



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 07:52 AM EDT

PDB ID : 5W2U  
Title : INFLUENZA VIRUS NEURAMINIDASE N9 IN COMPLEX WITH 7-DEOXYGENATED 2,3-DIFLUORO-N-ACETYLNEURAMINIC ACID  
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Deposited on : 2017-06-06  
Resolution : 2.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

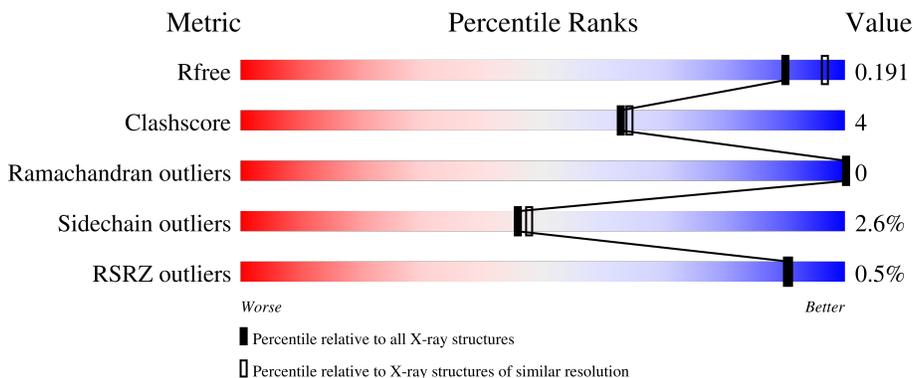
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	388	
2	B	8	
3	C	2	

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	NAG	C	2	-	-	-	X

## 2 Entry composition [i](#)

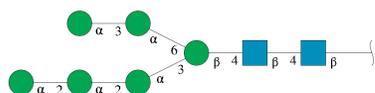
There are 9 unique types of molecules in this entry. The entry contains 3715 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	3094	1928	548	595	23	0	9	0

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



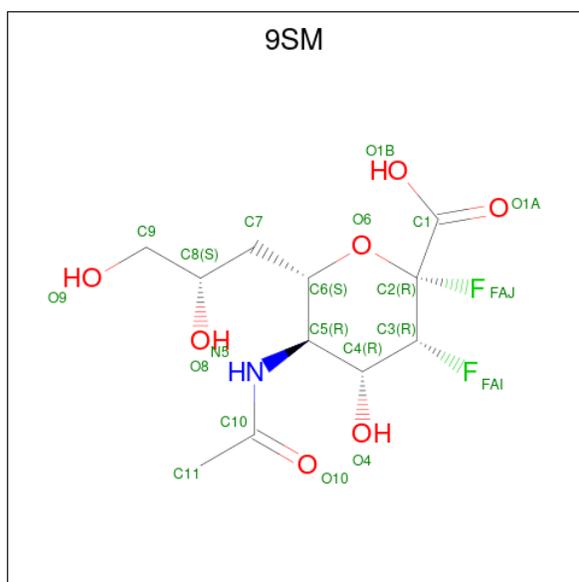
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	8	94	52	2	40	0	0	0

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



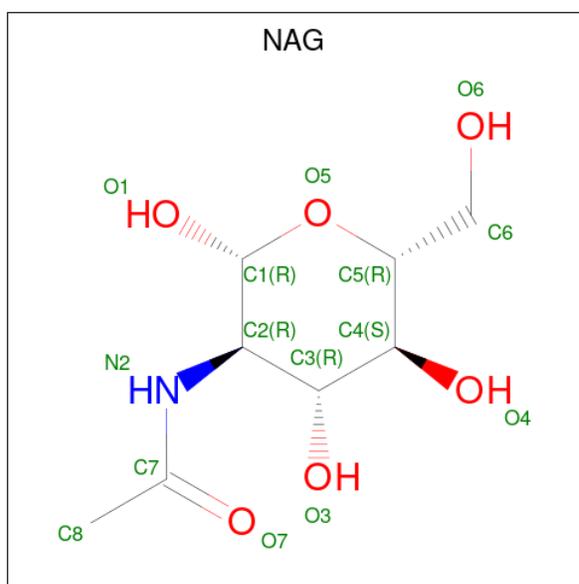
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	2	28	16	2	10	0	0	0

- Molecule 4 is (2R,3R,4R,5R,6S)-5-acetamido-6-[(2S)-2,3-bis(oxidanyl)propyl]-2,3-bis(fluoranyl)-4-oxidanyl-oxane-2-carboxylic acid (three-letter code: 9SM) (formula: C<sub>11</sub>H<sub>17</sub>F<sub>2</sub>NO<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	F	N			O
4	A	1	21	11	2	1	7	0	0

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

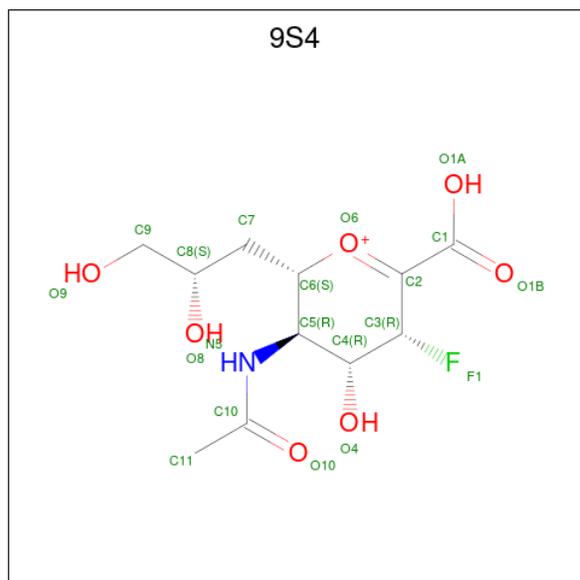


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

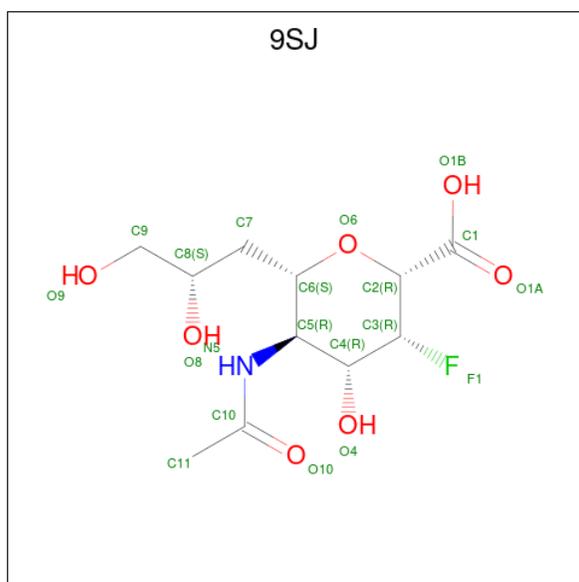
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		

- Molecule 7 is (2 {S},3 {R},4 {R},5 {R})-3-acetamido-2-[(2 {S})-2,3-bis(oxidanyl)propyl]-5-fluoranyl-4-oxidanyl-2,3,4,5-tetrahydropyran-1-ium-6-carboxylic acid (three-letter code: 9S4) (formula: C<sub>11</sub>H<sub>17</sub>FNO<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
7	A	1	Total	C	F	N	O	0	1
			20	11	1	1	7		

- Molecule 8 is 5-acetamido-2,6-anhydro-3,5,7-trideoxy-3-fluoro-D-threo-L-galacto-nononic acid (three-letter code: 9SJ) (formula: C<sub>11</sub>H<sub>18</sub>FNO<sub>7</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
8	A	1	20	11	1	1	7	0	1

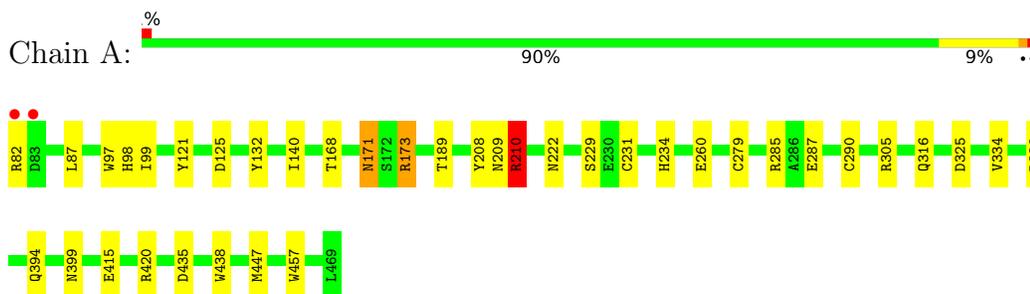
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	423	Total	O	0	0
			423	423		

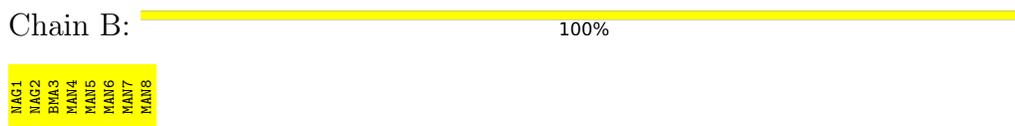
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

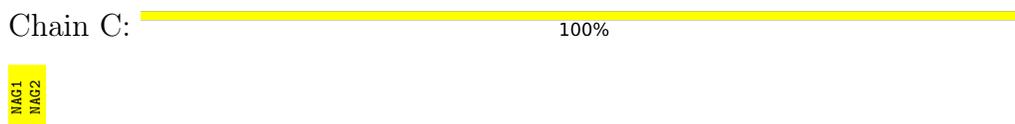
- Molecule 1: Neuraminidase



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.03Å 181.03Å 181.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.38 – 2.00 45.26 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.38-2.00) 99.6 (45.26-2.00)	Depositor EDS
$R_{merge}$	0.31	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.142 , 0.187 0.144 , 0.191	Depositor DCC
$R_{free}$ test set	1723 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 61.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3715	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 9SJ, 9S4, CA, 9SM, NAG, MAN, 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	1.09	3/3226 (0.1%)	0.96	10/4391 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	372	SER	CB-OG	-6.34	1.34	1.42
1	A	132	TYR	CE1-CZ	5.37	1.45	1.38
1	A	316	GLN	CD-NE2	5.06	1.45	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	ARG	NE-CZ-NH1	8.13	124.37	120.30
1	A	447[A]	MET	CG-SD-CE	7.62	112.40	100.20
1	A	447[B]	MET	CG-SD-CE	7.62	112.40	100.20
1	A	173	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	125	ASP	CB-CG-OD1	6.69	124.32	118.30
1	A	210	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	A	435	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	210	ARG	NE-CZ-NH2	5.41	123.01	120.30
1	A	339	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	325	ASP	CB-CG-OD1	5.34	123.11	118.30

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	3094	0	2925	27	1
2	B	94	0	79	0	0
3	C	28	0	25	0	0
4	A	21	0	0	0	0
5	A	14	0	13	1	0
6	A	1	0	0	0	0
7	A	20	0	0	0	0
8	A	20	0	0	0	0
9	A	423	0	0	4	7
All	All	3715	0	3042	27	7

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

All (27) 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:87:LEU:H	1:A:234:HIS:HD2	1.14	0.95
1:A:168:THR:H	1:A:171:ASN:HD21	1.14	0.88
1:A:173:ARG:HD3	1:A:210:ARG:NH1	1.92	0.84
1:A:87:LEU:H	1:A:234:HIS:CD2	2.03	0.76
1:A:285[B]:ARG:HD2	9:A:602:HOH:O	1.91	0.70
1:A:372:SER:HB2	1:A:399:ASN:ND2	2.07	0.69
1:A:140[B]:ILE:HD11	9:A:681:HOH:O	1.94	0.67
1:A:98:HIS:HE1	1:A:420:ARG:HH11	1.45	0.63
1:A:168:THR:H	1:A:171:ASN:ND2	1.94	0.62
1:A:168:THR:OG1	1:A:171:ASN:ND2	2.33	0.61
1:A:173:ARG:CD	1:A:210:ARG:NH1	2.64	0.60
1:A:97:TRP:H	1:A:394:GLN:HE22	1.50	0.60
1:A:168:THR:N	1:A:171:ASN:HD21	1.95	0.59
1:A:98:HIS:CE1	1:A:420:ARG:HH11	2.22	0.57
1:A:98:HIS:HD2	1:A:99:ILE:O	1.87	0.57
1:A:285[B]:ARG:NH2	9:A:601:HOH:O	2.16	0.55
1:A:285[B]:ARG:NH1	9:A:602:HOH:O	2.18	0.54
1:A:173:ARG:HD3	1:A:210:ARG:CZ	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:SER:HB2	1:A:399:ASN:HD21	1.74	0.52
1:A:171:ASN:HD22	1:A:171:ASN:H	1.57	0.51
1:A:279:CYS:HB3	1:A:290:CYS:HB3	1.95	0.48
1:A:121:TYR:CG	1:A:229:SER:HA	2.49	0.47
1:A:229:SER:HB3	1:A:350:LYS:HE2	1.96	0.46
1:A:287:GLU:OE2	1:A:305[B]:ARG:HD3	2.20	0.42
1:A:189:THR:HG21	1:A:209:ASN:HB2	2.01	0.42
1:A:438:TRP:CD1	5:A:512:NAG:H82	2.56	0.41
1:A:208:TYR:CZ	1:A:260:GLU:HA	2.56	0.41

All (7) 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)
9:A:650:HOH:O	9:A:982:HOH:O[15_555]	1.89	0.31
9:A:632:HOH:O	9:A:995:HOH:O[15_555]	1.92	0.28
9:A:953:HOH:O	9:A:964:HOH:O[9_555]	1.92	0.28
9:A:723:HOH:O	9:A:982:HOH:O[15_555]	1.97	0.23
9:A:993:HOH:O	9:A:995:HOH:O[15_555]	1.97	0.23
9:A:640:HOH:O	9:A:959:HOH:O[15_555]	2.06	0.14
1:A:171:ASN:CB	9:A:837:HOH:O[16_555]	2.14	0.06

## 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	394/388 (102%)	379 (96%)	15 (4%)	0	<b>100</b> <b>100</b>

There are no Ramachandran outliers to report.

### 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	350/341 (103%)	340 (97%)	10 (3%)	42 43

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82[A]	ARG
1	A	82[B]	ARG
1	A	171	ASN
1	A	210	ARG
1	A	222	ASN
1	A	231	CYS
1	A	334	VAL
1	A	372	SER
1	A	415	GLU
1	A	457	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	98	HIS
1	A	171	ASN
1	A	222	ASN
1	A	234	HIS
1	A	345	ASN
1	A	346	ASN
1	A	392	GLN
1	A	394	GLN
1	A	399	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

10 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	B	1	2,1	14,14,15	0.81	0	17,19,21	2.23	6 (35%)
2	NAG	B	2	2	14,14,15	0.79	1 (7%)	17,19,21	1.81	4 (23%)
2	BMA	B	3	2	11,11,12	0.76	0	15,15,17	1.48	5 (33%)
2	MAN	B	4	2	11,11,12	1.09	1 (9%)	15,15,17	2.40	5 (33%)
2	MAN	B	5	2	11,11,12	0.83	0	15,15,17	1.55	4 (26%)
2	MAN	B	6	2	11,11,12	0.98	0	15,15,17	1.14	1 (6%)
2	MAN	B	7	2	11,11,12	0.66	0	15,15,17	1.82	3 (20%)
2	MAN	B	8	2	11,11,12	1.01	0	15,15,17	2.15	5 (33%)
3	NAG	C	1	3,1	14,14,15	0.80	0	17,19,21	1.34	3 (17%)
3	NAG	C	2	3	14,14,15	1.34	3 (21%)	17,19,21	2.10	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	2/2/19/22	0/1/1/1
2	MAN	B	5	2	-	0/2/19/22	0/1/1/1
2	MAN	B	6	2	-	0/2/19/22	0/1/1/1
2	MAN	B	7	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	B	8	2	-	2/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	C1-C2	2.82	1.56	1.52
2	B	4	MAN	O5-C5	2.44	1.48	1.43
2	B	2	NAG	C1-C2	2.35	1.55	1.52
3	C	2	NAG	C2-N2	2.26	1.50	1.46
3	C	2	NAG	C3-C2	2.05	1.56	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C2-N2-C7	5.50	130.73	122.90
2	B	4	MAN	O2-C2-C1	-5.22	98.48	109.15
2	B	1	NAG	C1-C2-N2	-5.02	101.92	110.49
2	B	8	MAN	O5-C5-C6	4.28	113.91	107.20
2	B	7	MAN	O5-C5-C6	4.13	113.67	107.20
2	B	8	MAN	C1-O5-C5	4.10	117.75	112.19
2	B	4	MAN	C6-C5-C4	-3.99	103.66	113.00
2	B	4	MAN	C1-O5-C5	3.85	117.42	112.19
2	B	7	MAN	C1-O5-C5	3.84	117.40	112.19
2	B	1	NAG	C8-C7-N2	-3.76	109.73	116.10
2	B	4	MAN	O6-C6-C5	-3.76	98.40	111.29
2	B	2	NAG	C6-C5-C4	3.47	121.12	113.00
3	C	2	NAG	O5-C5-C6	3.40	112.53	107.20
2	B	2	NAG	O6-C6-C5	-3.27	100.06	111.29
2	B	8	MAN	C3-C4-C5	-3.21	104.51	110.24
2	B	1	NAG	C3-C4-C5	-3.15	104.62	110.24
2	B	1	NAG	C1-O5-C5	3.11	116.40	112.19
3	C	1	NAG	O6-C6-C5	-3.09	100.68	111.29
3	C	2	NAG	O4-C4-C3	3.05	117.41	110.35
2	B	5	MAN	O5-C5-C4	-3.03	103.45	110.83
2	B	7	MAN	O4-C4-C3	-3.03	103.35	110.35
2	B	2	NAG	C1-C2-N2	2.98	115.58	110.49
3	C	2	NAG	C1-O5-C5	2.71	115.86	112.19
2	B	1	NAG	O4-C4-C3	-2.67	104.17	110.35
2	B	1	NAG	C2-N2-C7	-2.59	119.22	122.90
2	B	2	NAG	C8-C7-N2	2.58	120.46	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	BMA	O5-C5-C4	-2.50	104.75	110.83
2	B	3	BMA	O2-C2-C3	-2.47	105.18	110.14
2	B	5	MAN	C1-C2-C3	-2.40	106.72	109.67
3	C	1	NAG	C8-C7-N2	2.40	120.16	116.10
2	B	5	MAN	O4-C4-C3	-2.39	104.81	110.35
2	B	8	MAN	O2-C2-C3	2.37	114.88	110.14
2	B	3	BMA	O5-C5-C6	2.33	110.85	107.20
2	B	3	BMA	O3-C3-C4	-2.29	105.05	110.35
2	B	5	MAN	O5-C5-C6	2.27	110.77	107.20
2	B	3	BMA	C6-C5-C4	-2.22	107.81	113.00
2	B	8	MAN	O5-C1-C2	-2.20	107.37	110.77
3	C	1	NAG	O5-C5-C6	2.11	110.51	107.20
2	B	4	MAN	O2-C2-C3	2.08	114.30	110.14
2	B	6	MAN	O2-C2-C1	-2.06	104.94	109.15

There are no chirality outliers.

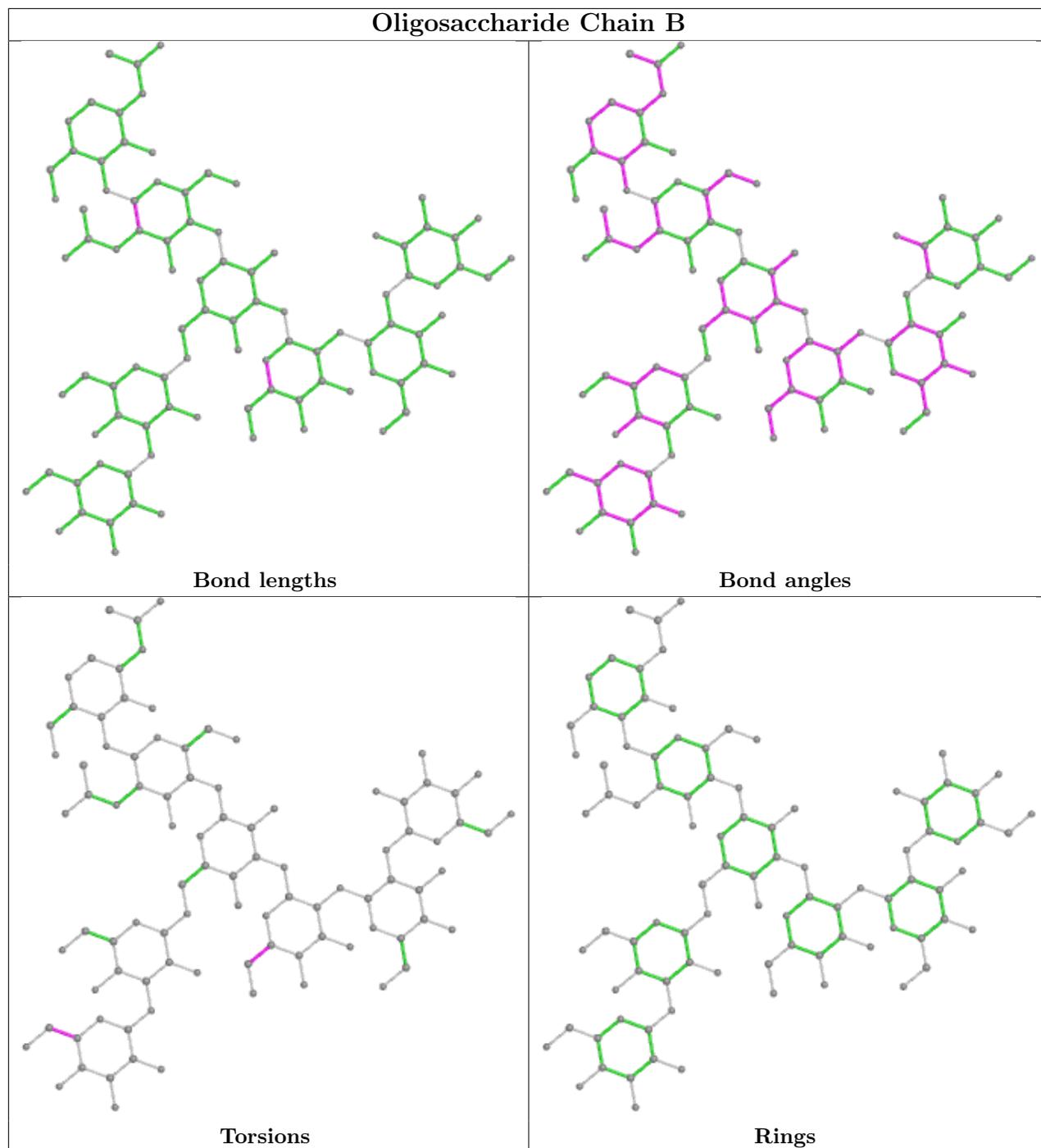
All (7) torsion outliers are listed below:

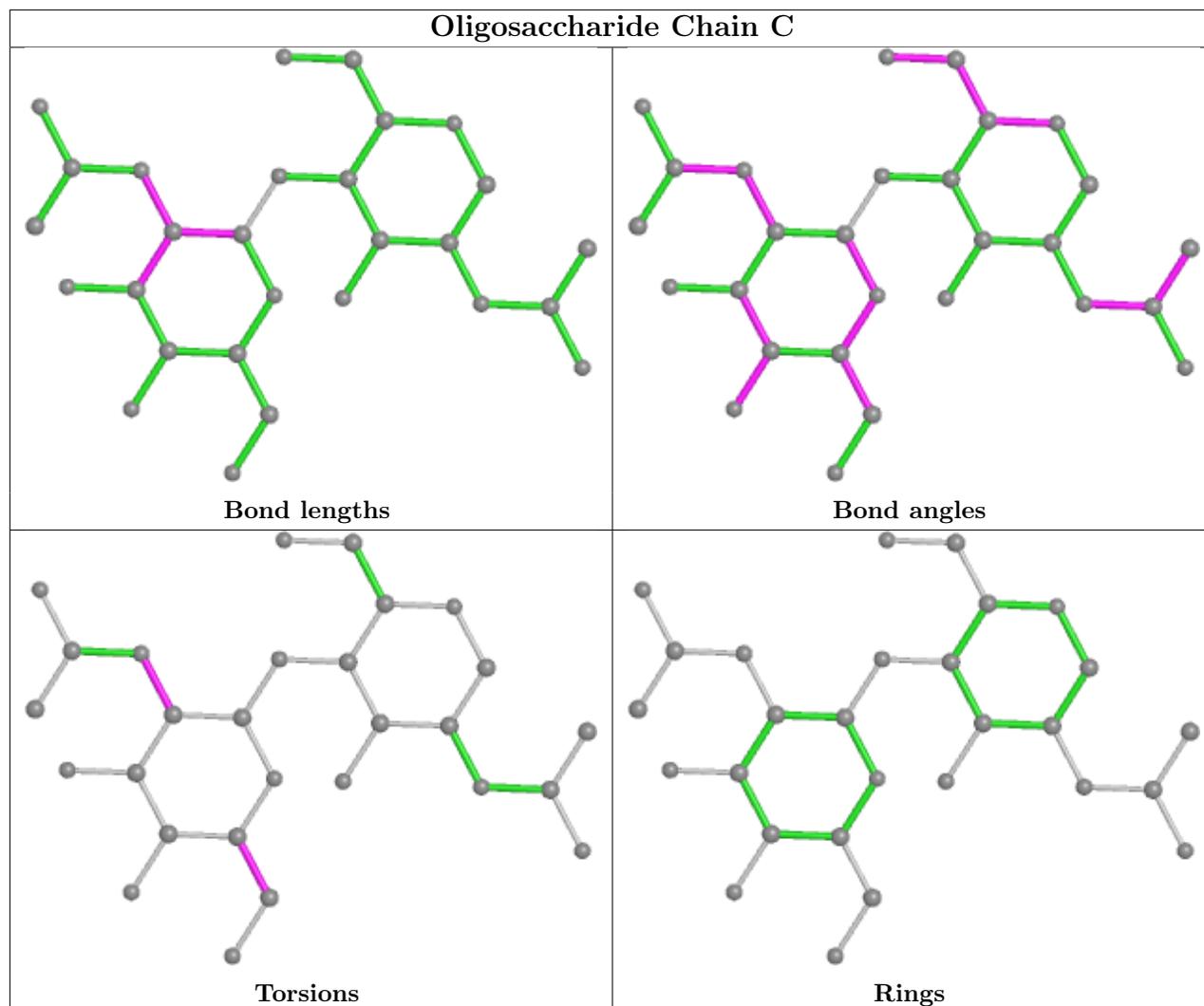
Mol	Chain	Res	Type	Atoms
2	B	8	MAN	O5-C5-C6-O6
2	B	8	MAN	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C3-C2-N2-C7
2	B	4	MAN	C4-C5-C6-O6
2	B	4	MAN	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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
5	NAG	A	512	1	14,14,15	0.68	0	17,19,21	2.01	7 (41%)
8	9SJ	A	515[A]	1	20,20,20	0.89	1 (5%)	22,28,28	2.86	10 (45%)
4	9SM	A	501	-	17,21,21	1.11	2 (11%)	17,31,31	2.96	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	9S4	A	514[B]	-	15,20,20	0.79	1 (6%)	15,28,28	1.76	5 (33%)

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	512	1	-	0/6/23/26	0/1/1/1
8	9SJ	A	515[A]	1	-	3/14/34/34	0/1/1/1
4	9SM	A	501	-	-	2/11/39/39	0/1/1/1
7	9S4	A	514[B]	-	-	0/10/34/34	0/0/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	515[A]	9SJ	F1-C3	-2.94	1.33	1.40
4	A	501	9SM	O1A-C1	2.43	1.30	1.22
4	A	501	9SM	O8-C8	2.08	1.49	1.43
7	A	514[B]	9S4	C5-N5	2.02	1.49	1.45

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	515[A]	9SJ	F1-C3-C2	-9.54	96.74	108.26
4	A	501	9SM	FAI-C3-C4	7.34	115.37	108.85
4	A	501	9SM	O8-C8-C7	5.12	120.80	109.18
5	A	512	NAG	C2-N2-C7	-4.97	115.83	122.90
8	A	515[A]	9SJ	C3-C2-C1	-4.46	106.00	112.15
4	A	501	9SM	C6-C7-C8	-4.29	104.99	114.61
7	A	514[B]	9S4	O1A-C1-C2	4.08	124.42	113.85
4	A	501	9SM	O6-C6-C7	-3.75	101.15	105.95
8	A	515[A]	9SJ	C6-C7-C8	-3.45	106.89	114.61
8	A	515[A]	9SJ	C4-C5-N5	-3.42	104.16	110.62
8	A	515[A]	9SJ	O1B-C1-C2	3.07	124.90	113.65
8	A	515[A]	9SJ	O6-C2-C1	-2.98	97.88	105.88
4	A	501	9SM	O4-C4-C3	-2.93	103.87	109.68
5	A	512	NAG	C8-C7-N2	2.80	120.84	116.10
5	A	512	NAG	O5-C1-C2	2.80	115.70	111.29
4	A	501	9SM	O4-C4-C5	-2.73	104.15	109.66
7	A	514[B]	9S4	C4-C5-N5	-2.69	105.54	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	514[B]	9S4	O4-C4-C3	-2.46	104.82	109.67
7	A	514[B]	9S4	O1A-C1-O1B	-2.45	118.01	123.61
5	A	512	NAG	C4-C3-C2	2.43	114.58	111.02
7	A	514[B]	9S4	C6-C7-C8	-2.42	109.19	114.61
8	A	515[A]	9SJ	O6-C2-C3	-2.38	104.77	109.33
5	A	512	NAG	O4-C4-C3	-2.37	104.88	110.35
8	A	515[A]	9SJ	F1-C3-C4	-2.35	106.77	108.85
8	A	515[A]	9SJ	O1A-C1-C2	-2.32	112.28	120.81
5	A	512	NAG	O5-C5-C6	2.31	110.83	107.20
5	A	512	NAG	O7-C7-N2	-2.10	118.10	121.95
8	A	515[A]	9SJ	C6-O6-C2	2.00	116.67	112.81

There are no chirality outliers.

All (5) torsion outliers are listed below:

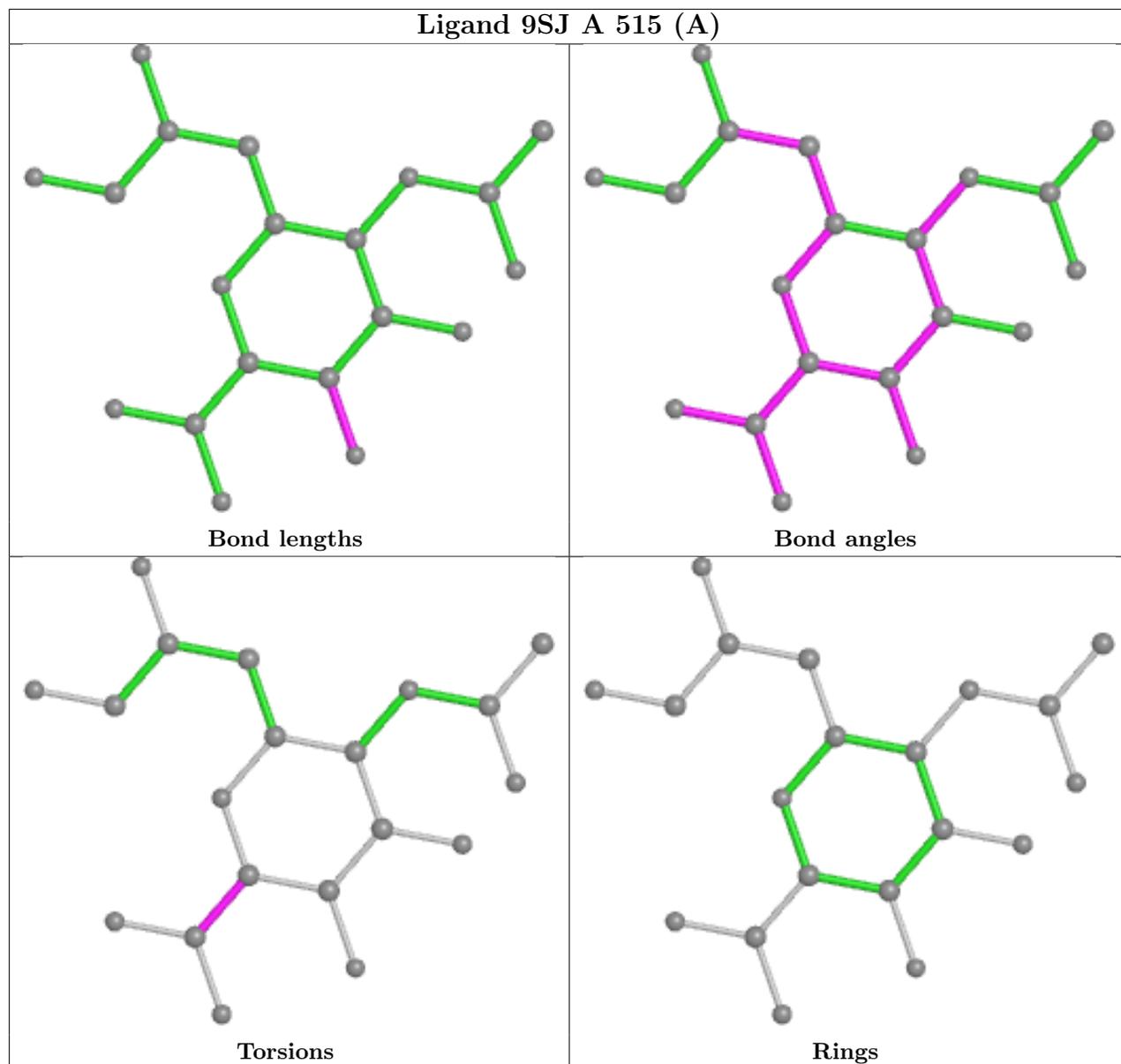
Mol	Chain	Res	Type	Atoms
4	A	501	9SM	C6-C7-C8-O8
4	A	501	9SM	C6-C7-C8-C9
8	A	515[A]	9SJ	O1A-C1-C2-C3
8	A	515[A]	9SJ	O1B-C1-C2-C3
8	A	515[A]	9SJ	O1A-C1-C2-O6

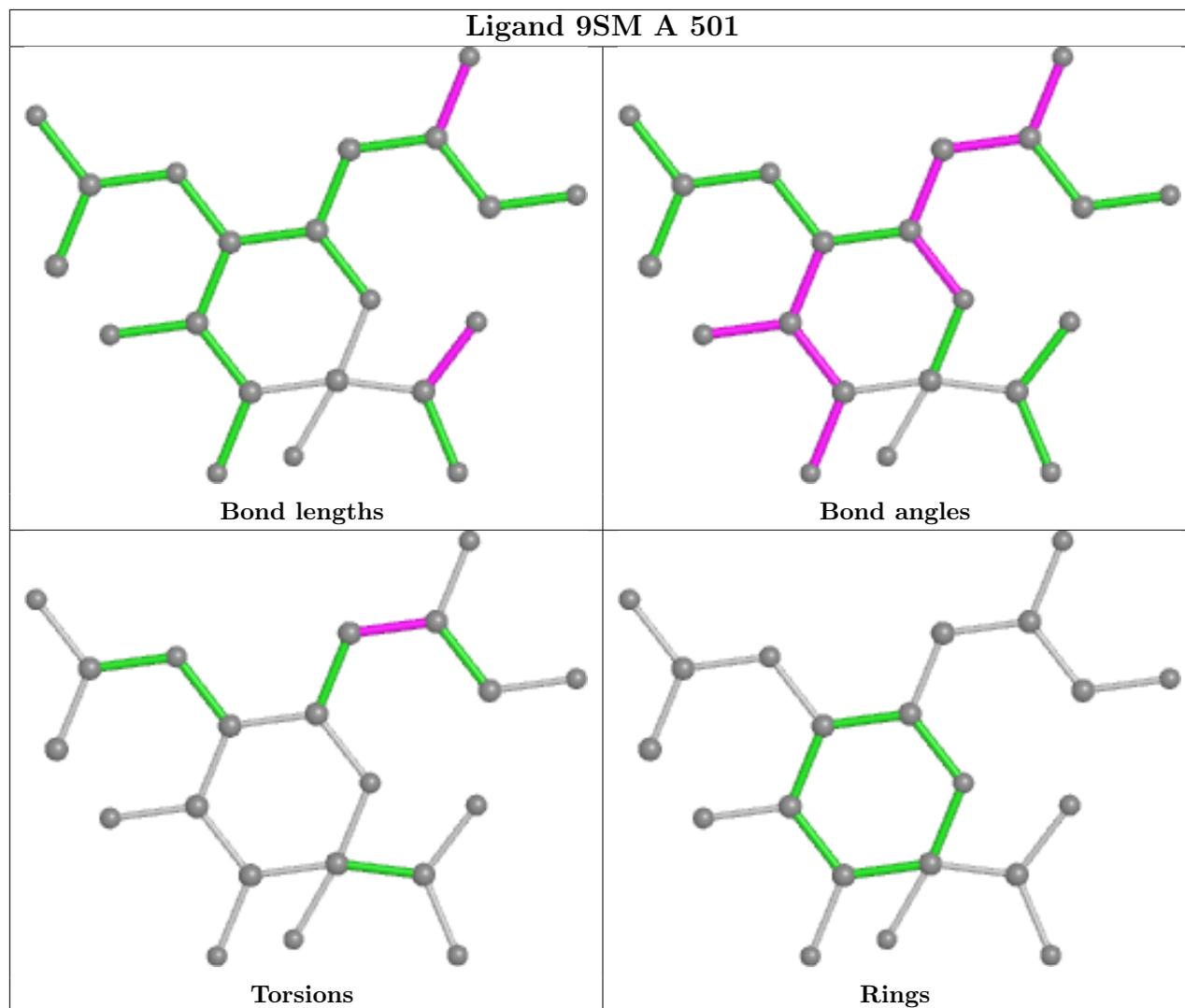
There are no ring outliers.

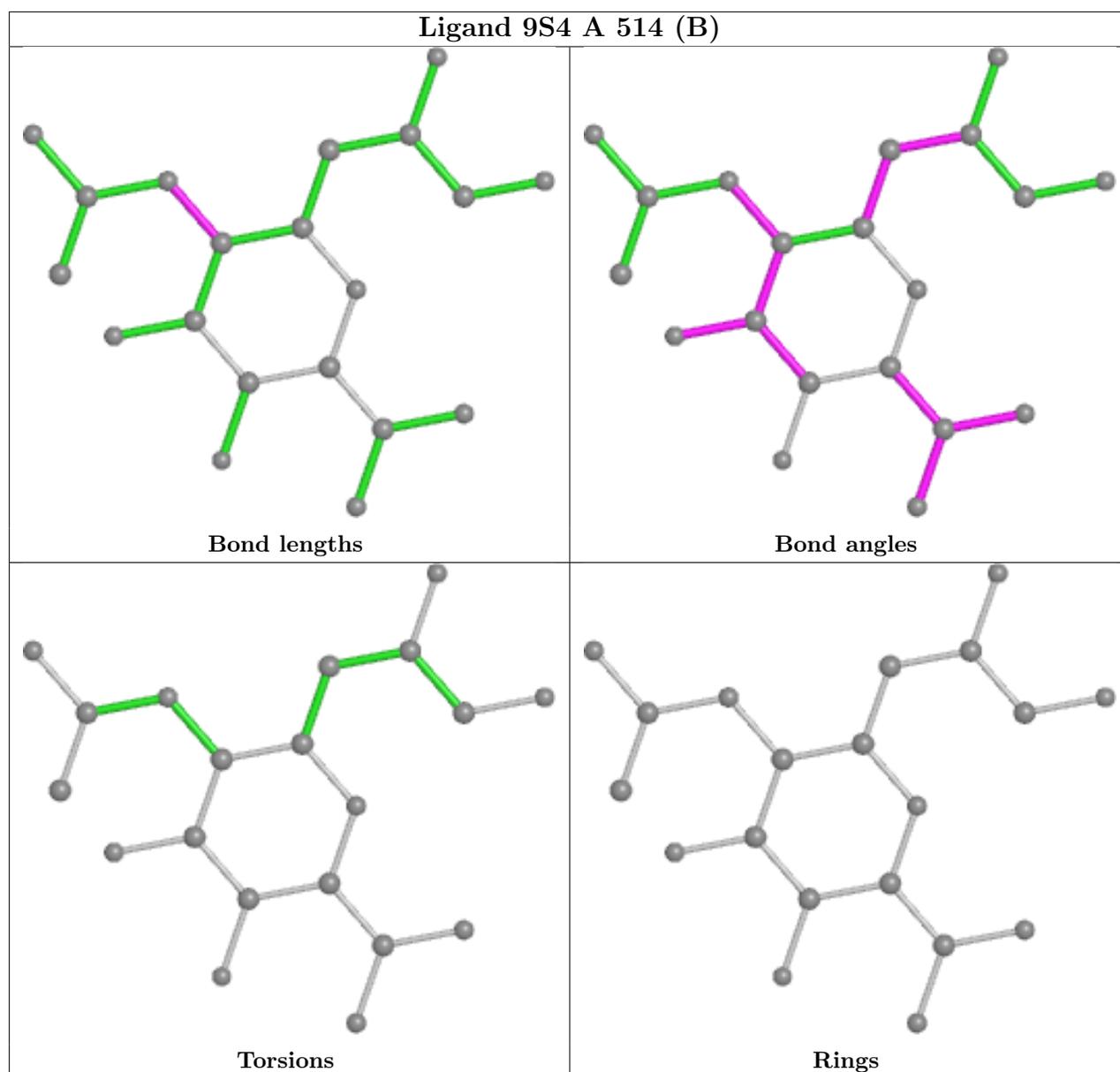
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	512	NAG	1	0

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	388/388 (100%)	-0.47	2 (0%) 91 90	17, 22, 32, 54	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82[A]	ARG	2.8
1	A	83	ASP	2.5

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

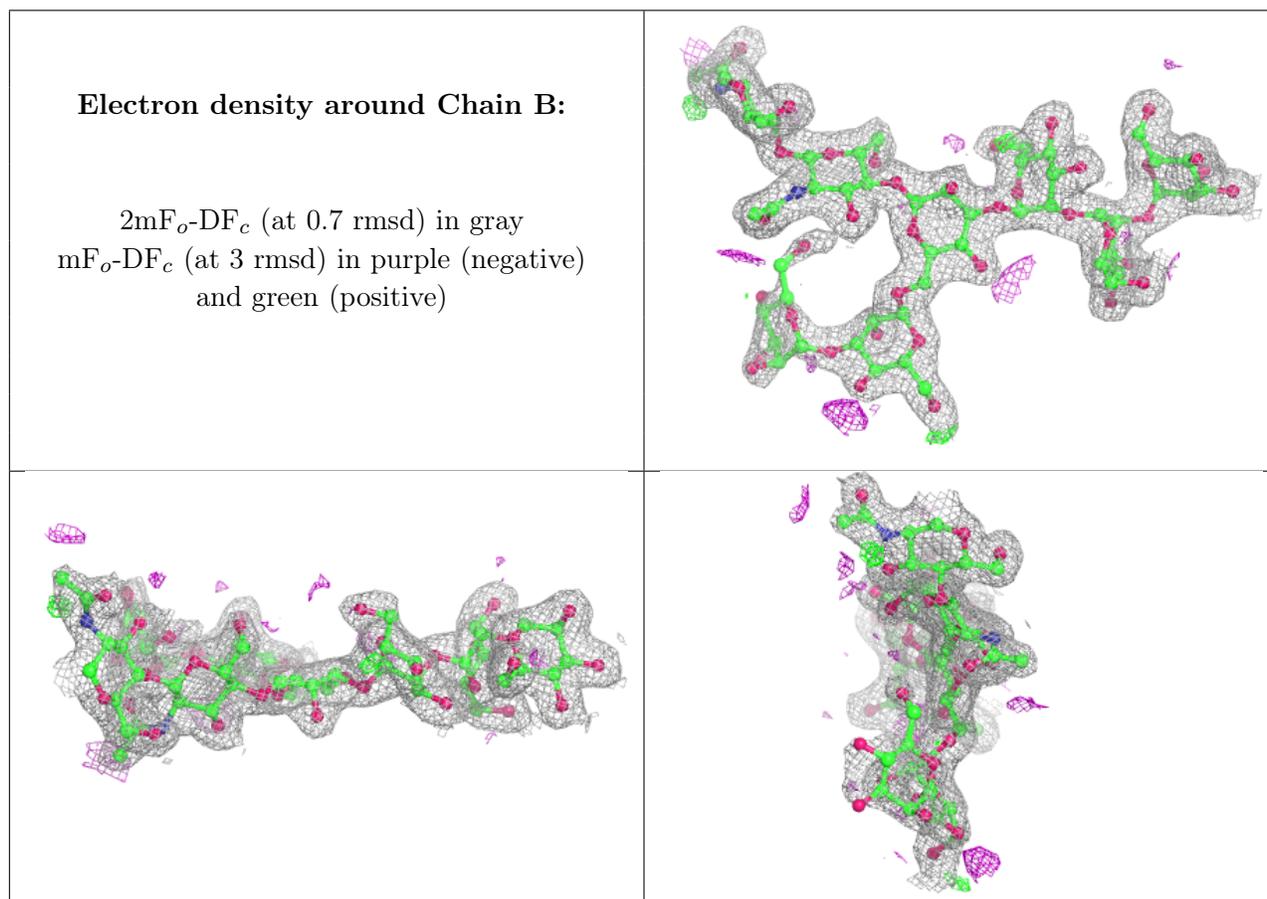
There are no non-standard protein/DNA/RNA residues in this entry.

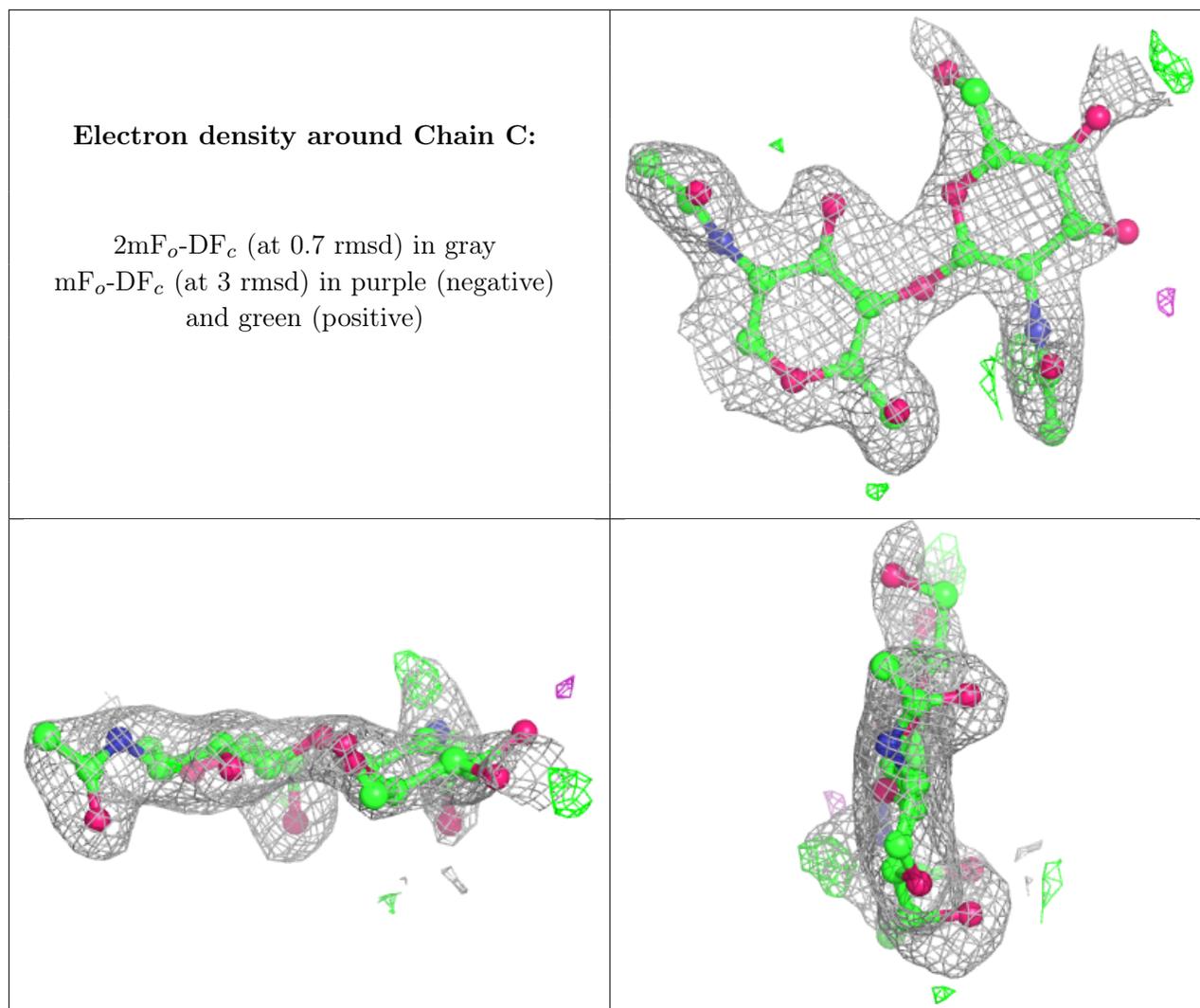
### 6.3 Carbohydrates [i](#)

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MAN	B	8	11/12	0.77	0.40	58,66,72,77	0
3	NAG	C	2	14/15	0.78	0.43	54,64,69,74	0
3	NAG	C	1	14/15	0.94	0.25	32,35,42,52	0
2	MAN	B	7	11/12	0.96	0.19	31,38,45,46	0
2	NAG	B	1	14/15	0.96	0.11	19,25,39,40	0
2	MAN	B	5	11/12	0.97	0.12	25,26,29,29	0
2	NAG	B	2	14/15	0.98	0.10	20,26,32,43	0
2	MAN	B	6	11/12	0.98	0.07	23,25,28,28	0
2	MAN	B	4	11/12	0.98	0.10	21,25,32,35	0
2	BMA	B	3	11/12	0.99	0.08	23,25,28,31	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.





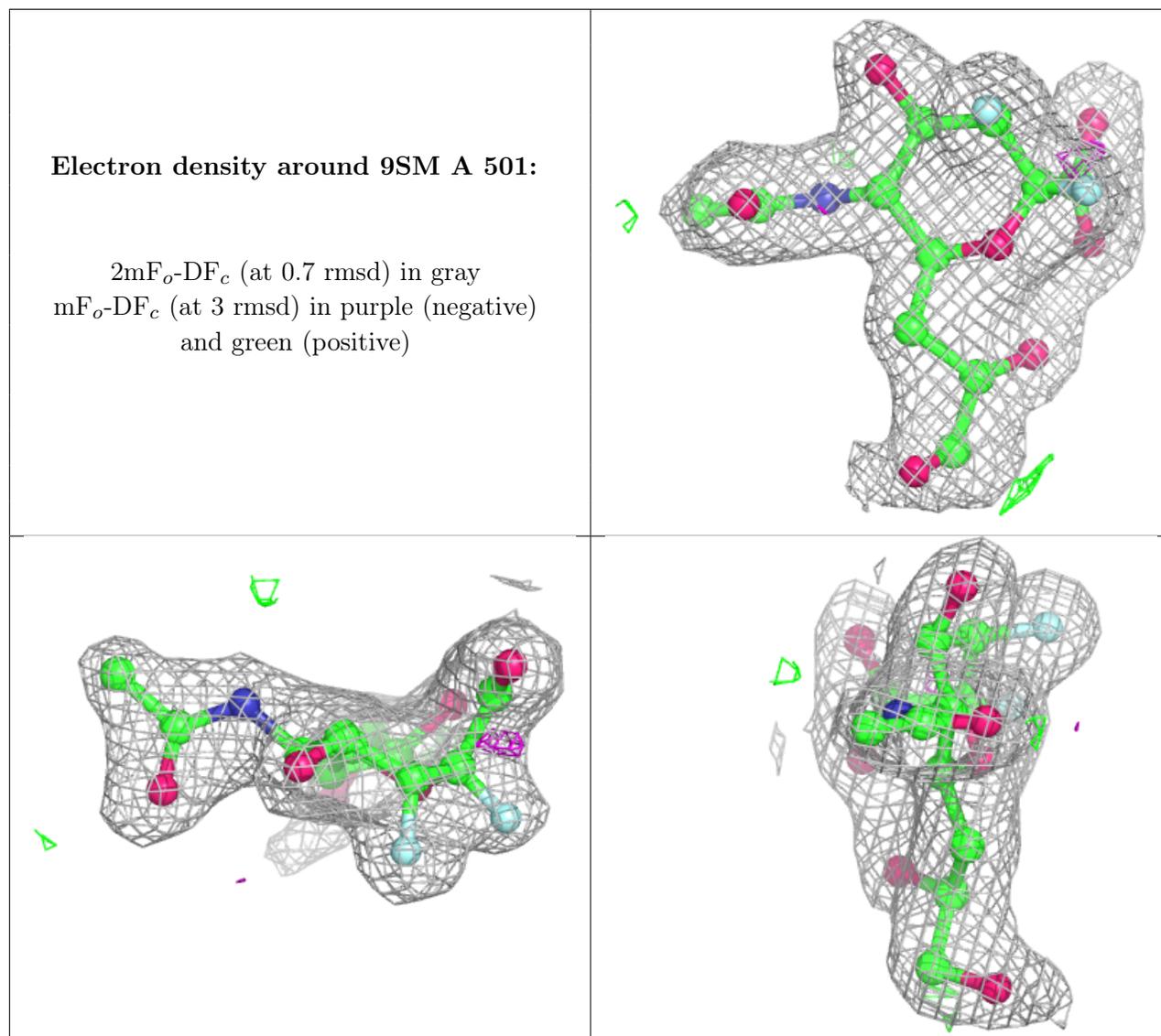
## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	9SM	A	501	21/21	0.93	0.19	28,38,43,50	0
5	NAG	A	512	14/15	0.93	0.33	45,52,63,65	0
7	9S4	A	514[B]	20/20	0.97	0.10	21,26,30,45	20
8	9SJ	A	515[A]	20/20	0.97	0.10	19,21,23,25	20
6	CA	A	513	1/1	0.99	0.05	25,25,25,25	0

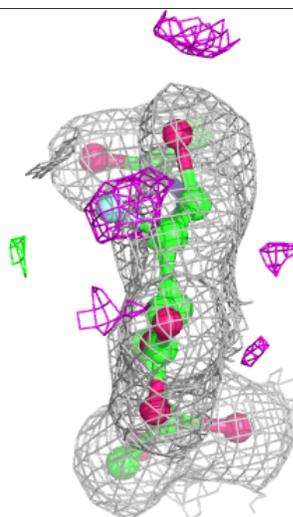
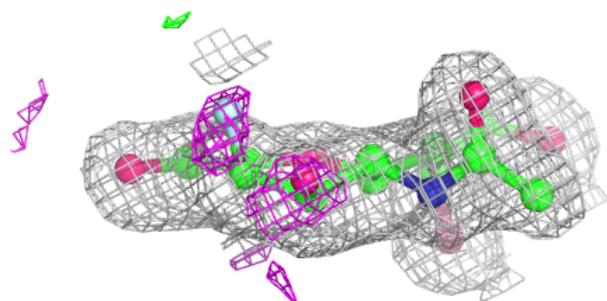
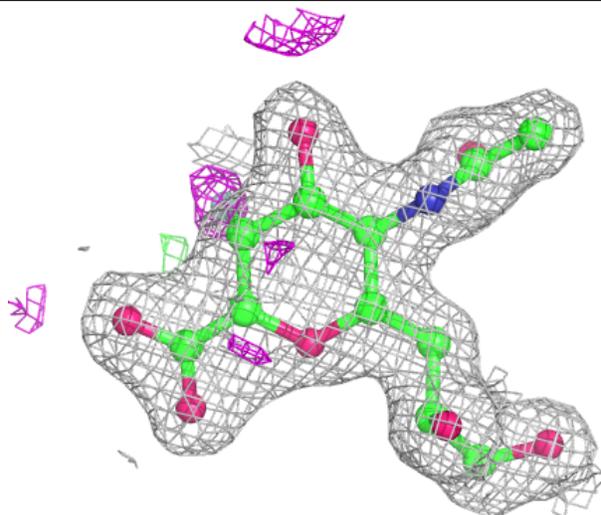
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

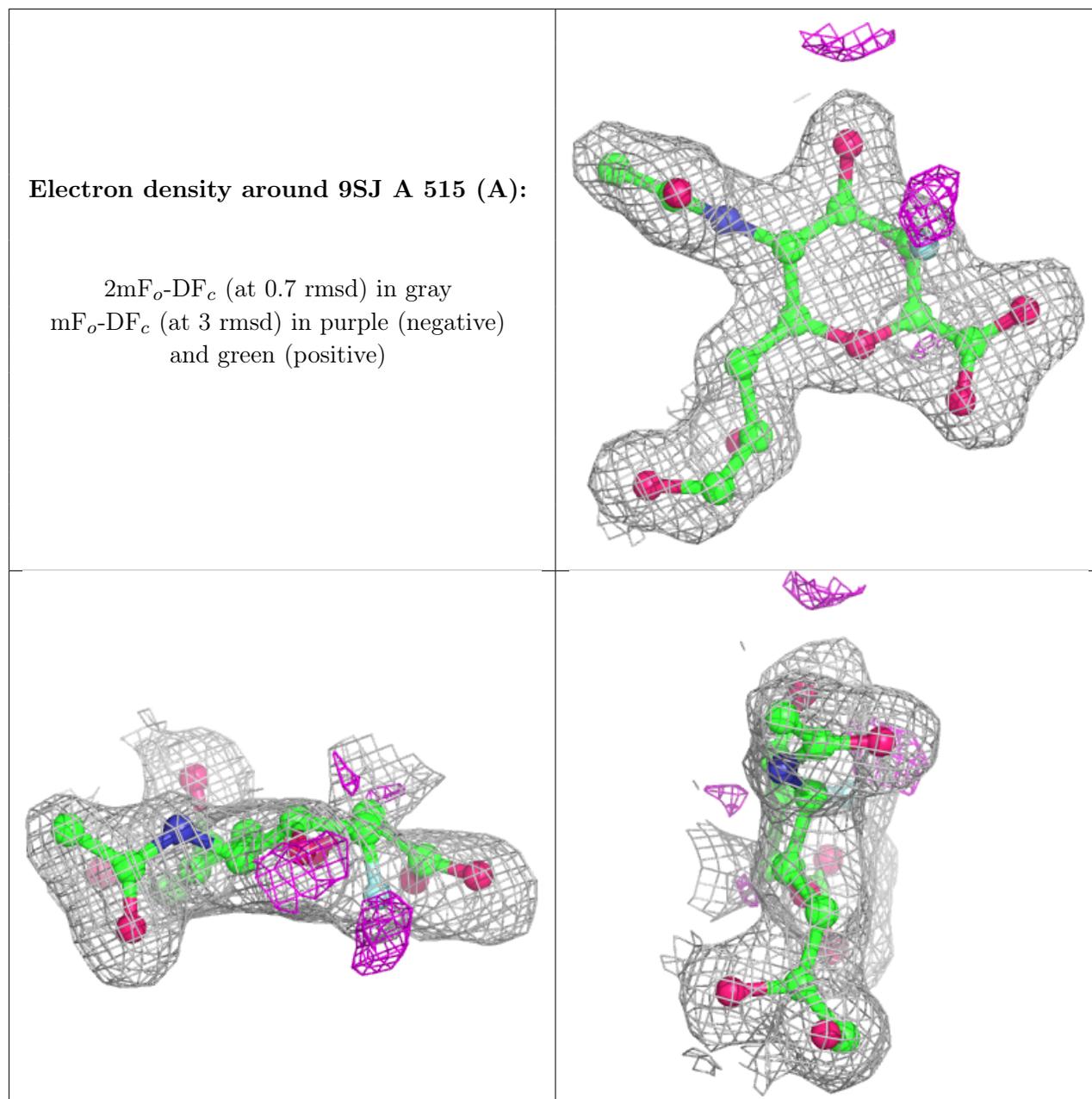
orientation to approximate a three-dimensional view.



**Electron density around 9S4 A 514 (B):**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.