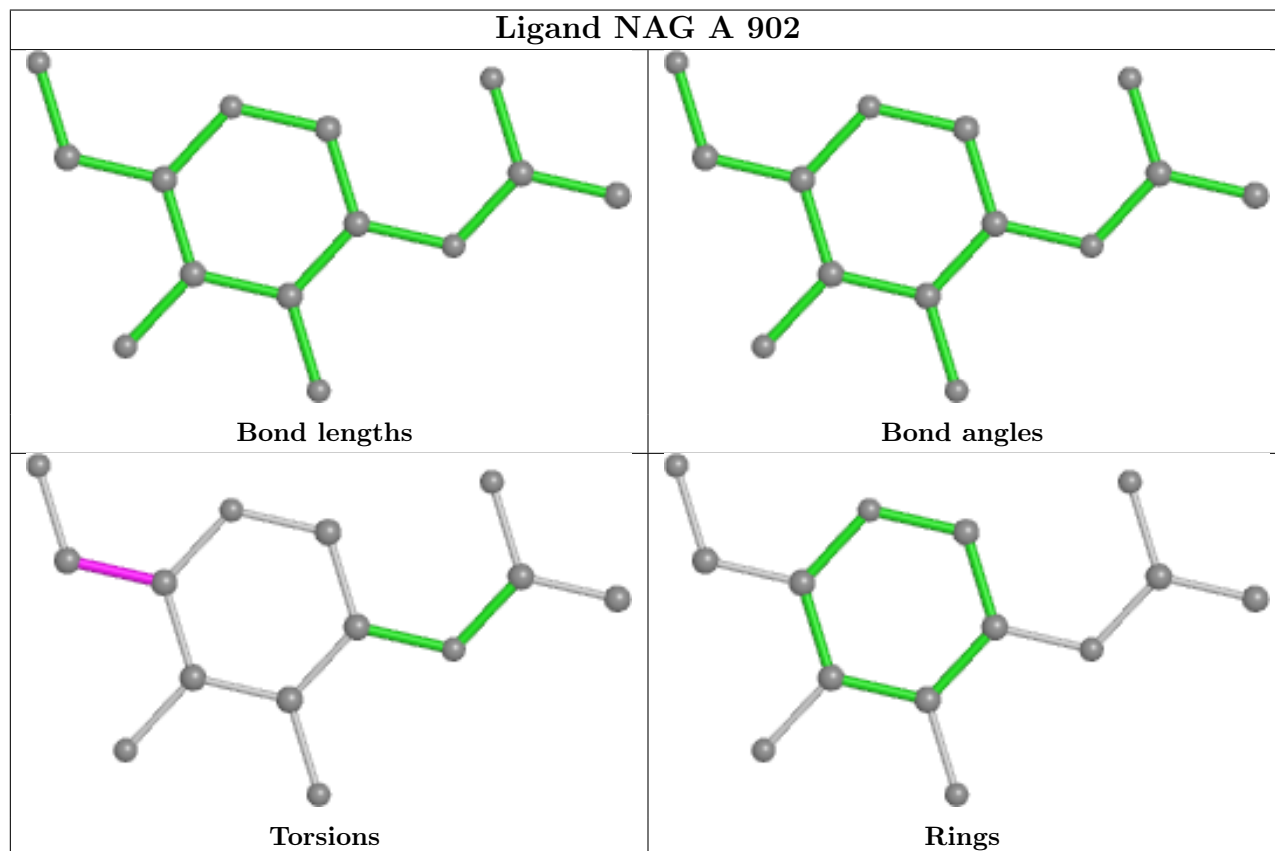
There are no ring outliers.

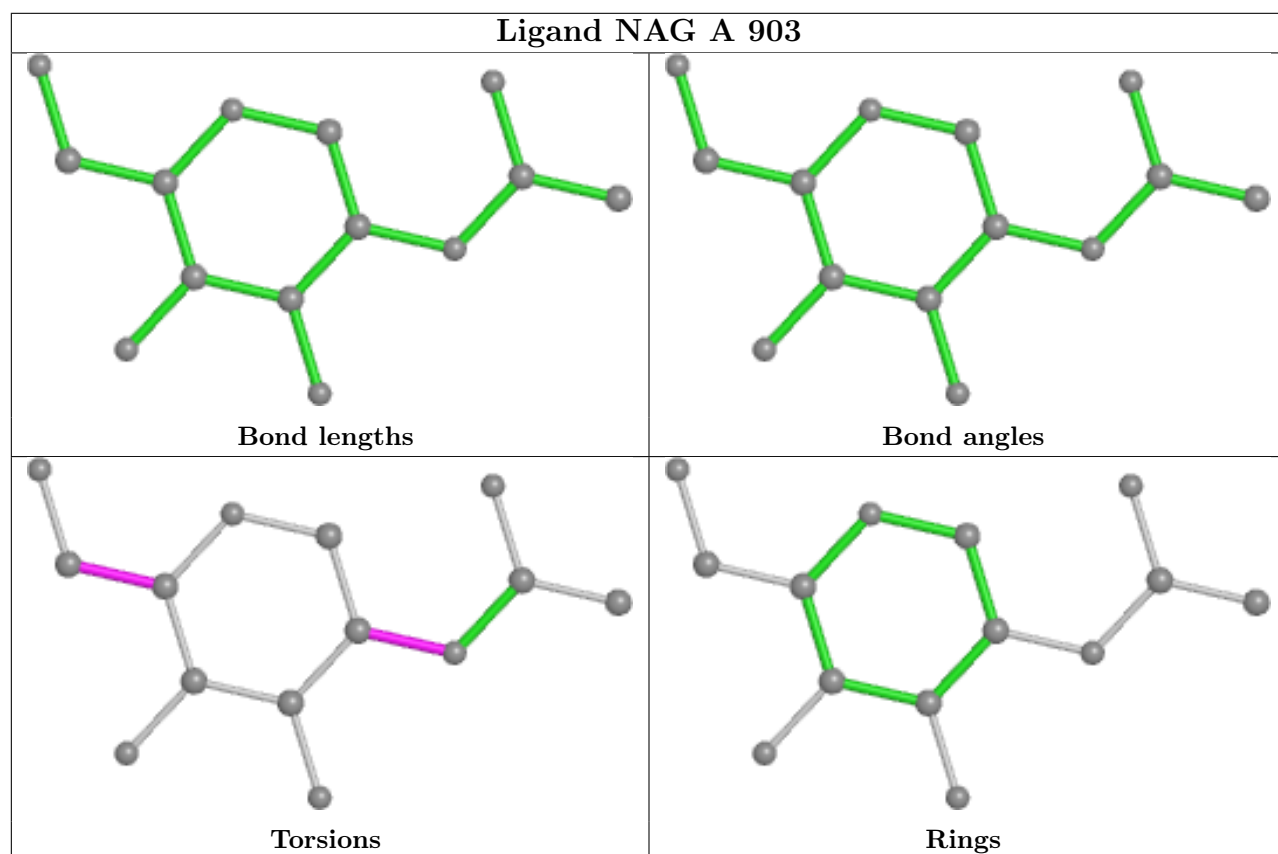
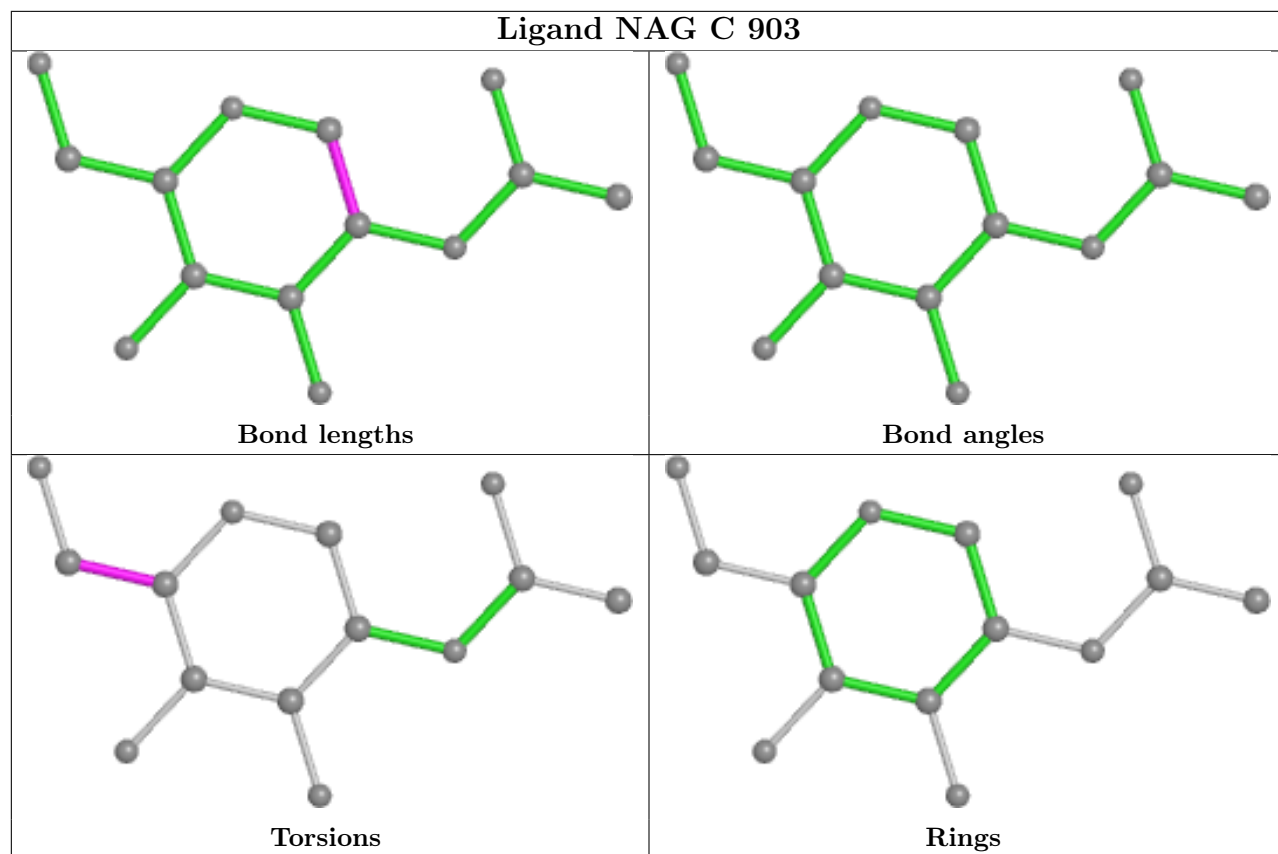
2 monomers are involved in 2 short contacts:

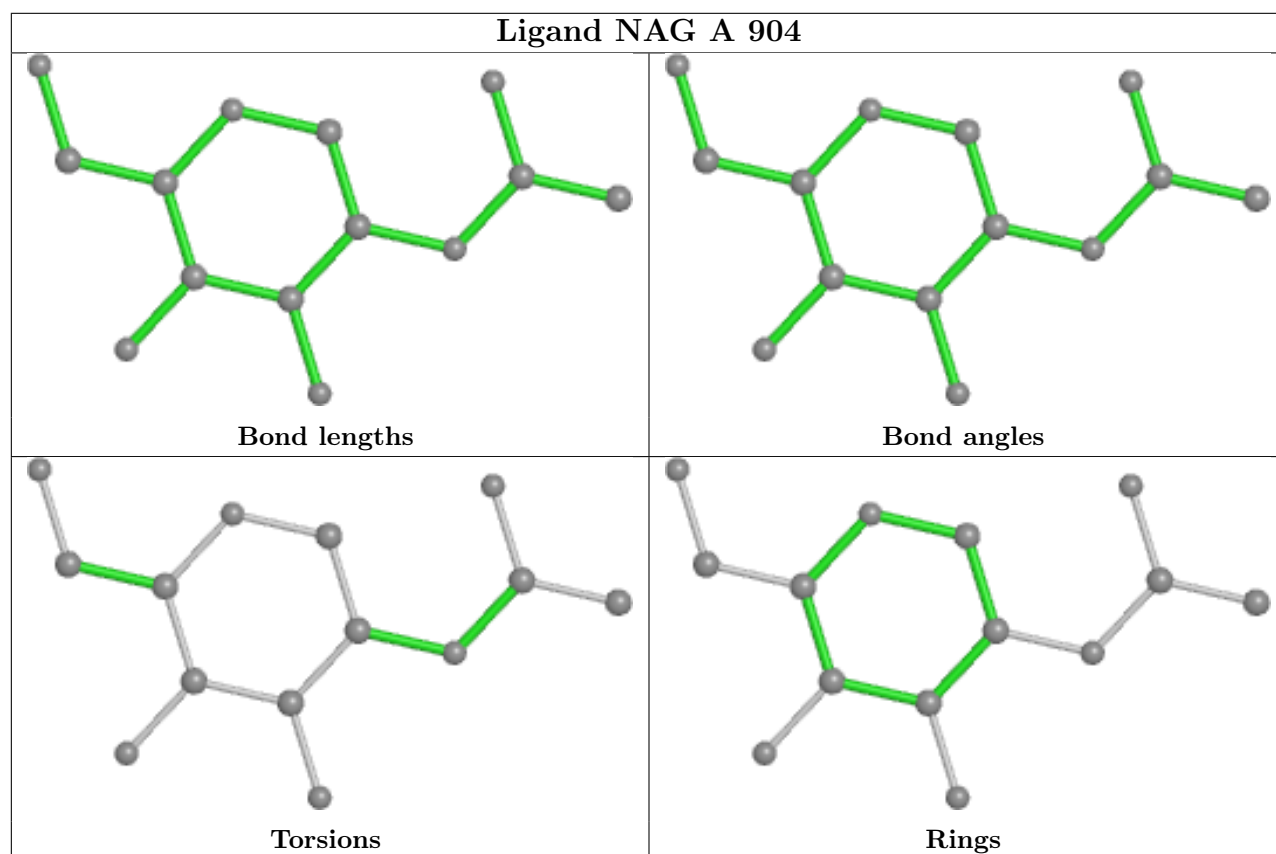
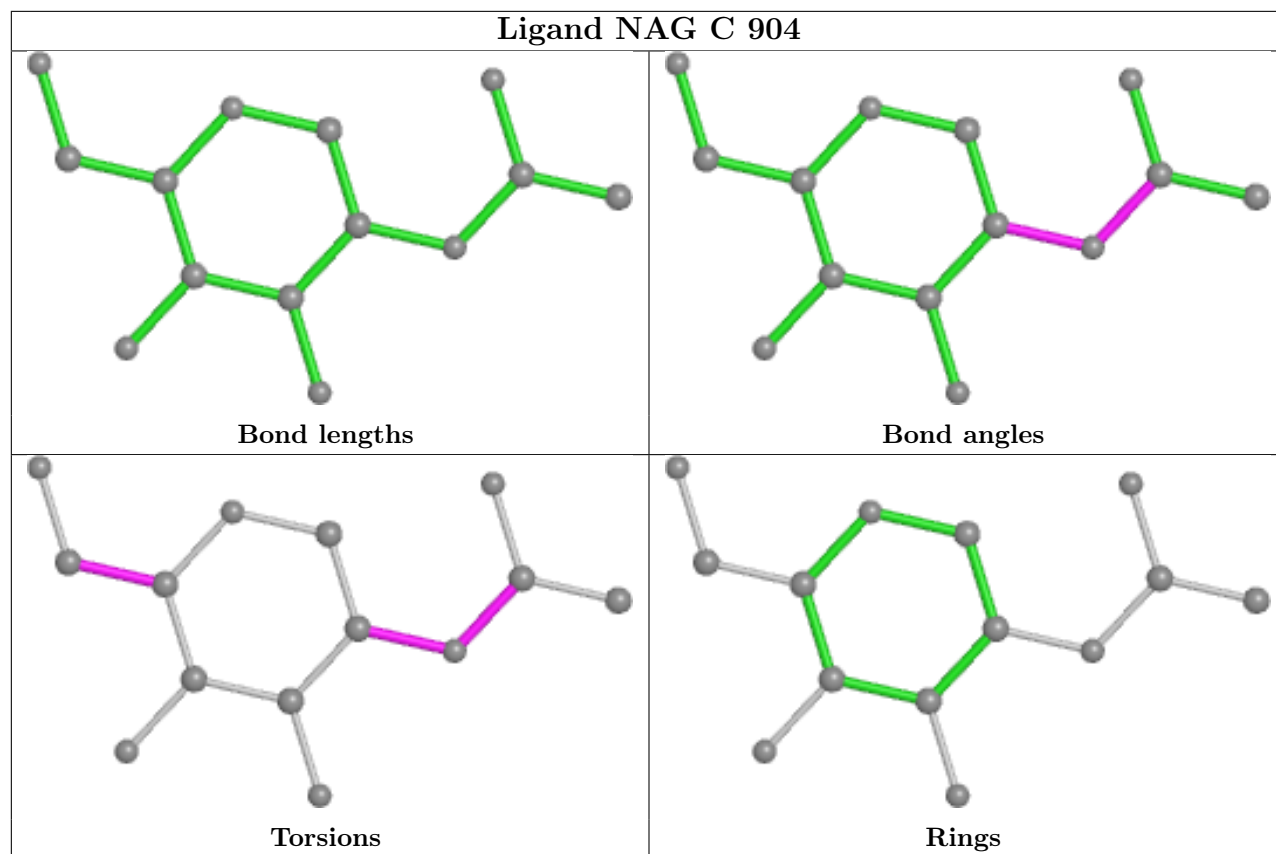
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	904	NAG	1	0
6	C	902	NAG	1	0

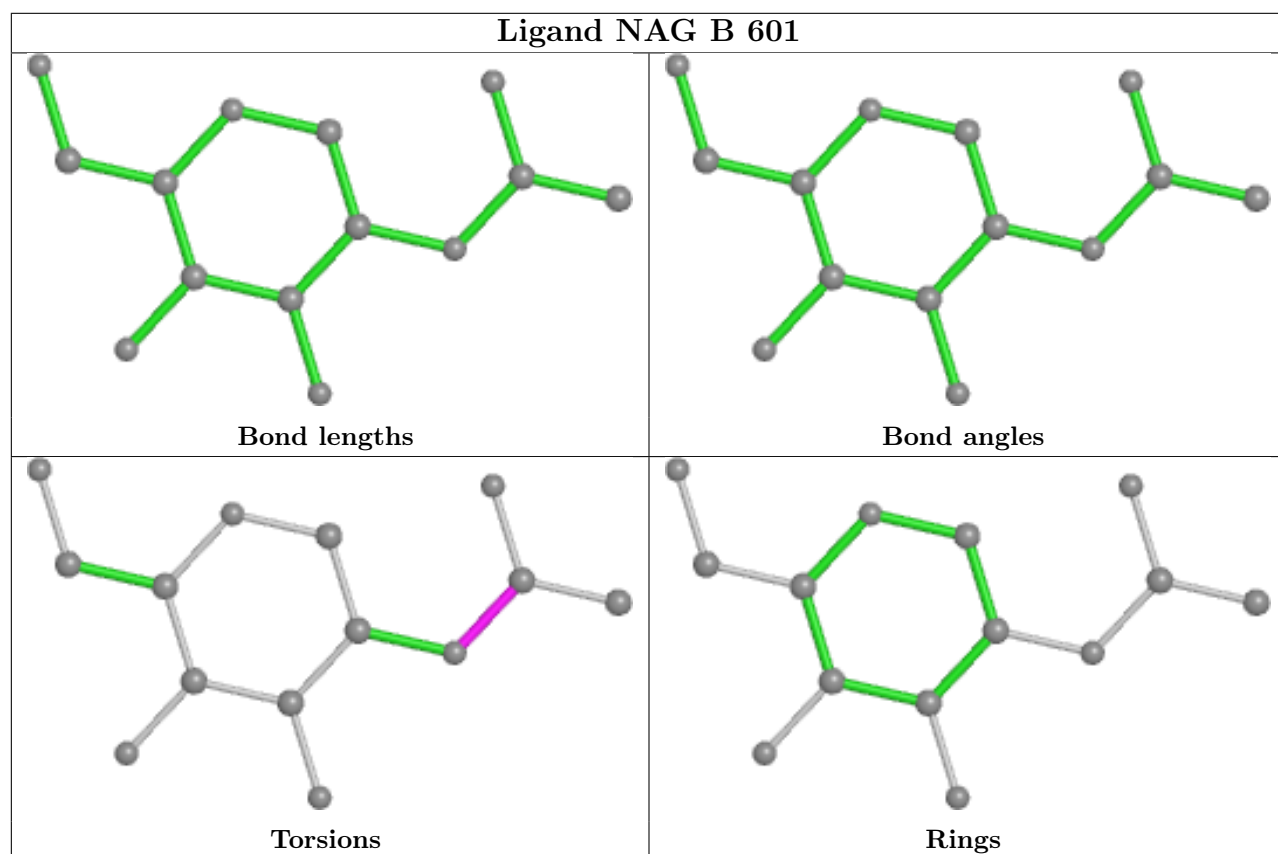
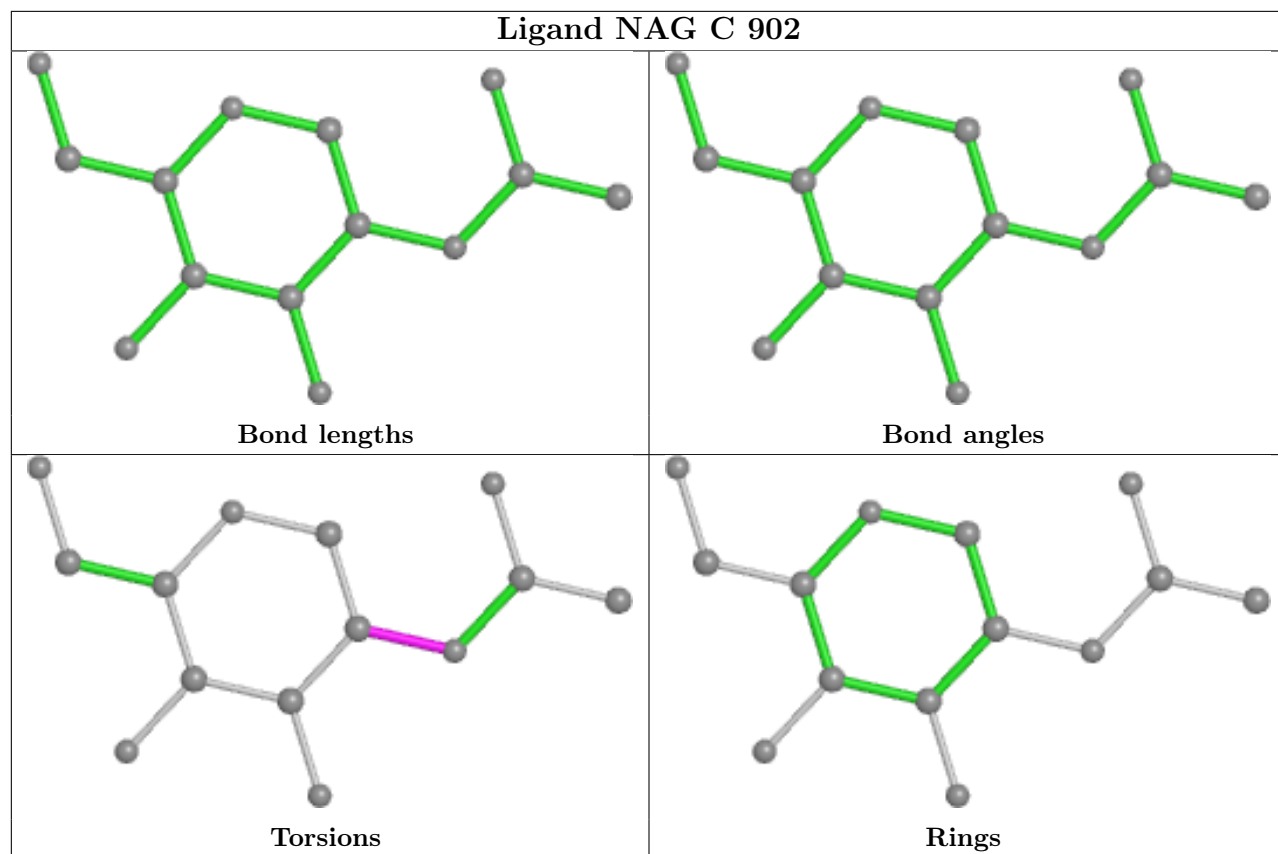
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	596/805 (74%)	-0.19	5 (0%) 86 82	46, 78, 133, 196	0
1	C	596/805 (74%)	-0.11	20 (3%) 45 42	45, 82, 143, 270	0
2	B	195/247 (78%)	0.36	18 (9%) 9 10	54, 99, 212, 280	0
2	D	195/247 (78%)	0.41	22 (11%) 5 6	57, 96, 212, 267	0
All	All	1582/2104 (75%)	-0.02	65 (4%) 37 35	45, 83, 175, 280	0

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	373	PRO	11.7
2	B	373	PRO	7.4
1	C	136	ASP	6.9
1	C	134	ASN	5.9
2	D	371	PHE	5.8

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.

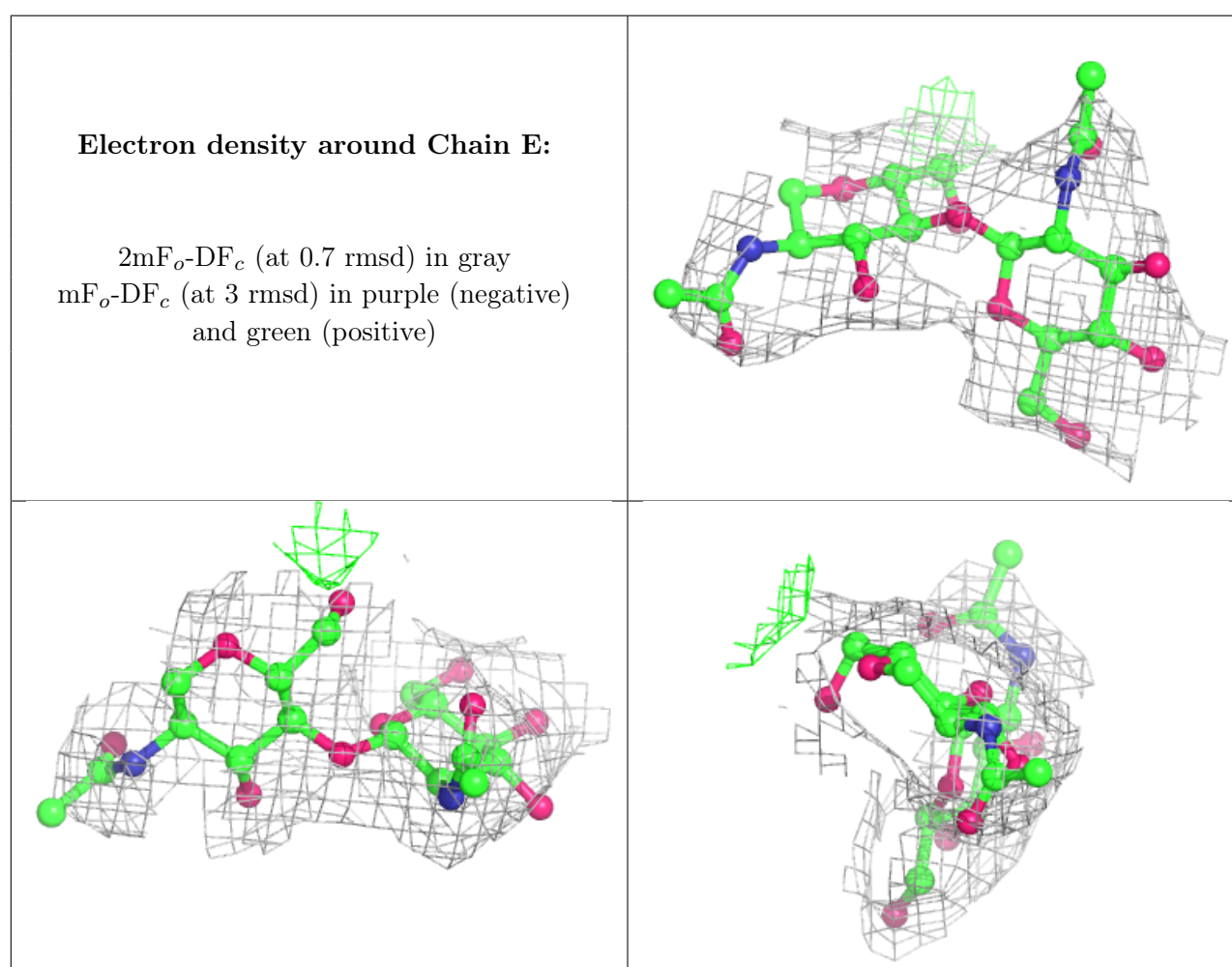
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	F	3	11/12	0.62	0.39	133,159,169,170	0
3	NAG	H	2	14/15	0.72	0.30	131,157,165,165	0

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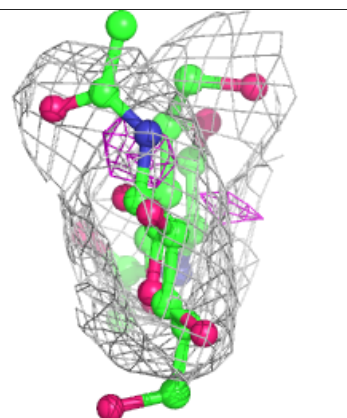
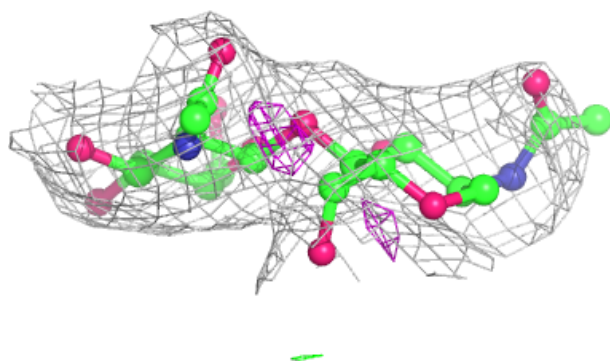
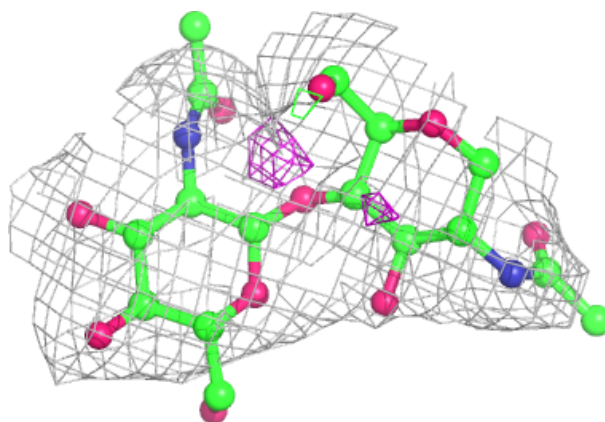
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	G	1	14/15	0.85	0.31	77,94,102,105	0
4	NAG	F	2	14/15	0.87	0.45	137,146,159,163	0
3	NAG	G	2	14/15	0.88	0.43	100,118,128,128	0
4	NAG	F	1	14/15	0.89	0.21	83,104,121,124	0
3	NAG	E	2	14/15	0.90	0.33	104,118,131,131	0
3	NAG	H	1	14/15	0.91	0.24	117,128,142,146	0
3	NAG	E	1	14/15	0.93	0.18	74,80,87,93	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.



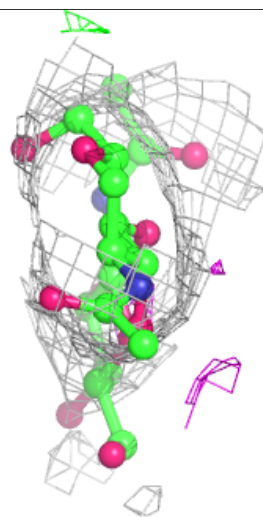
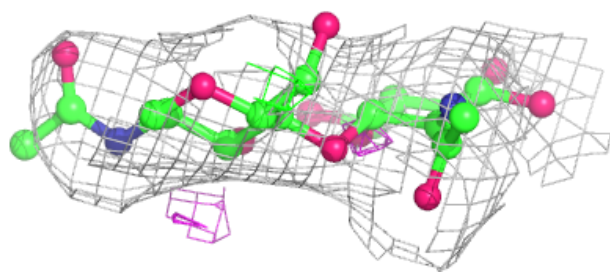
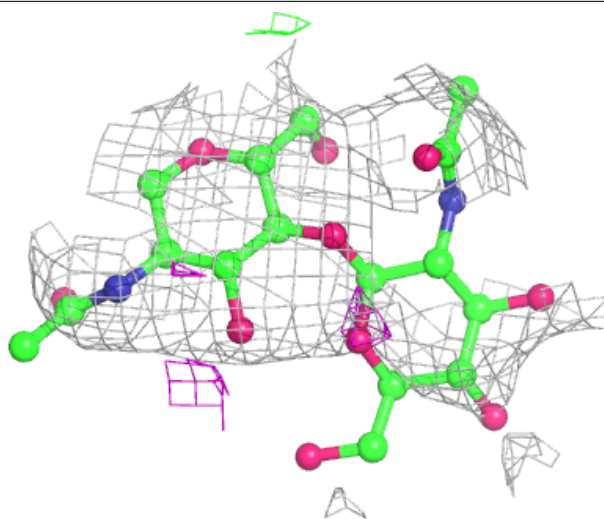
Electron density around Chain G:

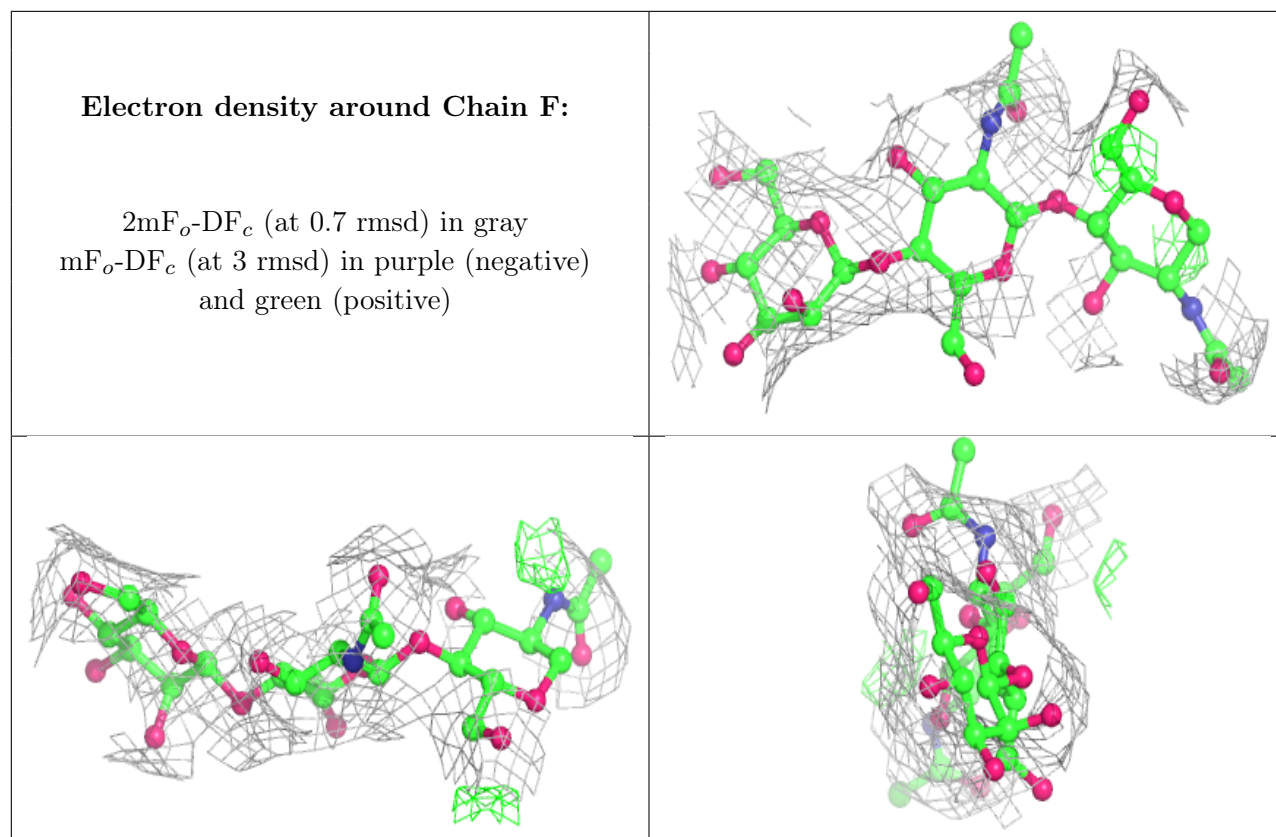
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

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





6.4 Ligands [i](#)

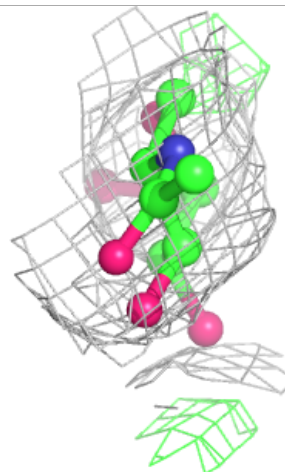
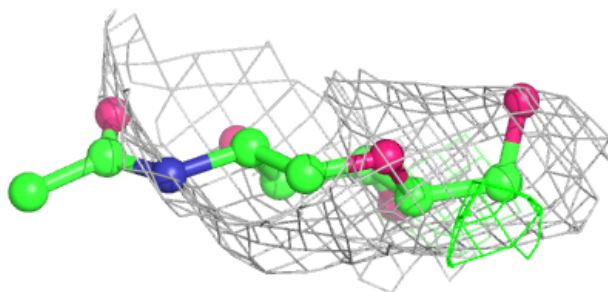
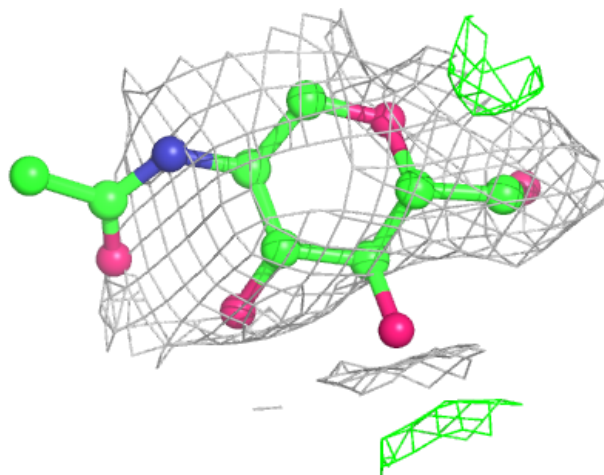
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists 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	NAG	C	902	14/15	0.58	0.36	153,177,186,189	0
6	NAG	C	904	14/15	0.66	0.38	117,132,141,150	0
6	NAG	A	903	14/15	0.68	0.48	166,184,193,205	0
6	NAG	A	904	14/15	0.69	0.32	135,158,174,178	0
6	NAG	B	601	14/15	0.71	0.42	139,159,166,167	0
6	NAG	C	903	14/15	0.72	0.31	102,123,134,139	0
6	NAG	A	902	14/15	0.83	0.20	113,123,131,144	0
5	ZN	A	901	1/1	0.97	0.09	74,74,74,74	0
5	ZN	C	901	1/1	0.98	0.12	58,58,58,58	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.

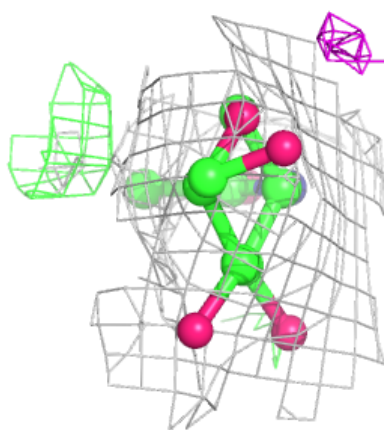
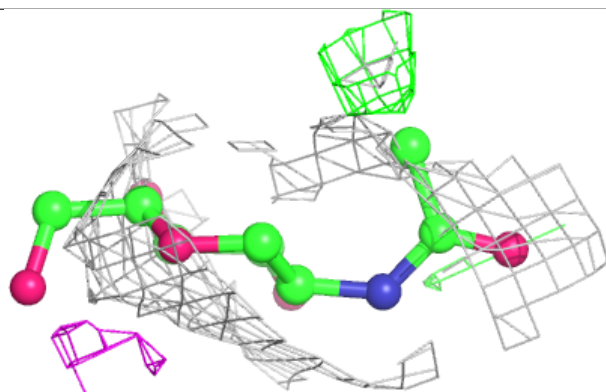
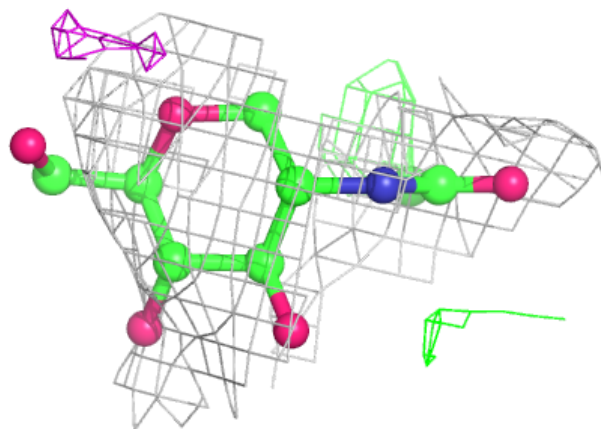
Electron density around NAG C 902:

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



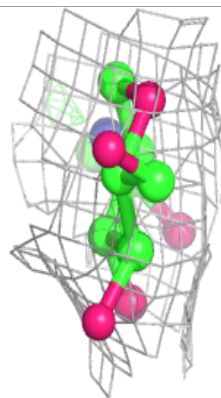
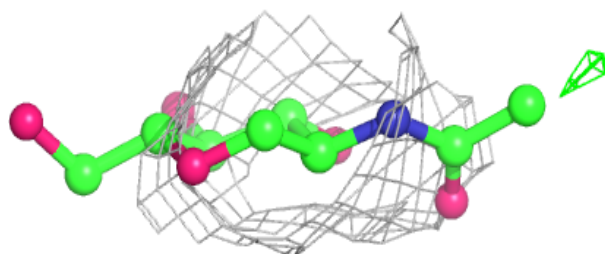
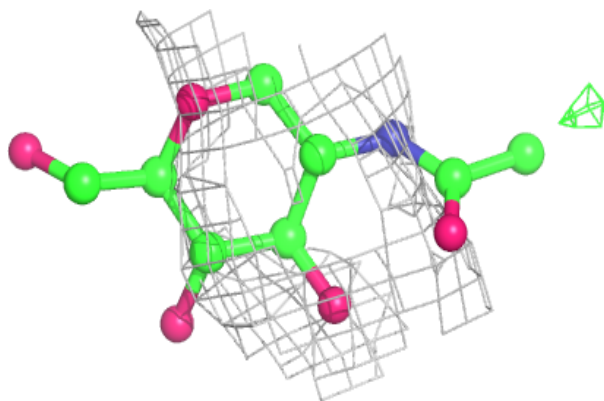
Electron density around NAG C 904:

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

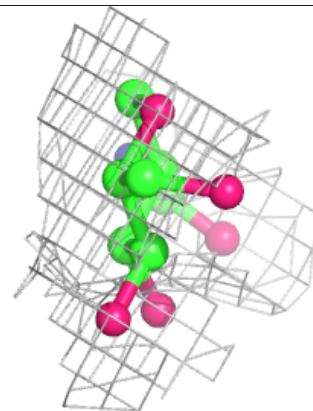
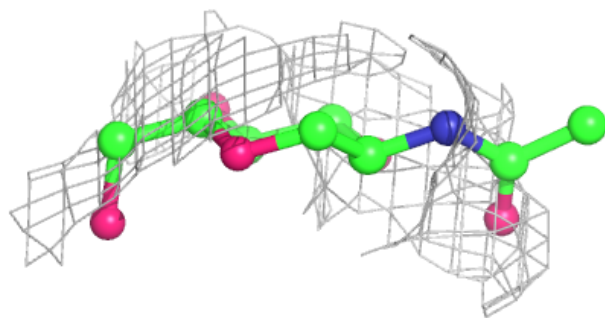
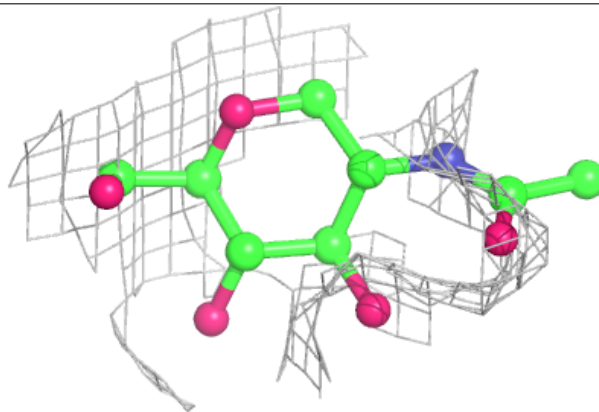


Electron density around NAG A 903:

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

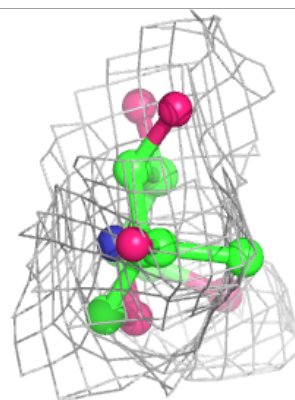
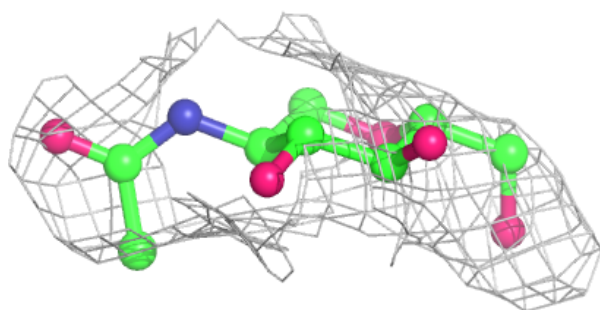
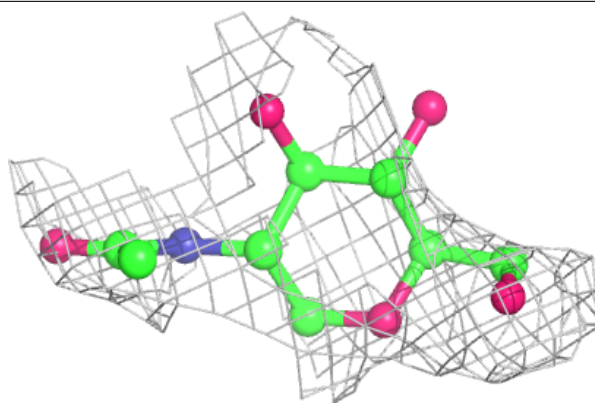
**Electron density around NAG A 904:**

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

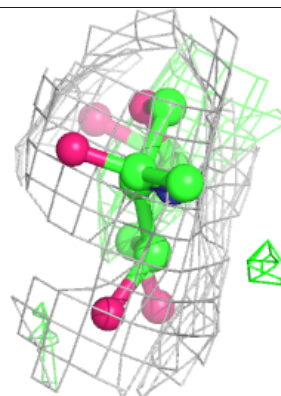
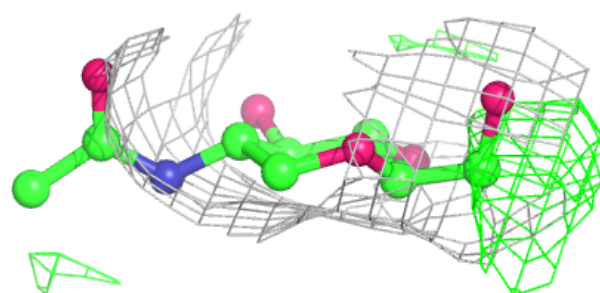
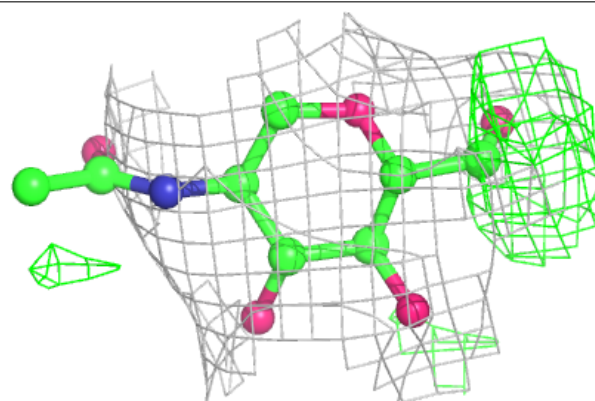


Electron density around NAG B 601:

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

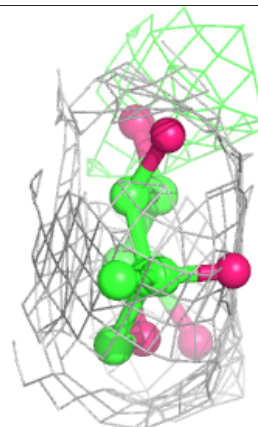
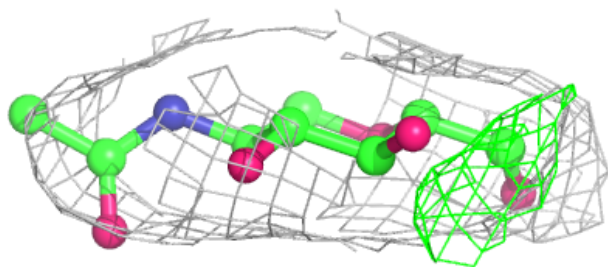
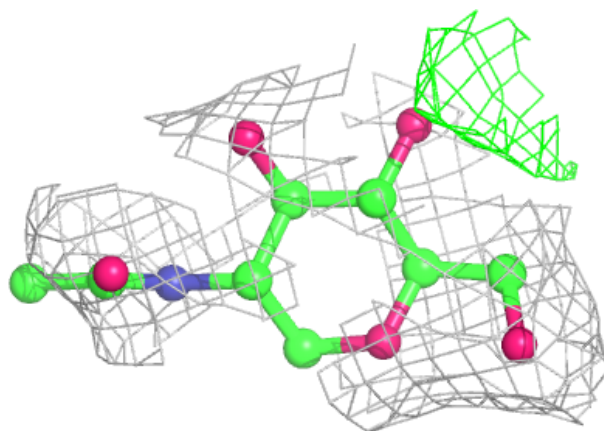
**Electron density around NAG C 903:**

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



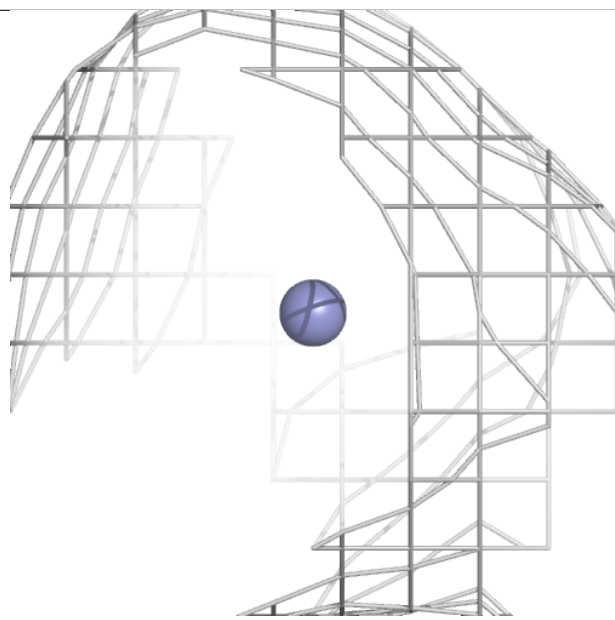
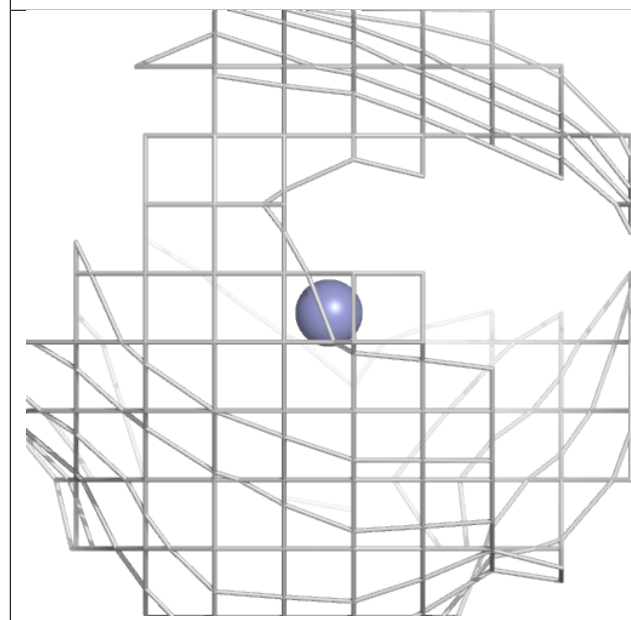
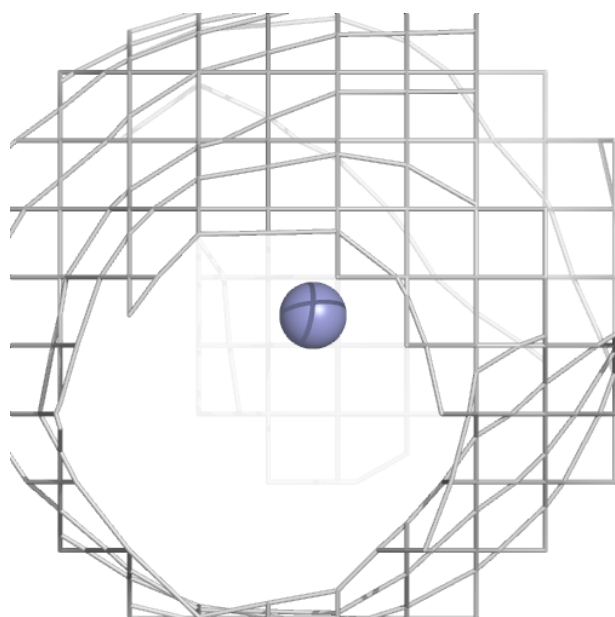
Electron density around NAG A 902:

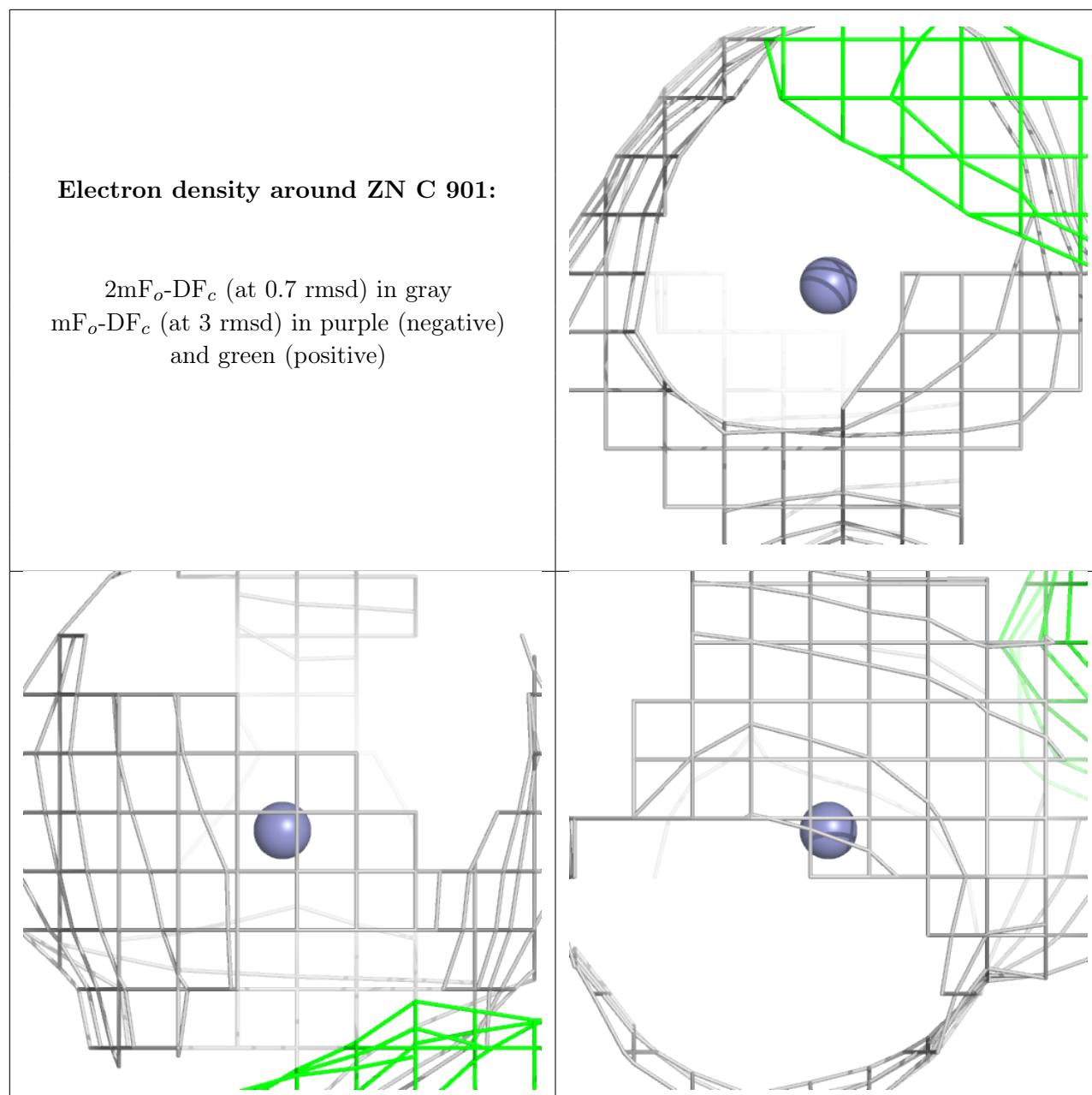
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN A 901:

$2mF_o-DF_c$ (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.