



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 11, 2023 – 04:11 PM JST

PDB ID : 8W6P  
Title : Crystal structure of dimeric murine SMPDL3A  
Authors : Zhang, C.; Liu, P.; Fan, S.; Hou, Y.  
Deposited on : 2023-08-29  
Resolution : 1.91 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)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

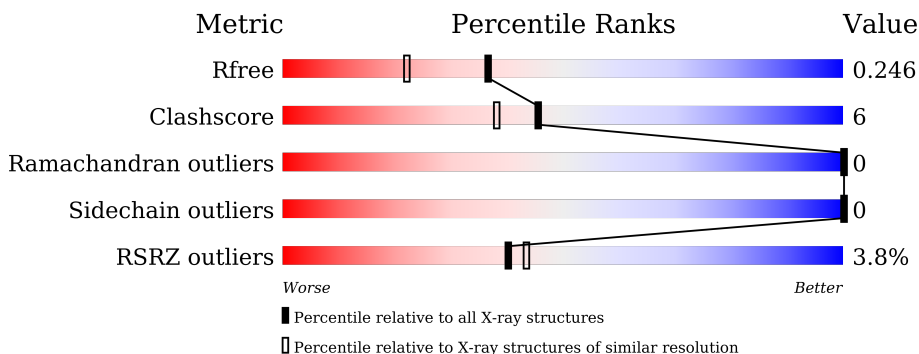
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.91 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	413	 3% 88% 11%
1	B	413	 5% 87% 13%
2	C	2	 50% 50%
2	E	2	 50% 50%
3	D	2	 100%
4	F	3	 67% 33%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
6	NAG	B	501	-	-	-	X

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 7618 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 Acid sphingomyelinase-like phosphodiesterase 3a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	412	3287	2118	535	620	14	0	0	0
1	B	413	3292	2121	536	621	14	0	0	0

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



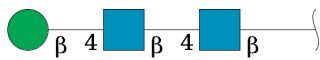
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0
2	E	2	28	16	2	10	0	0	0

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



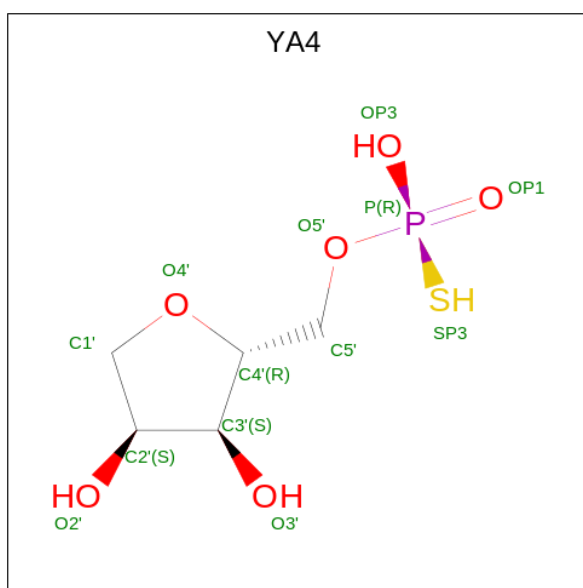
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	2	24	14	1	9	0	0	0

- 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.



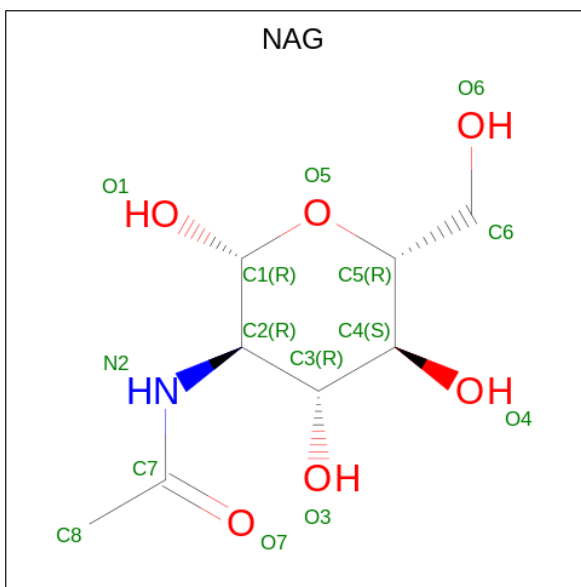
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	F	3	39	22	2	15	0	0	0

- Molecule 5 is [(2 {R},3 {S},4 {S})-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-sulfanyl-phosphinic acid (three-letter code: YA4) (formula: C<sub>5</sub>H<sub>11</sub>O<sub>6</sub>PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	O	P	S		
5	A	1	13	5	6	1	1	1	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).

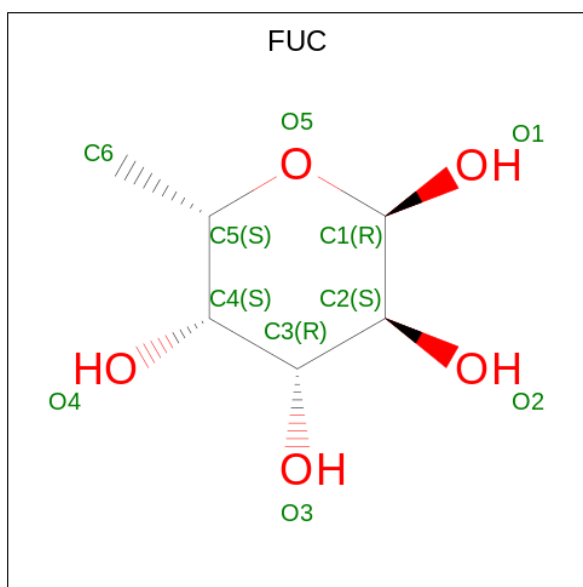


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
6	A	1	14	8	1	5	0	0
6	B	1	14	8	1	5	0	0
6	B	1	14	8	1	5	0	0
6	B	1	14	8	1	5	0	0
6	B	1	14	8	1	5	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

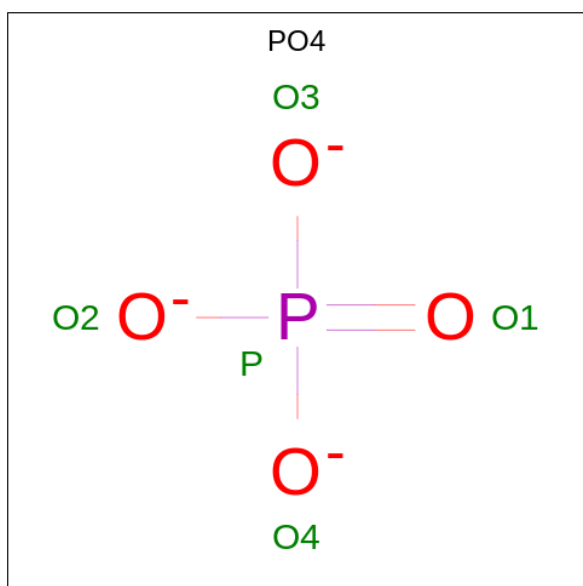
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
7	A	2	2	2	0	0
7	B	2	2	2	0	0

- Molecule 8 is alpha-L-fucopyranose (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 10 is water.

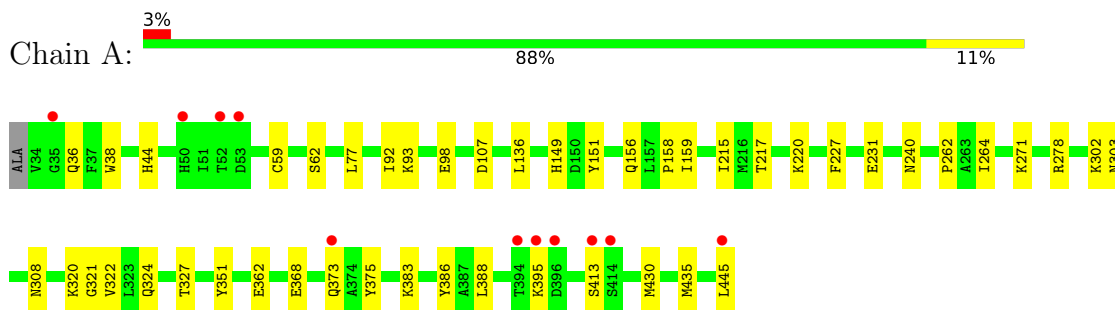
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
10	A	403	Total 403	O 403	0	0
10	B	401	Total 401	O 401	0	0



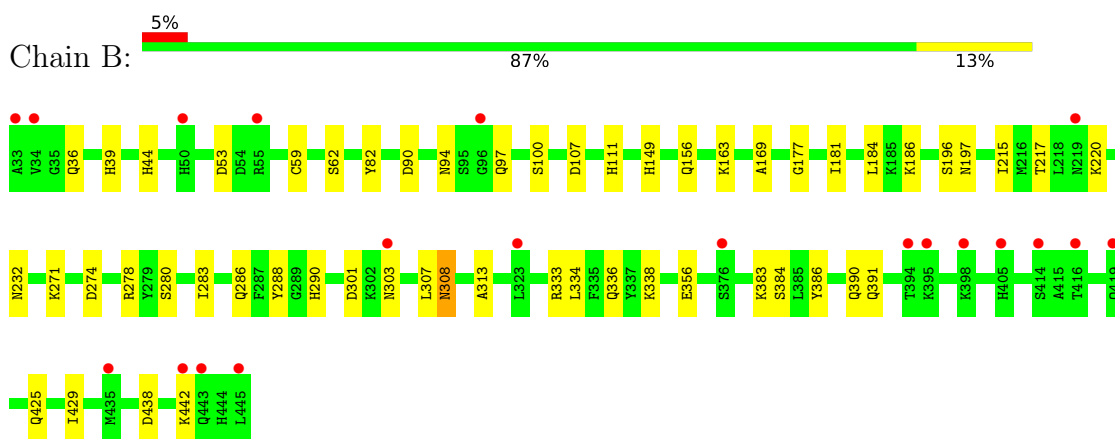
### 3 Residue-property plots [i](#)

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: Acid sphingomyelinase-like phosphodiesterase 3a



- Molecule 1: Acid sphingomyelinase-like phosphodiesterase 3a



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



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



MAG1  
MAG2

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

Chain D:  100%

MAG1  
FUC2

- 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:  67% 33%

MAG1  
MAG2  
BMA3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.22Å 122.22Å 79.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.27 – 1.91 20.27 – 1.91	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.27-1.91) 98.0 (20.27-1.91)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 1.90Å)	Xtrriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, $R_{free}$	0.218 , 0.246 0.218 , 0.246	Depositor DCC
$R_{free}$ test set	2001 reflections (2.23%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.0	Xtrriage
Anisotropy	0.216	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.058 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7618	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2627e-03.*

<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: ZN, BMA, PO4, YA4, FUC, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.47	0/3381	0.67	3/4618 (0.1%)
1	B	0.49	0/3386	0.68	3/4625 (0.1%)
All	All	0.48	0/6767	0.67	6/9243 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	LYS	CD-CE-NZ	-8.94	91.15	111.70
1	B	308	ASN	N-CA-CB	-6.32	99.23	110.60
1	B	308	ASN	CB-CA-C	5.72	121.84	110.40
1	A	308	ASN	N-CA-CB	5.42	120.36	110.60
1	A	435	MET	CB-CG-SD	-5.24	96.69	112.40
1	A	308	ASN	CB-CA-C	-5.04	100.31	110.40

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	3287	0	3189	35	3
1	B	3292	0	3195	47	0
2	C	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	28	0	25	0	0
3	D	24	0	22	1	0
4	F	39	0	34	0	0
5	A	13	0	0	1	3
6	A	28	0	26	1	0
6	B	56	0	50	1	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
8	B	10	0	10	0	0
9	B	5	0	0	1	0
10	A	403	0	0	12	0
10	B	401	0	0	22	0
All	All	7618	0	6576	86	3

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.

All (86) 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:383:LYS:HG2	10:A:858:HOH:O	1.43	1.16
1:B:82:TYR:OH	10:B:601:HOH:O	1.84	0.94
1:B:39:HIS:O	10:B:602:HOH:O	1.86	0.93
1:B:308:ASN:OD1	10:B:603:HOH:O	1.89	0.88
9:B:506:PO4:O2	10:B:604:HOH:O	1.94	0.84
1:A:413:SER:O	10:A:602:HOH:O	1.96	0.82
1:B:391:GLN:OE1	10:B:605:HOH:O	1.97	0.81
1:A:231:GLU:OE1	10:A:603:HOH:O	2.03	0.77
1:B:336:GLN:OE1	10:B:608:HOH:O	2.03	0.75
1:A:93:LYS:HE2	1:A:136:LEU:HD22	1.68	0.75
1:B:156:GLN:HE22	1:B:215:ILE:N	1.85	0.74
10:A:999:HOH:O	3:D:1:NAG:O4	2.04	0.74
1:B:156:GLN:HE22	1:B:215:ILE:H	1.36	0.74
1:A:240:ASN:ND2	10:A:608:HOH:O	2.19	0.73
1:A:362:GLU:OE1	10:A:604:HOH:O	2.07	0.72
1:A:217:THR:HA	1:A:220:LYS:HD2	1.72	0.70
1:B:44:HIS:CE1	10:B:604:HOH:O	2.44	0.69
1:B:36:GLN:HB3	1:B:334:LEU:HD11	1.75	0.69
1:B:274:ASP:OD2	10:B:606:HOH:O	2.12	0.68
6:A:502:NAG:O3	10:A:606:HOH:O	2.13	0.66
1:B:53:ASP:OD2	10:B:611:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:VAL:O	10:A:607:HOH:O	2.15	0.64
1:B:97:GLN:NE2	10:B:614:HOH:O	2.17	0.64
1:B:271:LYS:NZ	10:B:619:HOH:O	2.30	0.63
1:A:59:CYS:SG	1:A:62:SER:HB3	2.38	0.63
1:B:232:ASN:ND2	10:B:609:HOH:O	2.09	0.62
1:A:156:GLN:HE22	1:A:215:ILE:H	1.48	0.62
1:B:283:ILE:HB	1:B:308:ASN:HD21	1.66	0.59
1:B:356:GLU:OE1	10:B:613:HOH:O	2.17	0.59
1:B:149:HIS:CD2	10:B:604:HOH:O	2.56	0.59
1:B:303:ASN:ND2	10:B:623:HOH:O	2.36	0.59
1:A:321:GLY:H	1:A:324:GLN:NE2	2.01	0.57
1:B:290:HIS:HA	10:B:639:HOH:O	2.04	0.57
1:A:227:PHE:O	1:A:231:GLU:HG3	2.06	0.56
1:B:338:LYS:HE2	10:B:878:HOH:O	2.06	0.54
1:A:36:GLN:HG3	1:A:98:GLU:O	2.06	0.54
1:B:36:GLN:OE1	1:B:334:LEU:HD21	2.07	0.54
1:B:301:ASP:HB3	1:B:307:LEU:HD11	1.90	0.53
1:A:302:LYS:HG2	10:A:715:HOH:O	2.08	0.53
1:B:278:ARG:NH2	10:B:606:HOH:O	2.02	0.52
1:B:90:ASP:O	1:B:94:ASN:ND2	2.39	0.52
1:A:395:LYS:N	1:A:395:LYS:HD2	2.25	0.52
1:A:44:HIS:CE1	1:A:107:ASP:HB3	2.44	0.52
1:B:220:LYS:CG	10:B:629:HOH:O	2.59	0.51
6:B:503:NAG:O6	10:B:607:HOH:O	2.02	0.51
1:B:338:LYS:HD3	10:B:803:HOH:O	2.11	0.50
1:B:307:LEU:O	1:B:308:ASN:HB2	2.10	0.50
1:B:438:ASP:O	1:B:442:LYS:HG2	2.11	0.49
1:B:163:LYS:N	1:B:163:LYS:HD3	2.28	0.49
1:B:425:GLN:O	1:B:429:ILE:HG13	2.12	0.49
1:A:445:LEU:C	10:A:619:HOH:O	2.50	0.49
1:B:386:TYR:O	1:B:390:GLN:HG2	2.12	0.49
1:B:286:GLN:NE2	1:B:288:TYR:OH	2.45	0.48
1:A:156:GLN:NE2	1:A:215:ILE:HG12	2.30	0.47
1:A:373:GLN:HG2	10:A:929:HOH:O	2.13	0.47
1:B:44:HIS:CE1	1:B:107:ASP:HB3	2.50	0.47
1:B:169:ALA:HA	1:B:184:LEU:HD23	1.96	0.47
1:B:156:GLN:NE2	1:B:156:GLN:HA	2.29	0.47
1:B:44:HIS:CE1	1:B:111:HIS:CE1	3.03	0.46
1:B:220:LYS:HG3	10:B:629:HOH:O	2.15	0.46
1:A:156:GLN:HE22	1:A:215:ILE:N	2.11	0.46
1:A:227:PHE:CE2	1:A:271:LYS:HD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:ALA:HB2	1:B:333:ARG:HD2	1.99	0.45
1:A:38:TRP:CE2	1:A:92:ILE:HG23	2.52	0.45
1:A:159:ILE:HD13	1:A:220:LYS:CE	2.46	0.45
1:A:386:TYR:HD1	1:A:430:MET:HE1	1.82	0.45
1:B:59:CYS:SG	1:B:62:SER:HB3	2.57	0.45
1:B:100:SER:HB2	1:B:196:SER:OG	2.18	0.43
1:B:196:SER:OG	1:B:197:ASN:ND2	2.51	0.43
1:A:320:LYS:HB3	1:A:327:THR:HB	2.00	0.43
1:A:62:SER:HA	1:A:77:LEU:O	2.18	0.43
1:A:156:GLN:CD	10:A:611:HOH:O	2.57	0.43
1:B:383:LYS:HG3	1:B:384:SER:N	2.34	0.43
1:A:151:TYR:CZ	1:A:158:PRO:HD3	2.55	0.42
1:B:177:GLY:O	1:B:181:ILE:HG12	2.19	0.42
1:A:351:TYR:CD1	1:A:368:GLU:HB2	2.55	0.42
1:A:375:TYR:HB3	1:A:388:LEU:CD1	2.50	0.41
1:B:280:SER:HA	1:B:308:ASN:HD22	1.85	0.41
1:A:321:GLY:H	1:A:324:GLN:HE21	1.68	0.41
1:B:217:THR:HA	1:B:220:LYS:HD2	2.03	0.41
1:A:262:PRO:HB2	1:A:264:ILE:O	2.20	0.41
1:A:278:ARG:HH11	1:A:278:ARG:HD3	1.71	0.41
1:B:156:GLN:NE2	1:B:215:ILE:H	2.11	0.41
1:A:375:TYR:HB3	1:A:388:LEU:HD13	2.03	0.41
1:A:149:HIS:NE2	5:A:501:YA4:SP3	2.66	0.40
1:B:280:SER:HA	1:B:308:ASN:ND2	2.36	0.40

All (3) 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:303:ASN:ND2	5:A:501:YA4:C2'[4_554]	1.79	0.41
1:A:303:ASN:CG	5:A:501:YA4:O2'[4_554]	1.97	0.23
1:A:303:ASN:OD1	5:A:501:YA4:O2'[4_554]	2.19	0.01

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	410/413 (99%)	390 (95%)	20 (5%)	0	100	100
1	B	411/413 (100%)	387 (94%)	24 (6%)	0	100	100
All	All	821/826 (99%)	777 (95%)	44 (5%)	0	100	100

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	367/367 (100%)	367 (100%)	0	100	100
1	B	367/367 (100%)	367 (100%)	0	100	100
All	All	734/734 (100%)	734 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	324	GLN
1	B	156	GLN
1	B	286	GLN
1	B	308	ASN
1	B	373	GLN

### 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
2	NAG	C	1	1,2	14,14,15	0.32	0	17,19,21	0.95	1 (5%)
2	NAG	C	2	2	14,14,15	0.16	0	17,19,21	0.39	0
3	NAG	D	1	3,1	14,14,15	0.41	0	17,19,21	0.66	0
3	FUC	D	2	3	10,10,11	1.67	3 (30%)	14,14,16	1.37	2 (14%)
2	NAG	E	1	1,2	14,14,15	0.33	0	17,19,21	0.57	0
2	NAG	E	2	2	14,14,15	0.27	0	17,19,21	1.66	3 (17%)
4	NAG	F	1	1,4	14,14,15	0.28	0	17,19,21	0.48	0
4	NAG	F	2	4	14,14,15	0.44	0	17,19,21	0.54	0
4	BMA	F	3	4	11,11,12	0.86	0	15,15,17	1.11	1 (6%)

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	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	FUC	D	2	3	-	-	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	FUC	O5-C5	2.93	1.49	1.43
3	D	2	FUC	C2-C3	2.63	1.56	1.52
3	D	2	FUC	O5-C1	-2.60	1.39	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C1-O5-C5	4.15	117.82	112.19
2	E	2	NAG	C2-N2-C7	3.79	128.29	122.90
2	C	1	NAG	C1-O5-C5	3.30	116.67	112.19
4	F	3	BMA	C1-O5-C5	2.91	116.13	112.19
2	E	2	NAG	C1-C2-N2	2.75	115.19	110.49
3	D	2	FUC	O2-C2-C1	2.38	114.02	109.15
3	D	2	FUC	O5-C5-C4	2.28	113.60	109.52

There are no chirality outliers.

All (3) torsion outliers are listed below:

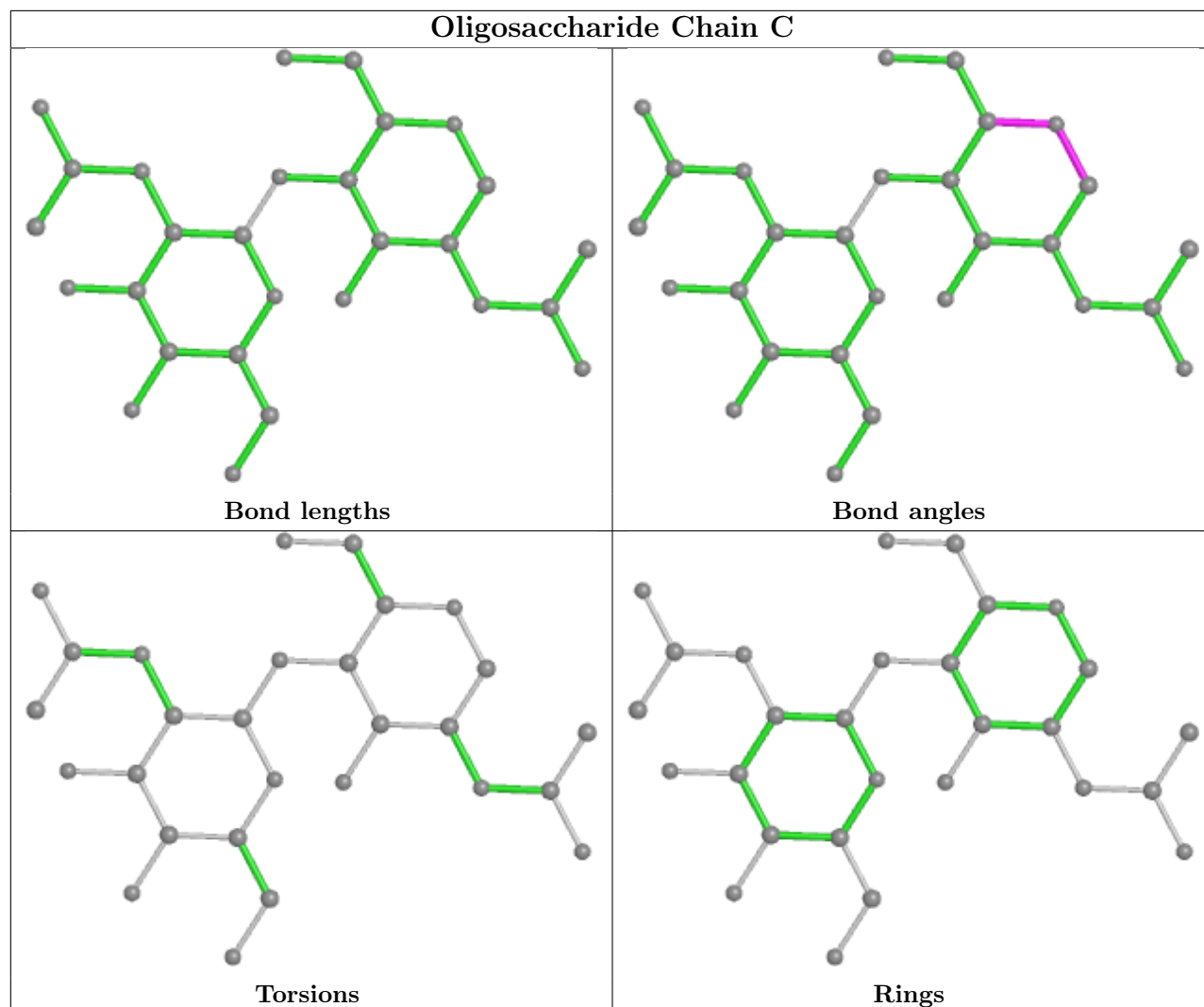
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C3-C2-N2-C7
2	E	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6

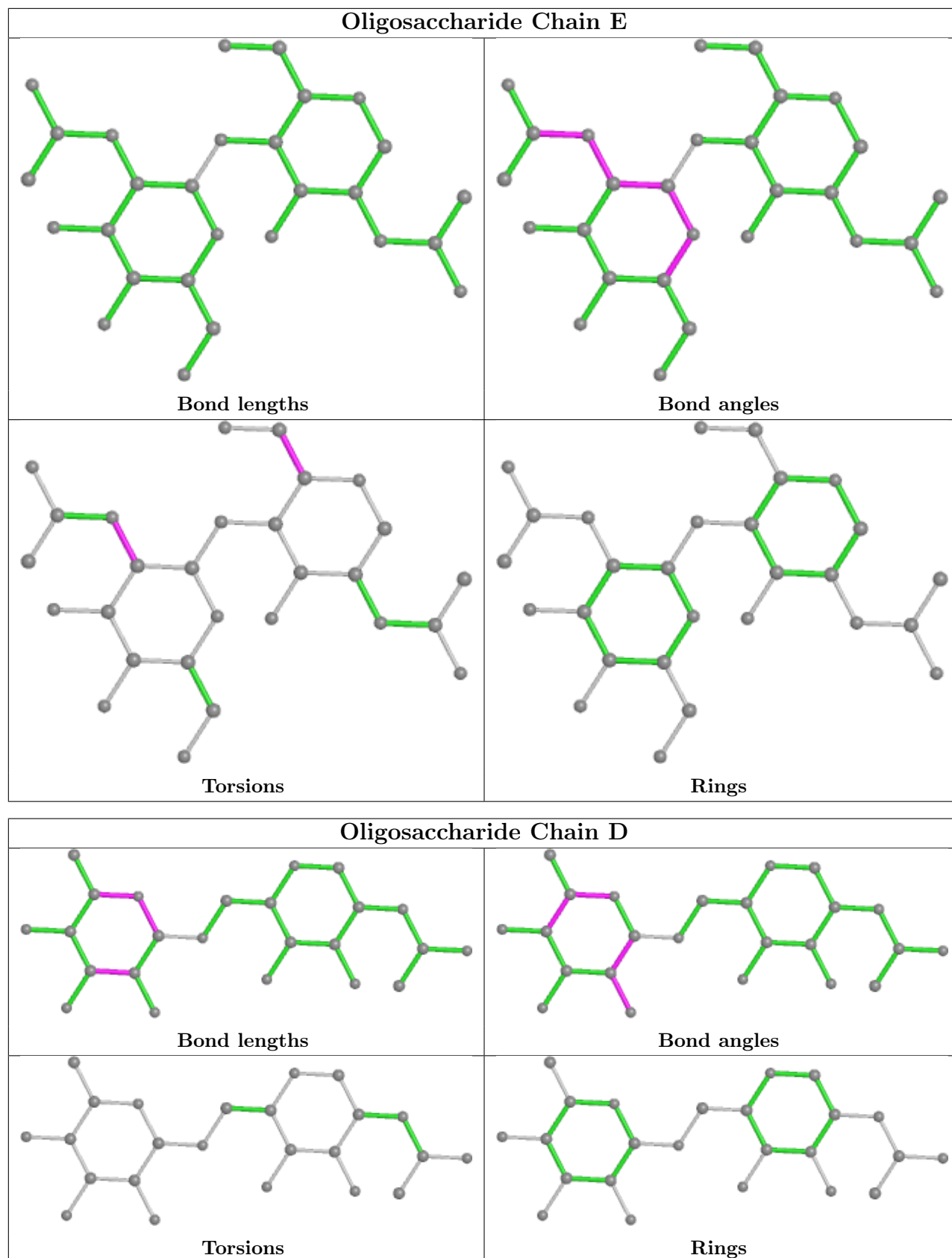
There are no ring outliers.

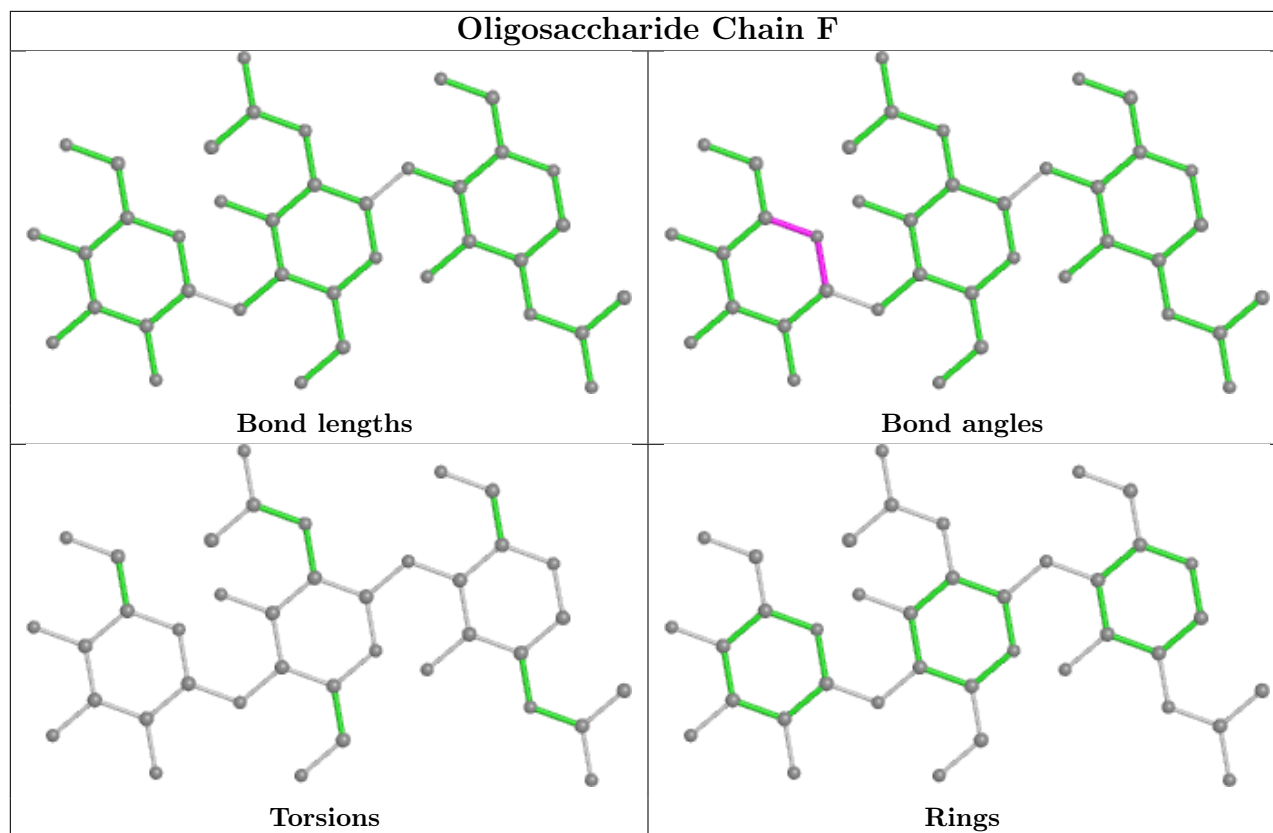
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	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 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	$\# Z  > 2$
9	PO4	B	506	7	4,4,4	0.87	0	6,6,6	1.07	0
8	FUC	B	502	6	10,10,11	1.11	1 (10%)	14,14,16	1.46	4 (28%)
6	NAG	B	505	6,1	14,14,15	0.48	0	17,19,21	0.70	0
6	NAG	B	501	6	14,14,15	0.50	0	17,19,21	0.66	0
6	NAG	B	504	8,1	14,14,15	0.49	0	17,19,21	0.66	0
6	NAG	A	503	1	14,14,15	0.51	0	17,19,21	0.55	0
6	NAG	A	502	1	14,14,15	0.39	0	17,19,21	0.69	1 (5%)
6	NAG	B	503	1	14,14,15	0.76	1 (7%)	17,19,21	0.55	0
5	YA4	A	501	7,1	11,13,13	1.07	1 (9%)	13,19,19	1.08	1 (7%)

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
8	FUC	B	502	6	-	-	0/1/1/1
6	NAG	B	505	6,1	-	0/6/23/26	0/1/1/1
6	NAG	B	501	6	-	3/6/23/26	0/1/1/1
6	NAG	B	504	8,1	-	2/6/23/26	0/1/1/1
6	NAG	A	503	1	-	0/6/23/26	0/1/1/1
6	NAG	A	502	1	-	2/6/23/26	0/1/1/1
6	NAG	B	503	1	-	0/6/23/26	0/1/1/1
5	YA4	A	501	7,1	-	2/5/19/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	502	FUC	C1-C2	2.81	1.58	1.52
5	A	501	YA4	P-OP3	2.41	1.63	1.56
6	B	503	NAG	C1-C2	2.32	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	502	FUC	C1-O5-C5	2.81	119.15	112.78
5	A	501	YA4	C1'-C2'-C3'	2.61	105.60	101.63
8	B	502	FUC	O5-C5-C4	2.55	114.10	109.52
8	B	502	FUC	C1-C2-C3	2.16	112.32	109.67
8	B	502	FUC	O2-C2-C1	2.08	113.40	109.15
6	A	502	NAG	C1-O5-C5	2.05	114.96	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	504	NAG	C4-C5-C6-O6
6	A	502	NAG	O5-C5-C6-O6
6	B	501	NAG	O5-C5-C6-O6
6	B	504	NAG	O5-C5-C6-O6
6	B	501	NAG	C4-C5-C6-O6
6	A	502	NAG	C4-C5-C6-O6
5	A	501	YA4	O4'-C4'-C5'-O5'

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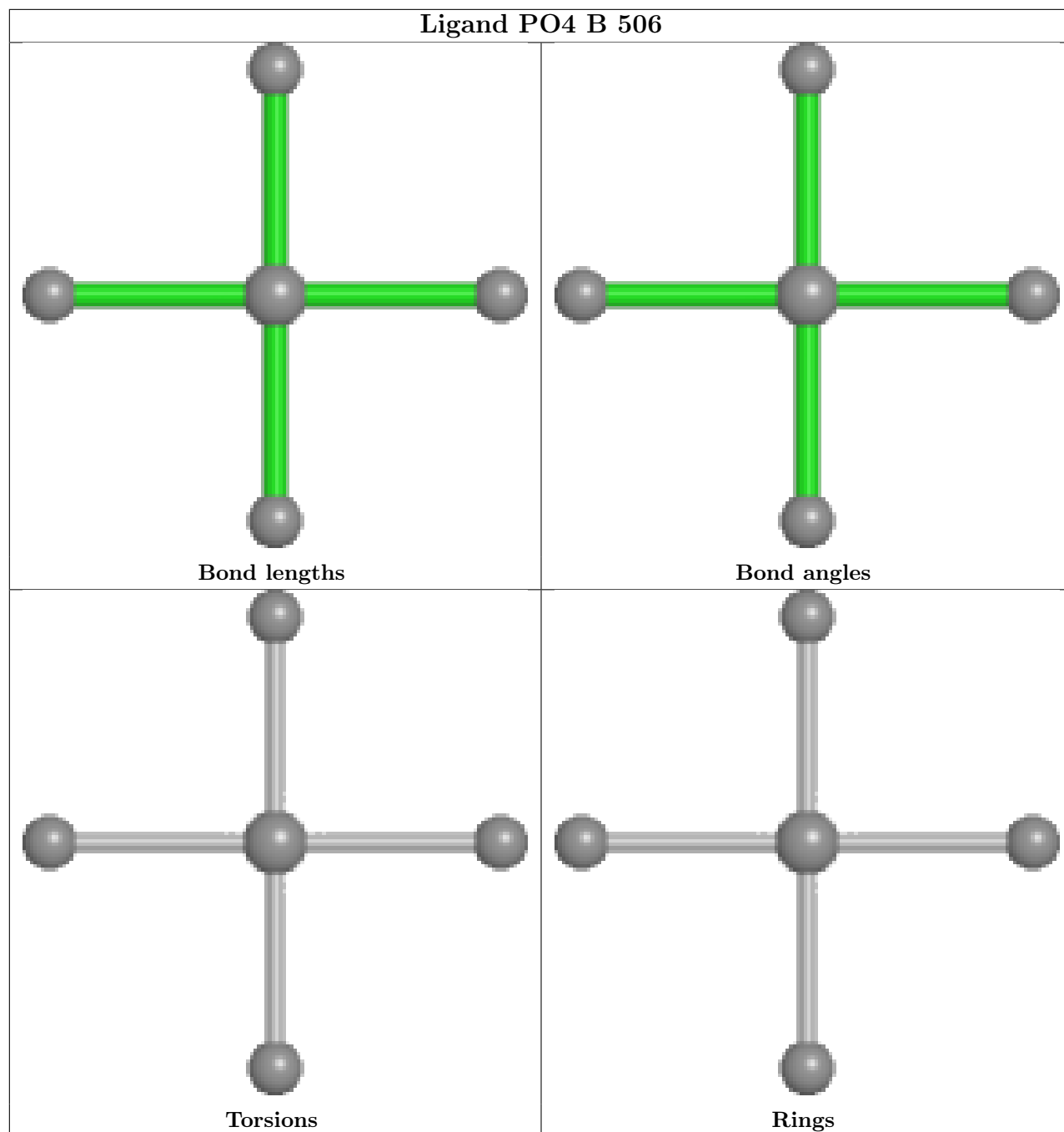
Mol	Chain	Res	Type	Atoms
6	B	501	NAG	C3-C2-N2-C7
5	A	501	YA4	C3'-C4'-C5'-O5'

There are no ring outliers.

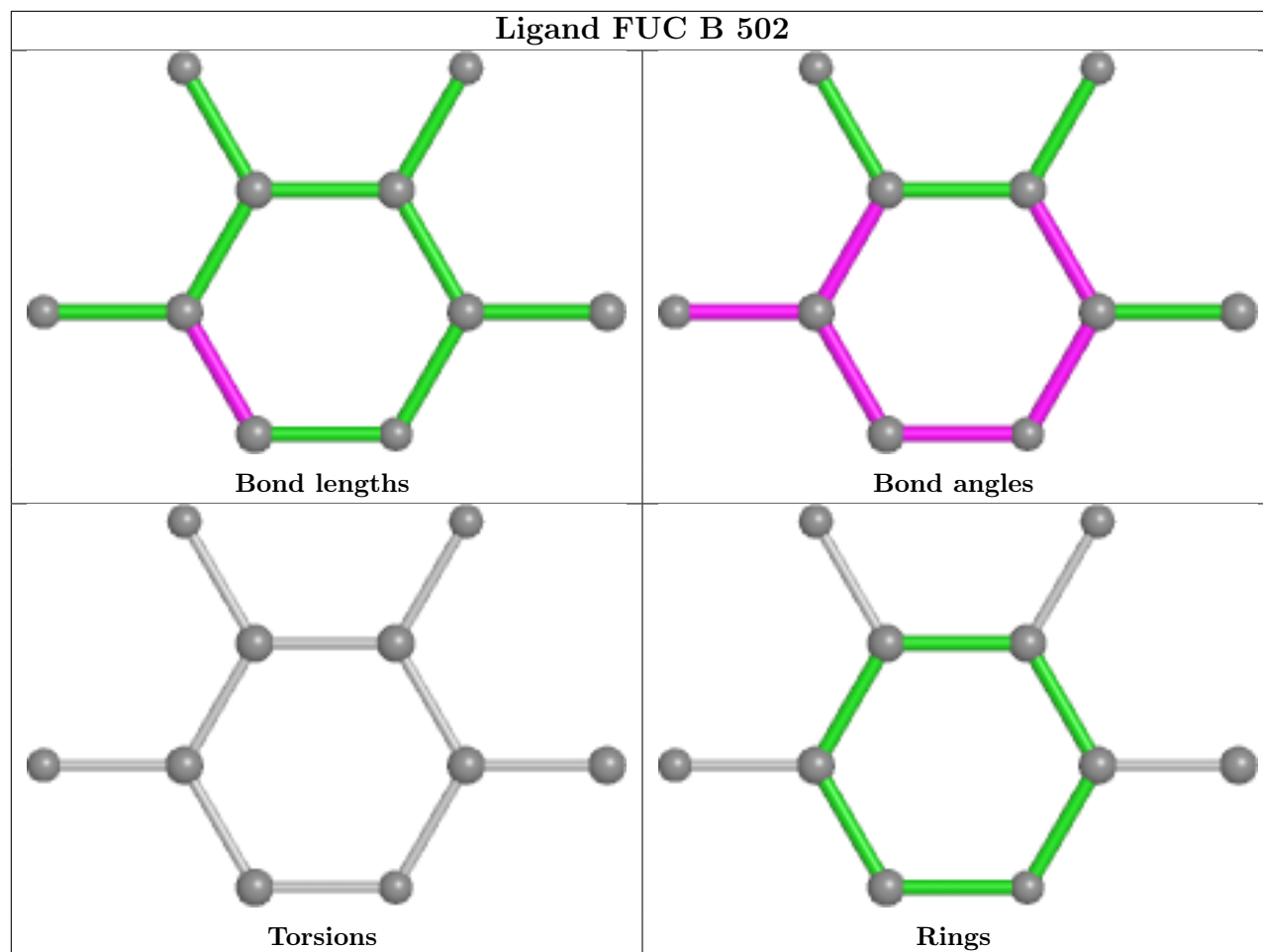
4 monomers are involved in 7 short contacts:

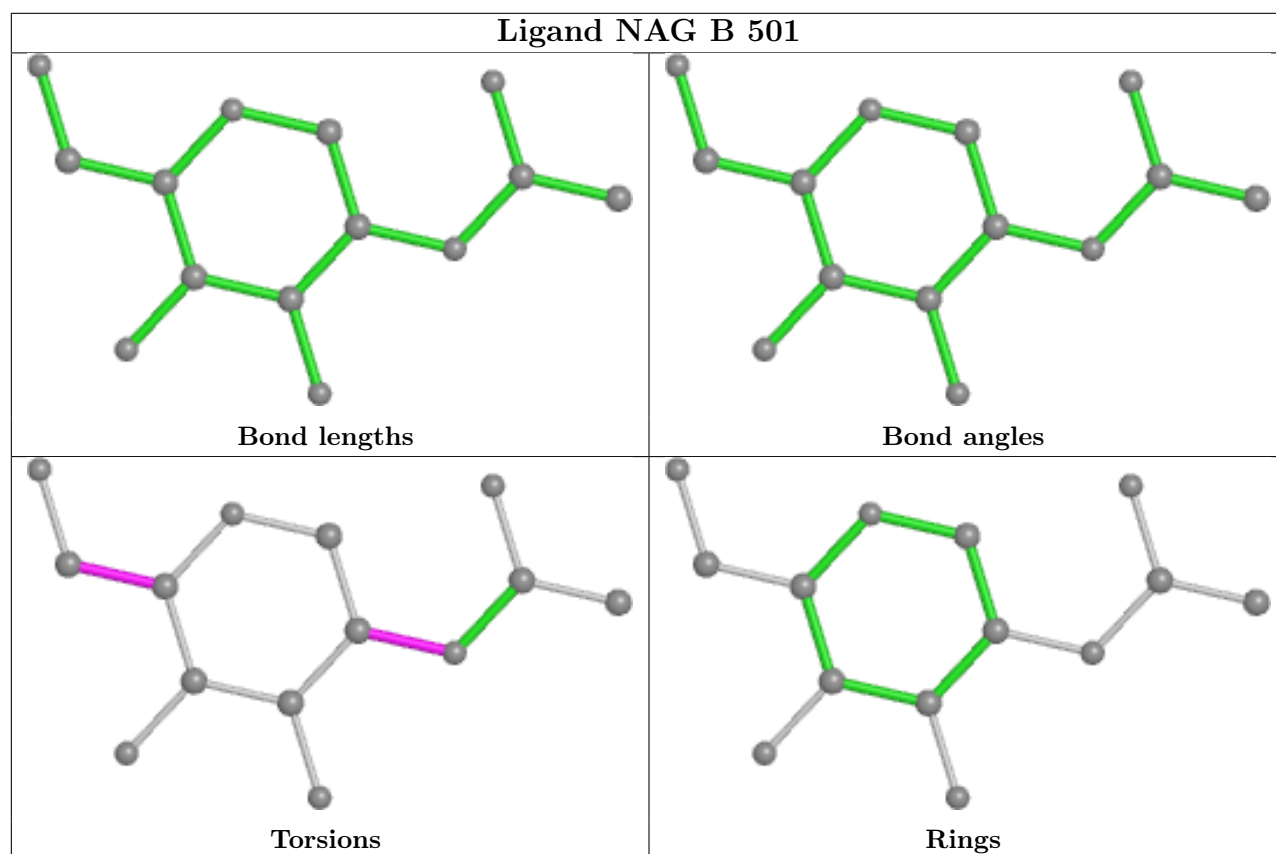
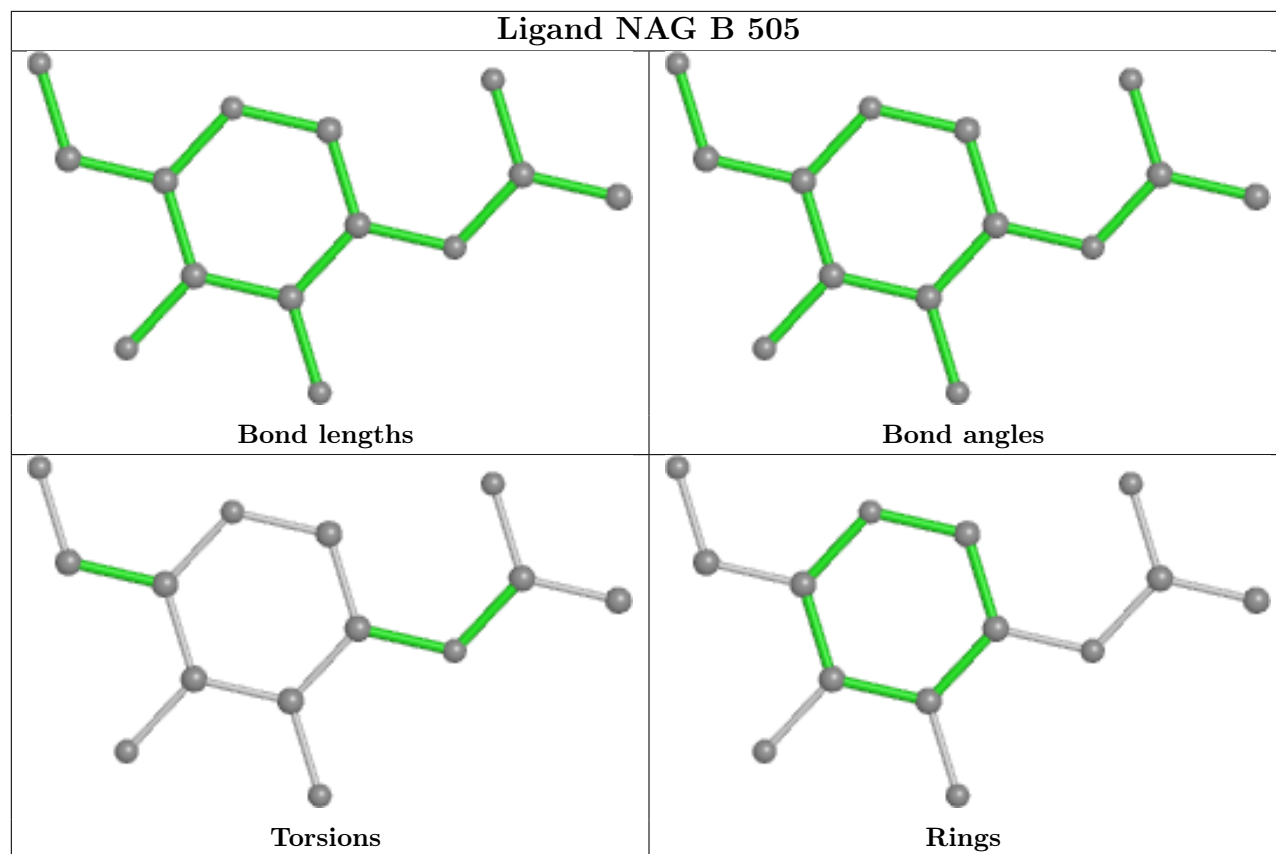
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	506	PO4	1	0
6	A	502	NAG	1	0
6	B	503	NAG	1	0
5	A	501	YA4	1	3

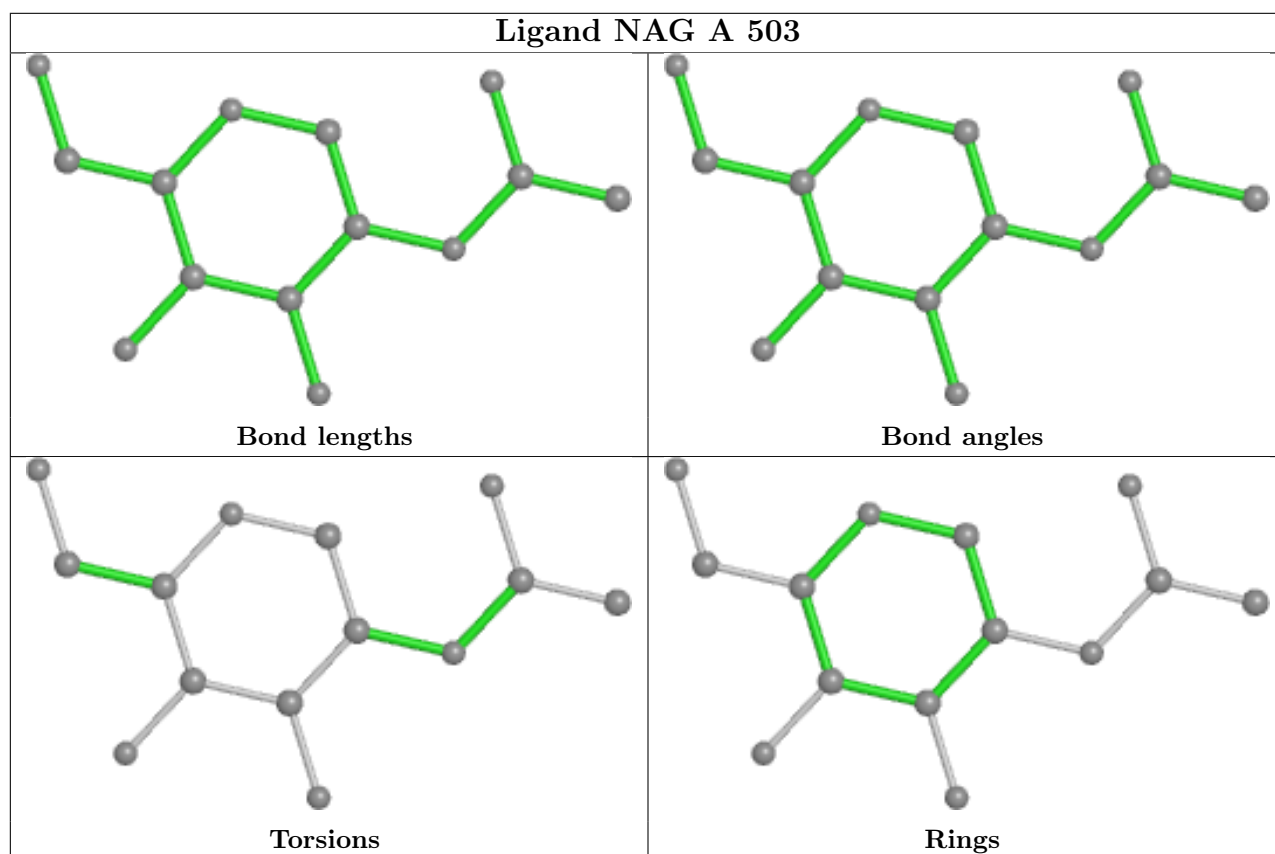
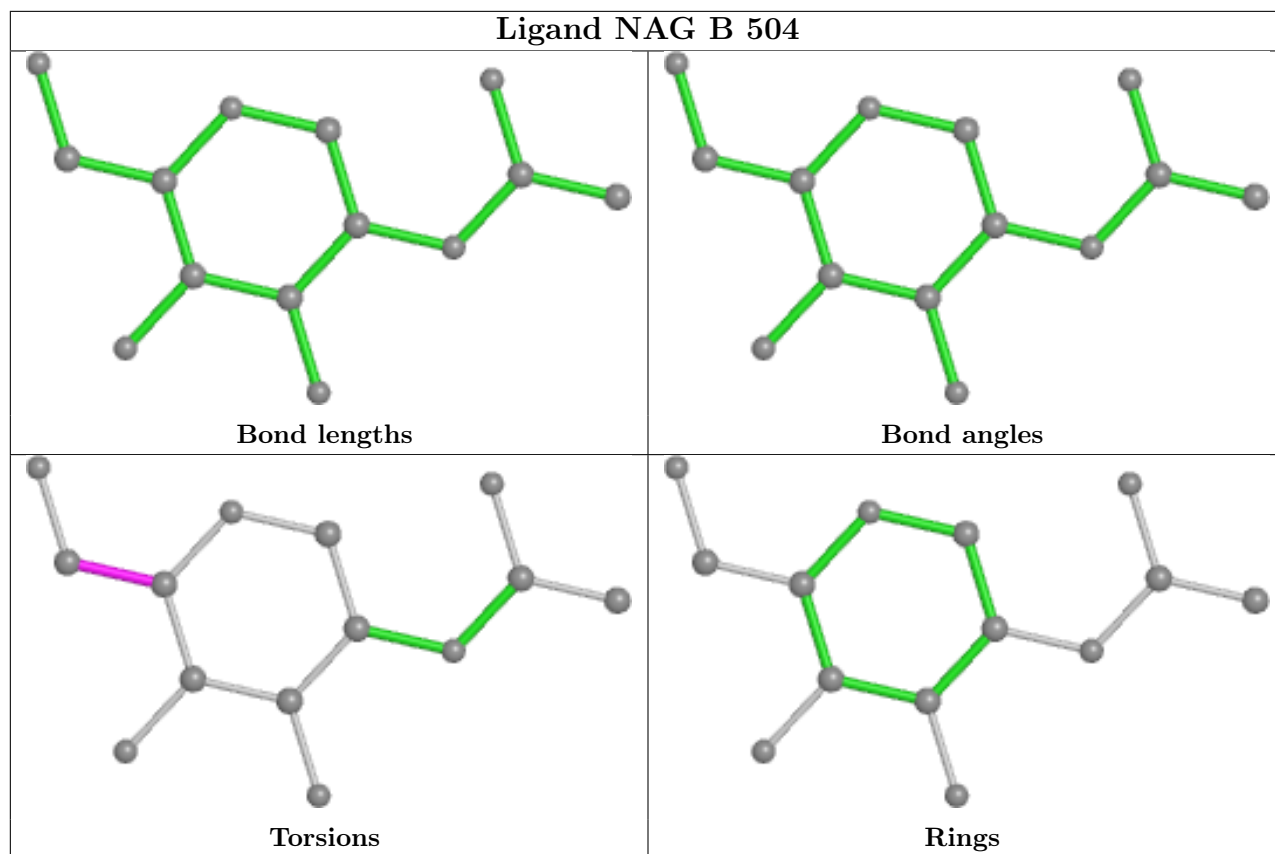
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

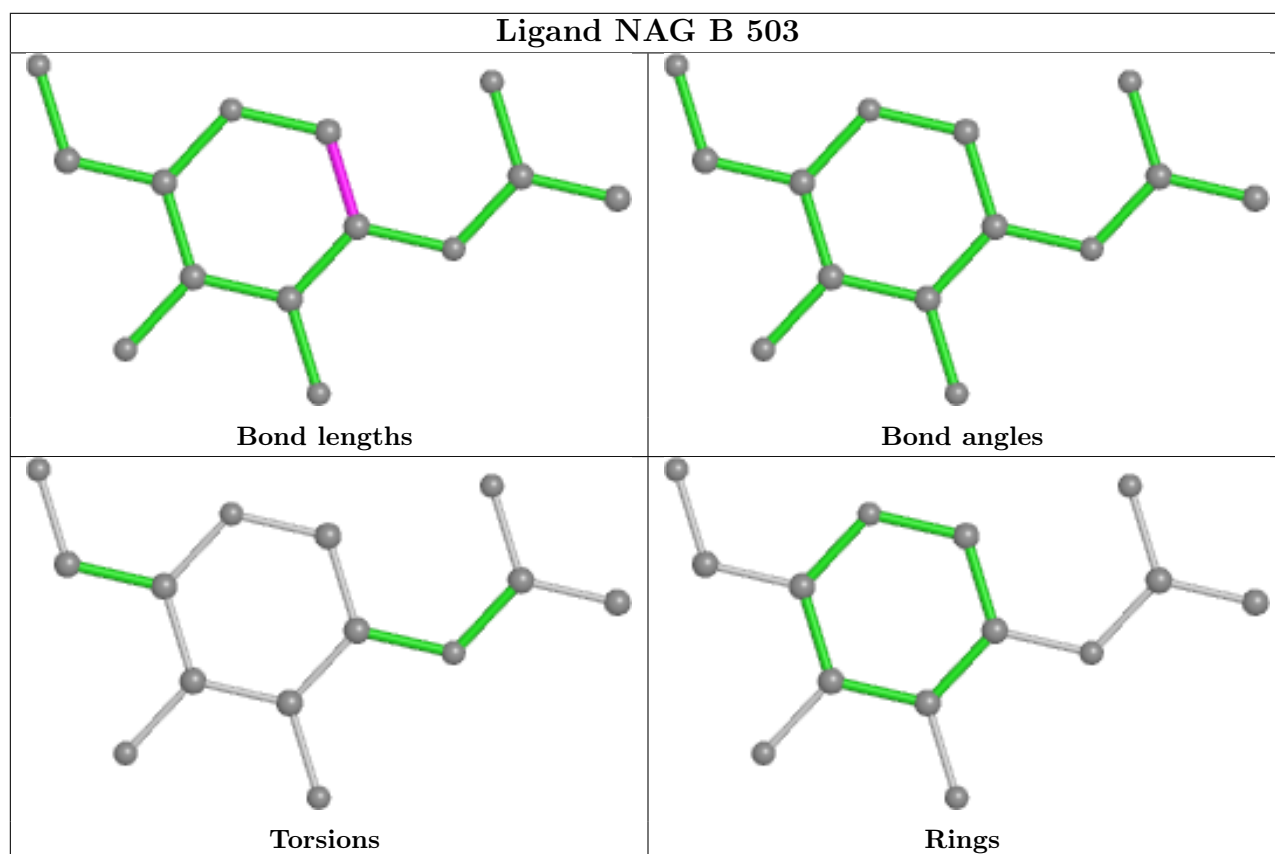
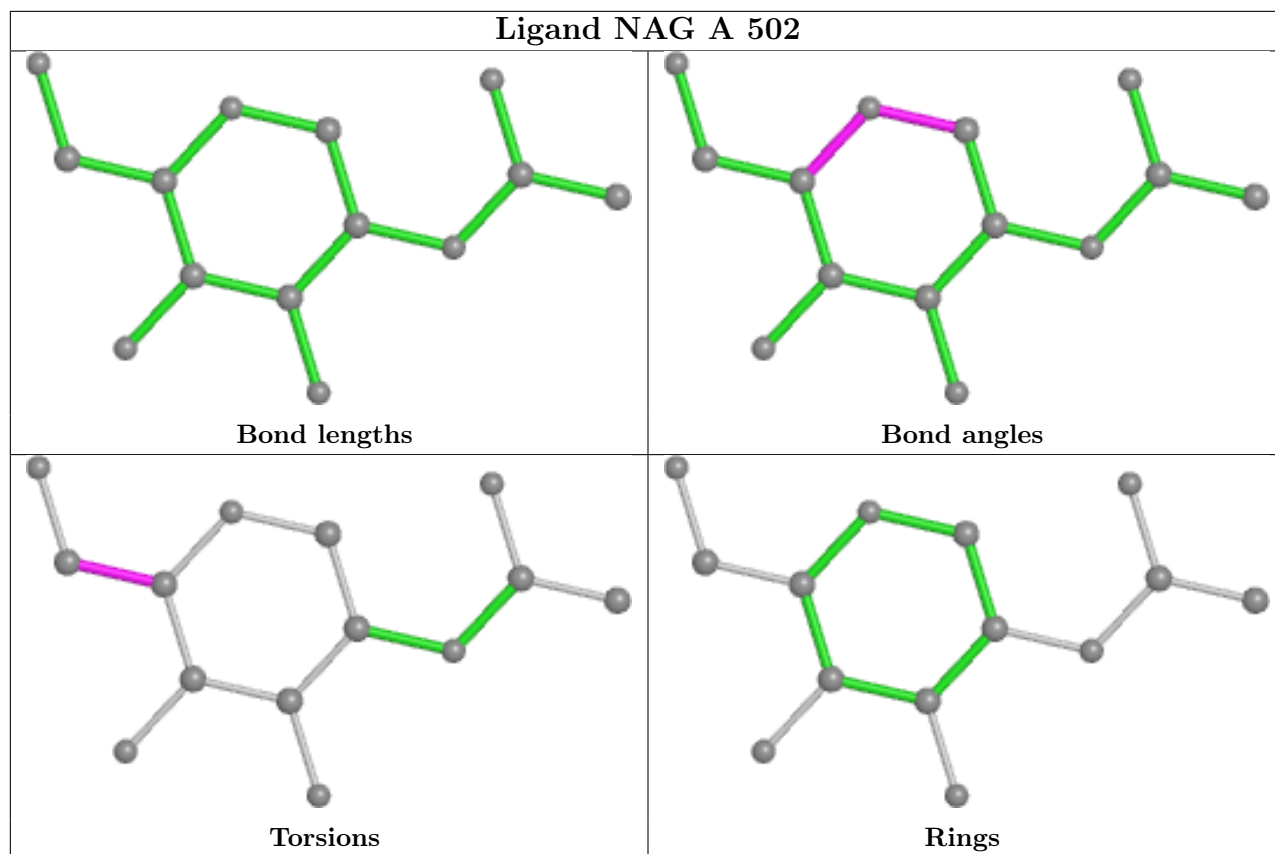


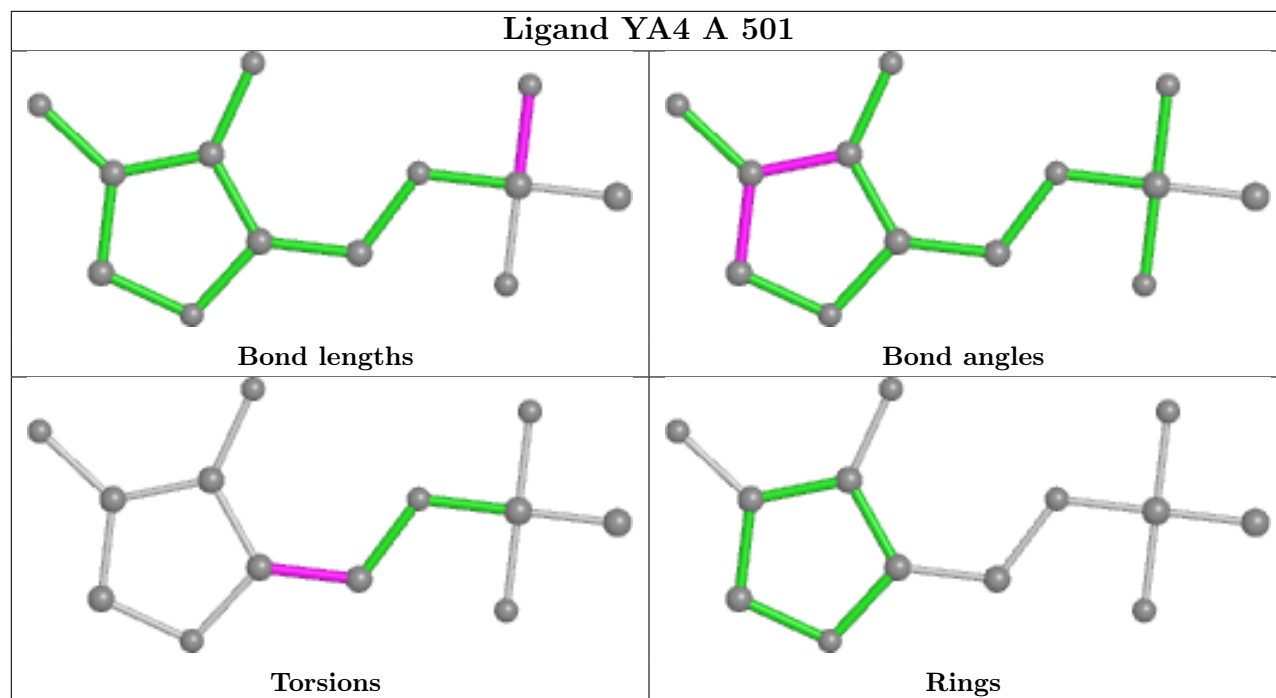












## 5.7 Other polymers [i](#)

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

### 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, 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	412/413 (99%)	0.26	11 (2%) 54 57	16, 27, 43, 52	0
1	B	413/413 (100%)	0.34	20 (4%) 30 34	17, 28, 43, 69	0
All	All	825/826 (99%)	0.30	31 (3%) 40 43	16, 28, 43, 69	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	33	ALA	8.2
1	B	34	VAL	7.7
1	B	395	LYS	4.1
1	A	50	HIS	3.8
1	A	445	LEU	3.3
1	A	414	SER	3.2
1	A	35	GLY	3.1
1	B	419	GLN	3.0
1	B	394	THR	3.0
1	A	395	LYS	2.9
1	B	398	LYS	2.9
1	A	394	THR	2.8
1	B	414	SER	2.7
1	B	376	SER	2.5
1	B	96	GLY	2.4
1	B	445	LEU	2.4
1	A	413	SER	2.3
1	A	373	GLN	2.3
1	B	443	GLN	2.3
1	B	50	HIS	2.2
1	B	303	ASN	2.2
1	B	416	THR	2.2
1	B	323	LEU	2.2
1	B	55	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	52	THR	2.1
1	B	219	ASN	2.1
1	A	53	ASP	2.0
1	B	442	LYS	2.0
1	B	435	MET	2.0
1	A	396	ASP	2.0
1	B	405	HIS	2.0

## 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](#)

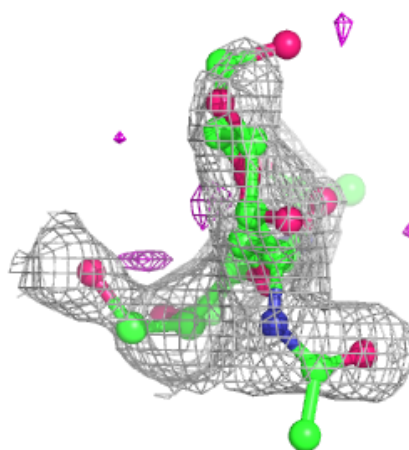
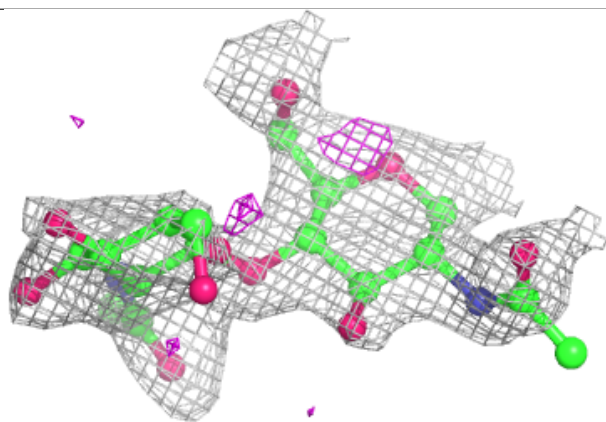
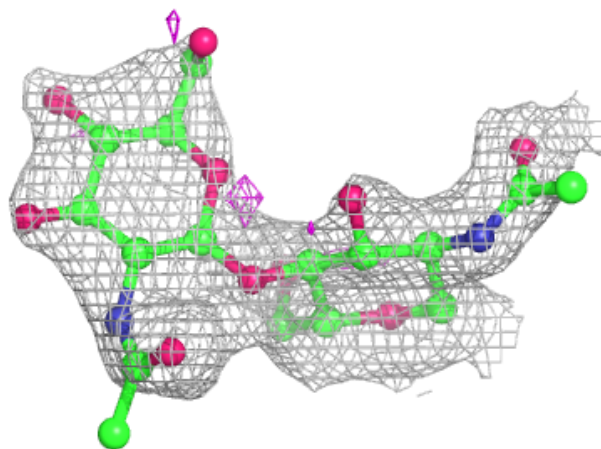
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	FUC	D	2	10/11	0.68	0.36	46,52,54,58	0
4	BMA	F	3	11/12	0.68	0.37	56,63,68,69	0
2	NAG	E	2	14/15	0.74	0.39	49,60,67,68	0
2	NAG	C	1	14/15	0.81	0.32	41,51,58,64	0
2	NAG	C	2	14/15	0.83	0.44	69,71,77,78	0
4	NAG	F	2	14/15	0.87	0.23	42,49,60,62	0
2	NAG	E	1	14/15	0.87	0.16	38,42,48,52	0
3	NAG	D	1	14/15	0.89	0.17	32,40,45,50	0
4	NAG	F	1	14/15	0.89	0.14	30,33,38,43	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 C:**

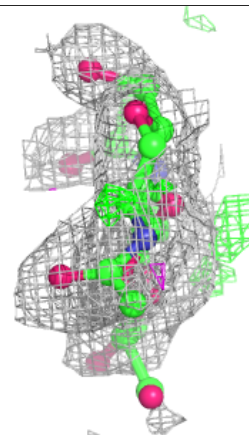
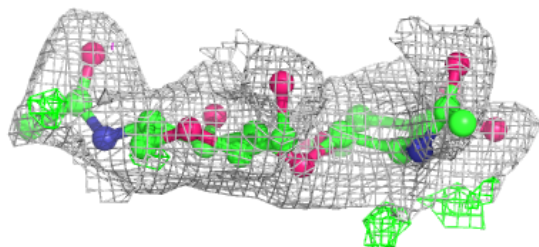
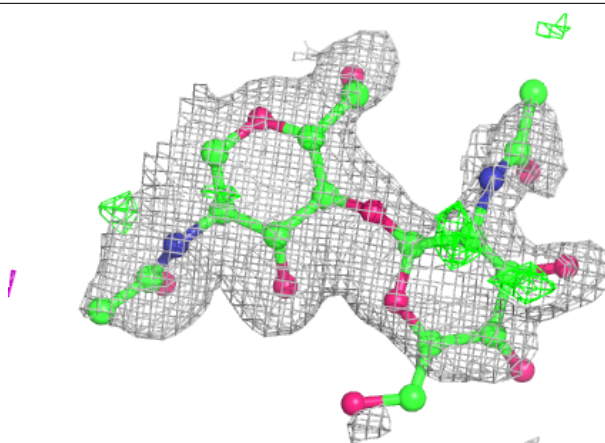
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



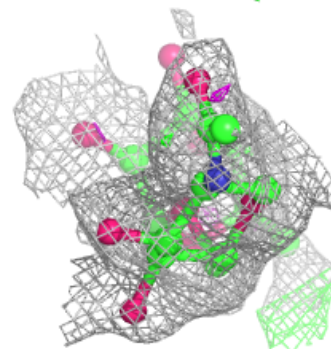
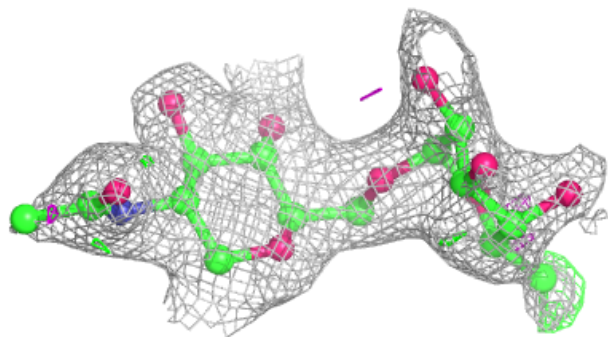
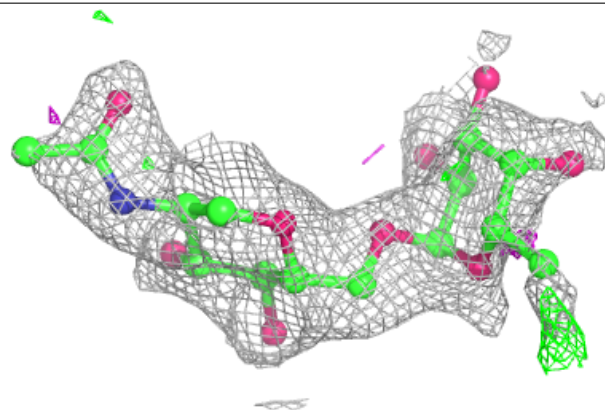


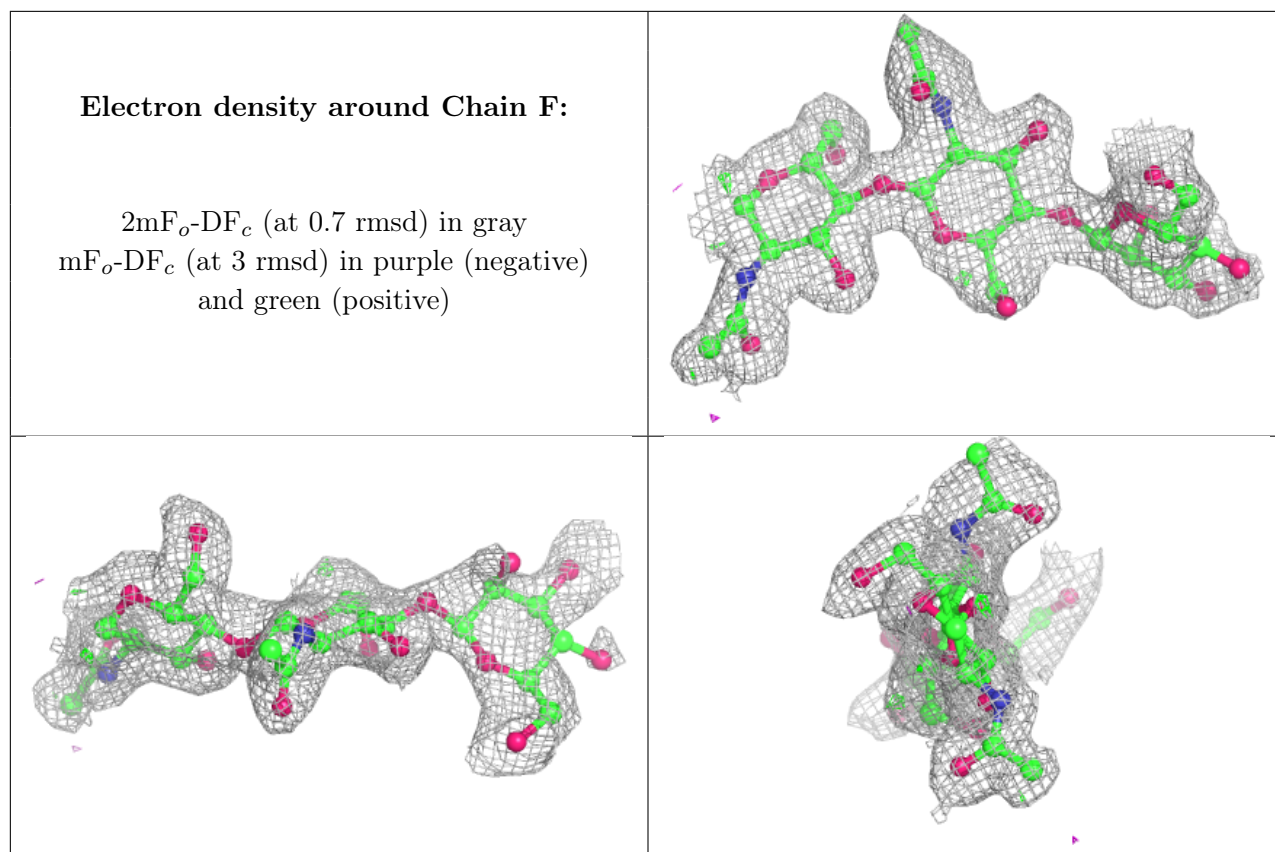
**Electron density around Chain E:**

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

**Electron density around Chain D:**

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



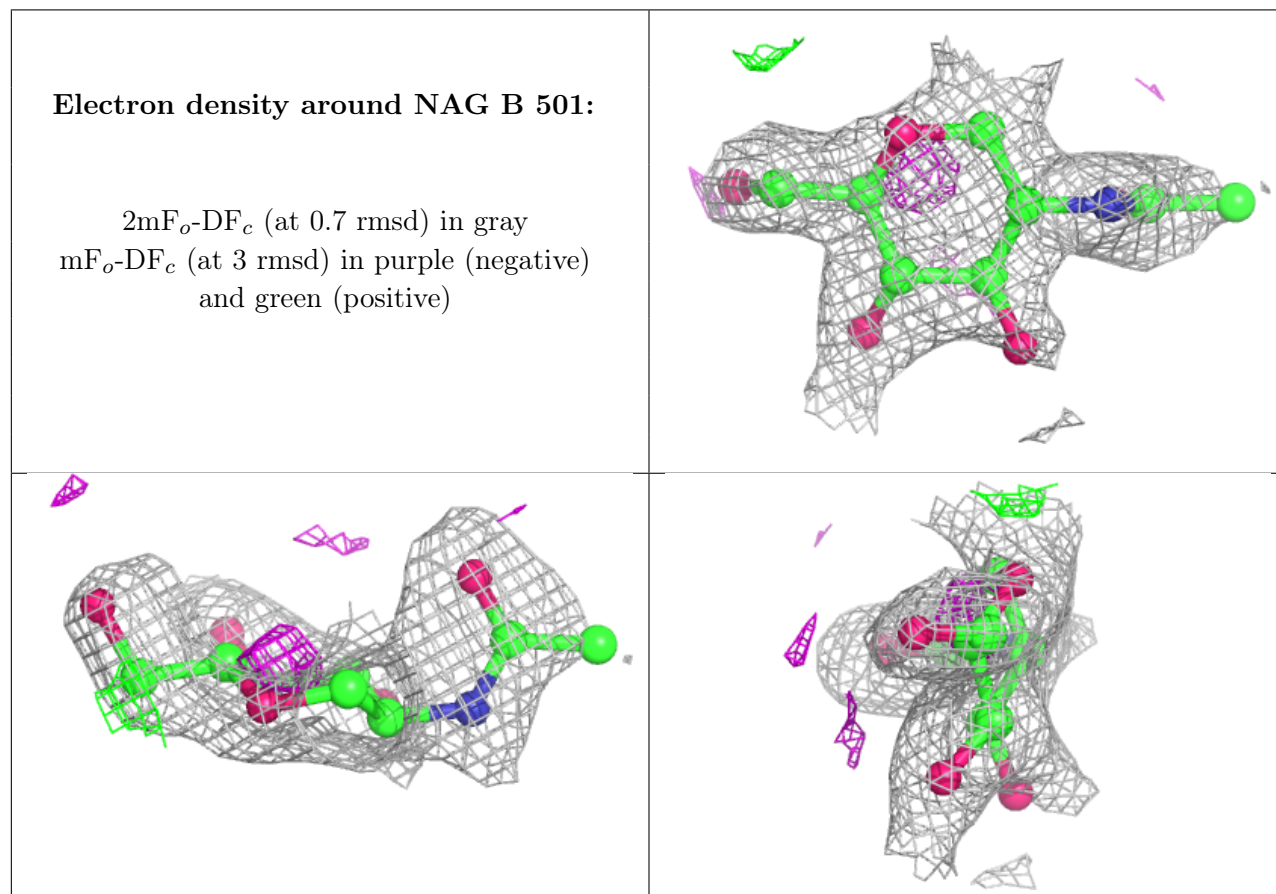


## 6.4 Ligands [i](#)

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, 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.

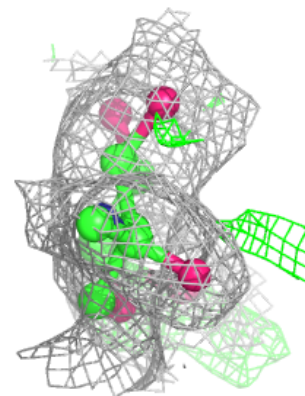
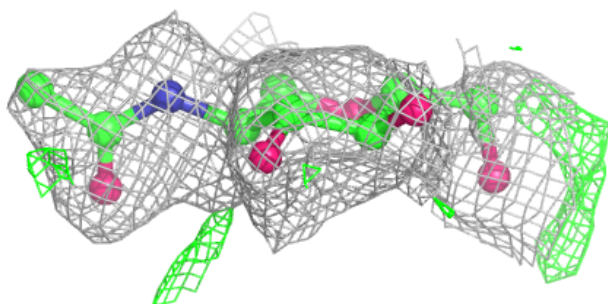
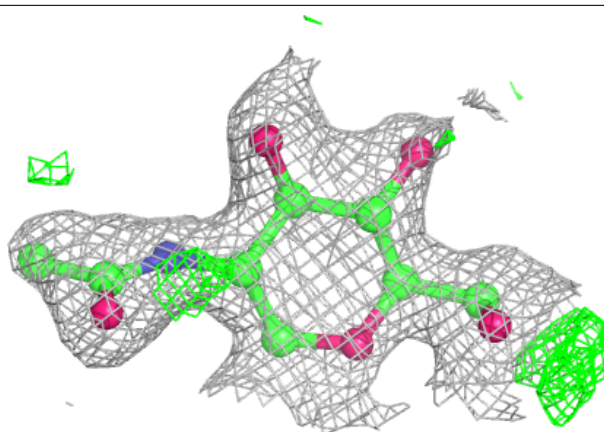
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	B	501	14/15	0.73	0.45	50,55,59,64	0
6	NAG	B	503	14/15	0.79	0.23	34,49,56,62	0
6	NAG	A	502	14/15	0.81	0.24	38,47,52,55	0
8	FUC	B	502	10/11	0.82	0.35	59,61,63,63	0
6	NAG	B	505	14/15	0.88	0.17	37,39,46,49	0
6	NAG	B	504	14/15	0.89	0.23	33,40,52,53	0
6	NAG	A	503	14/15	0.90	0.14	33,37,48,52	0
5	YA4	A	501	13/13	0.93	0.16	25,34,41,41	9
9	PO4	B	506	5/5	0.95	0.10	28,28,34,36	0
7	ZN	B	508	1/1	0.97	0.12	36,36,36,36	0
7	ZN	A	504	1/1	0.98	0.10	33,33,33,33	0
7	ZN	B	507	1/1	0.99	0.04	29,29,29,29	0
7	ZN	A	505	1/1	1.00	0.02	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.

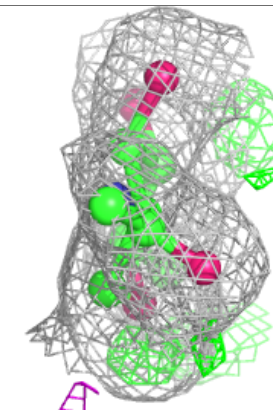
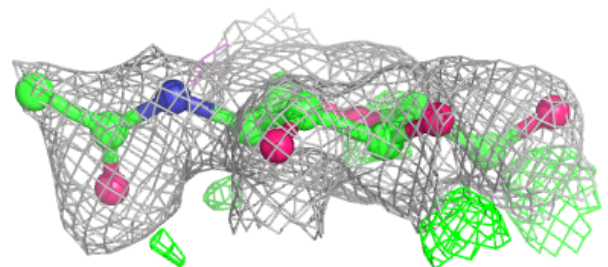
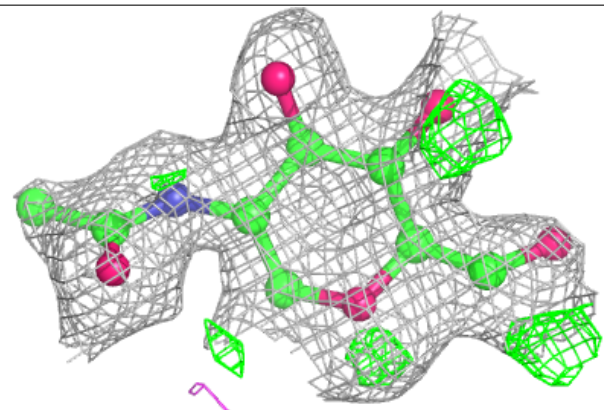


**Electron density around NAG B 503:**

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

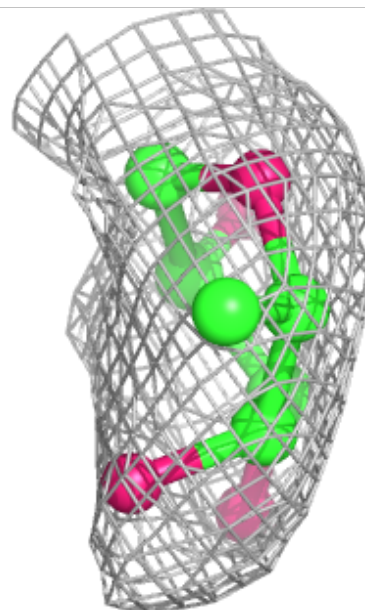
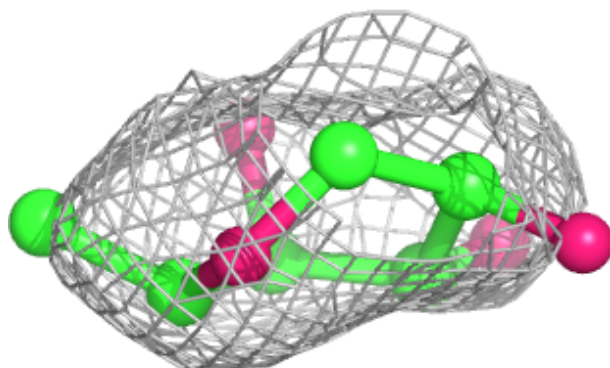
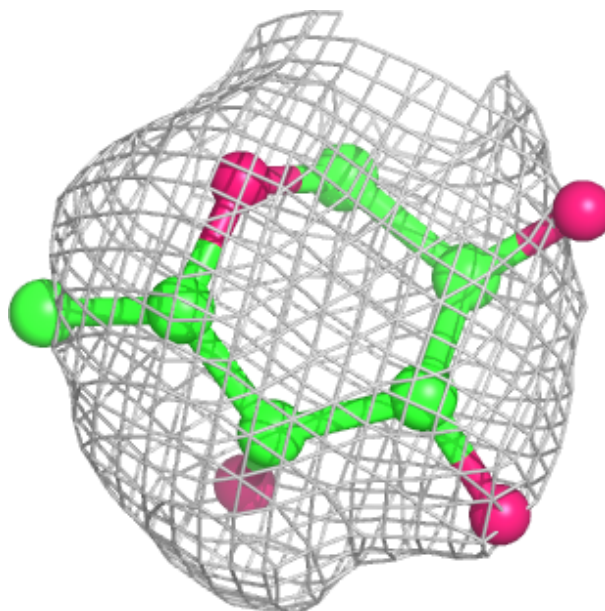
**Electron density around NAG A 502:**

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



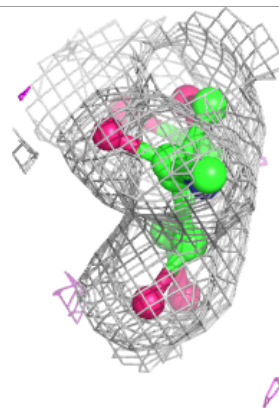
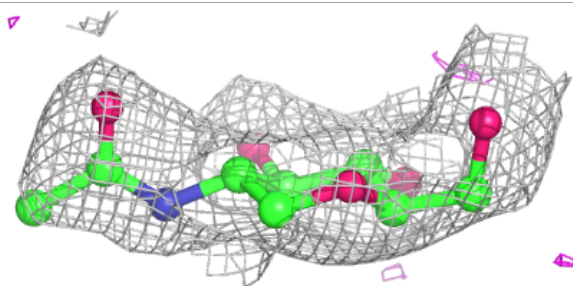
**Electron density around FUC B 502:**

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

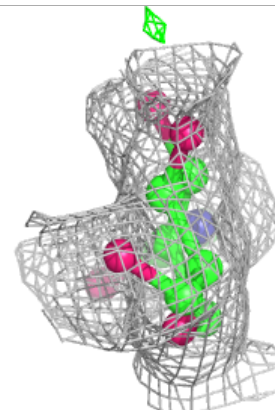
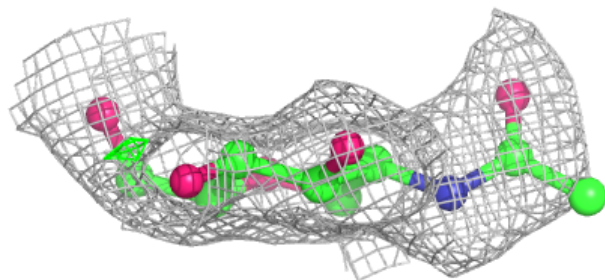
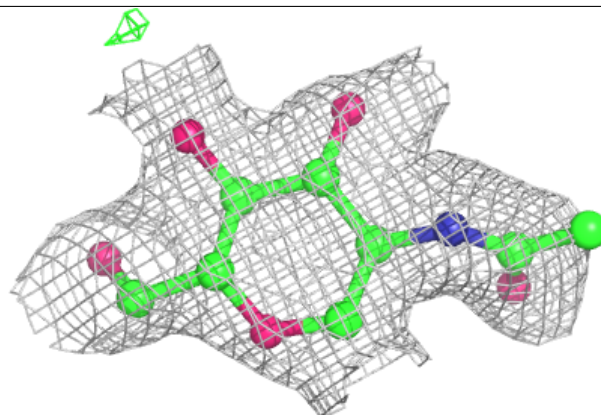


**Electron density around NAG B 505:**

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

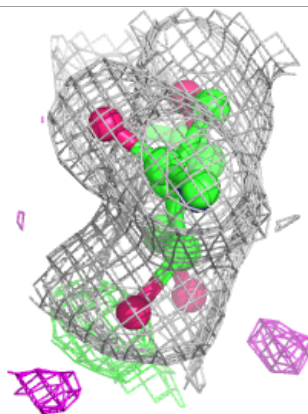
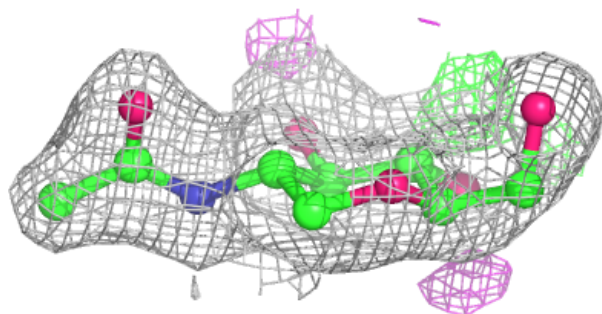
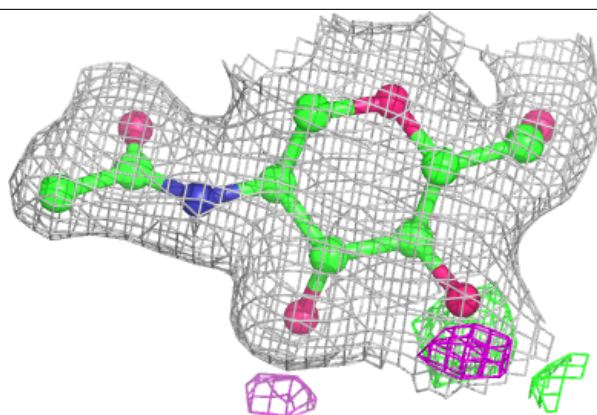
**Electron density around NAG B 504:**

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



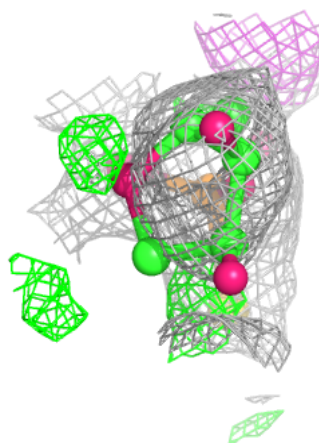
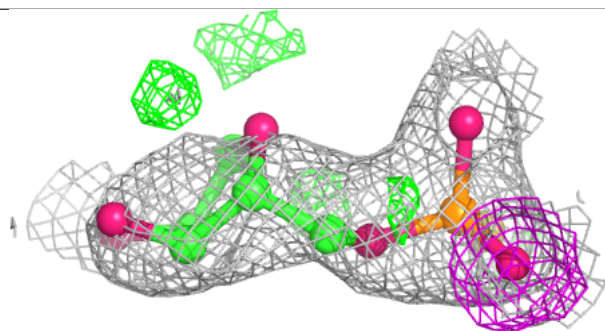
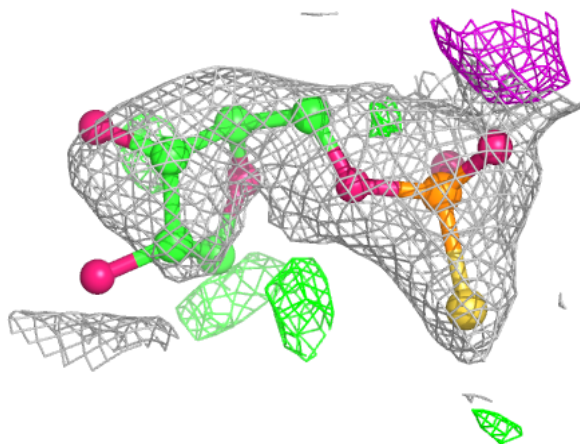
**Electron density around NAG A 503:**

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



**Electron density around YA4 A 501:**

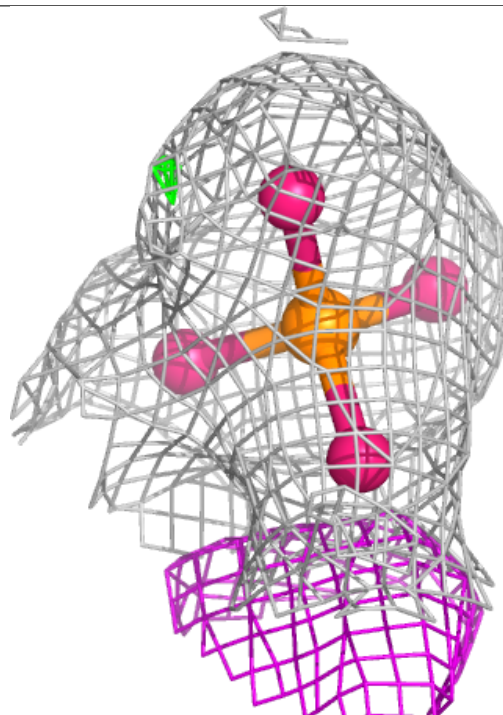
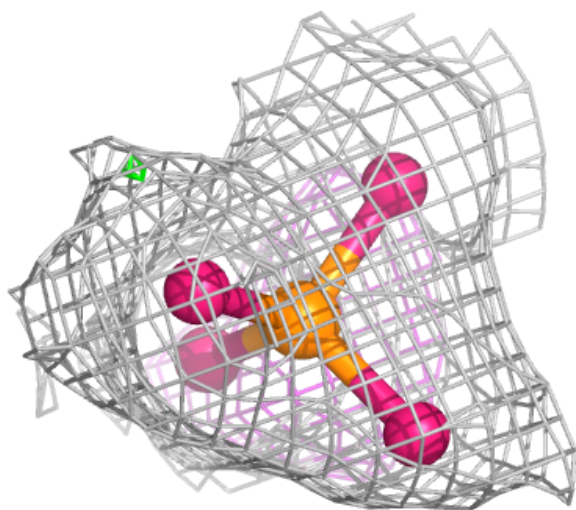
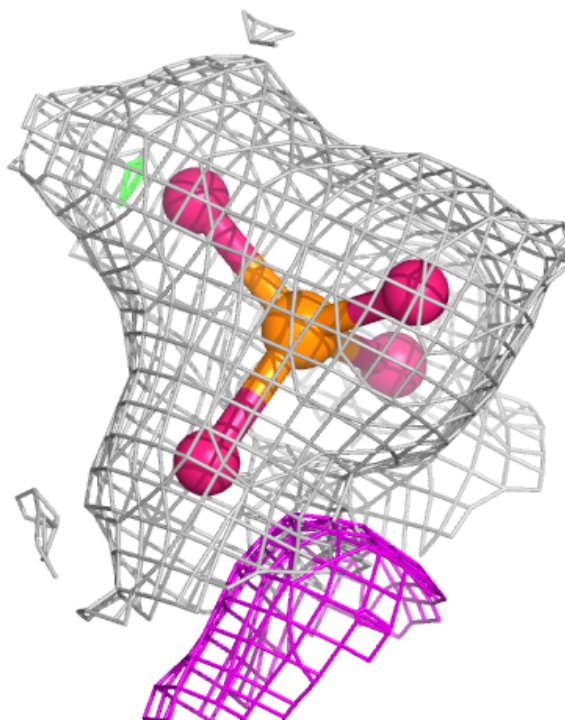
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





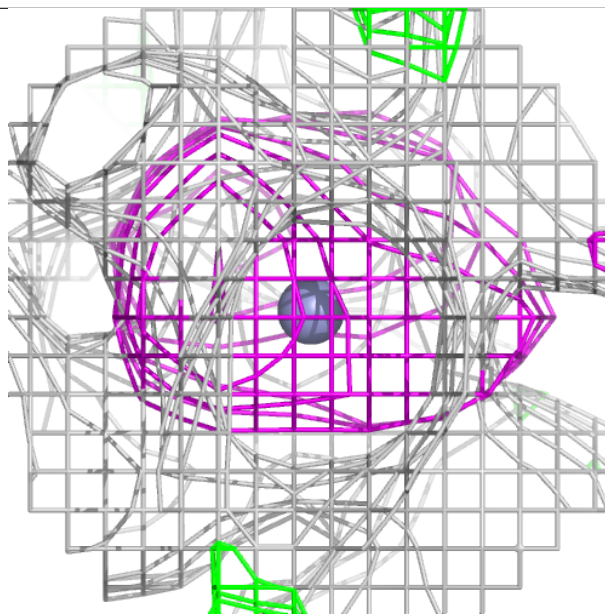
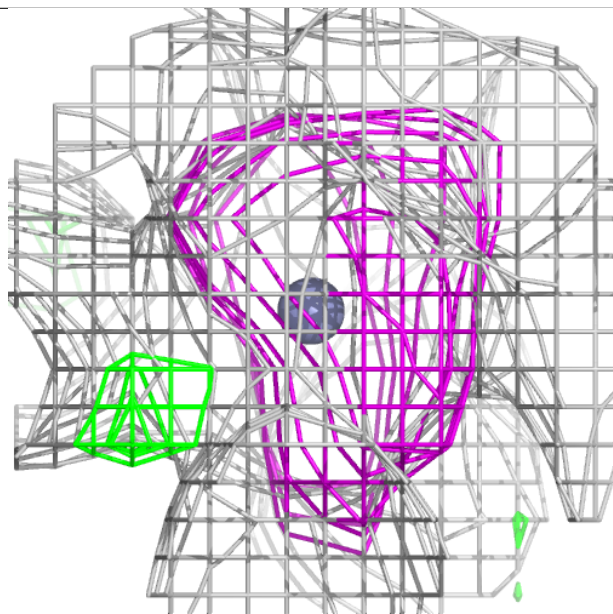
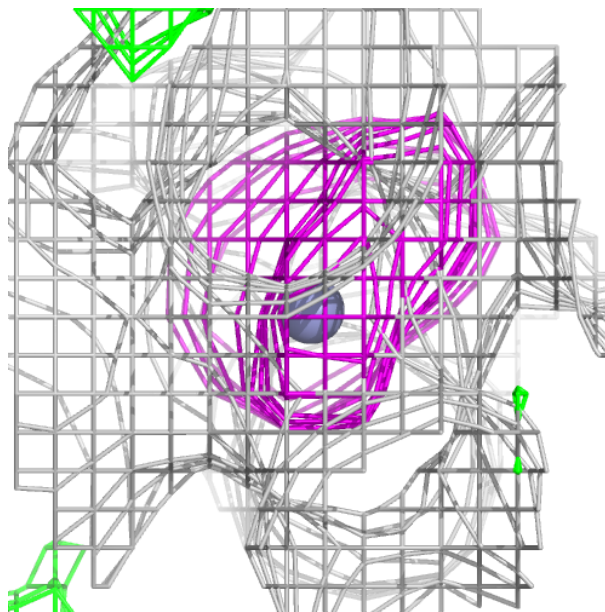
**Electron density around PO4 B 506:**

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



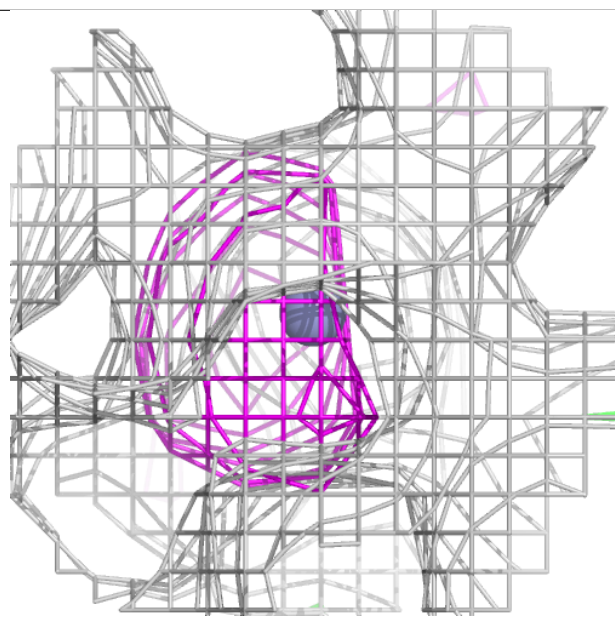
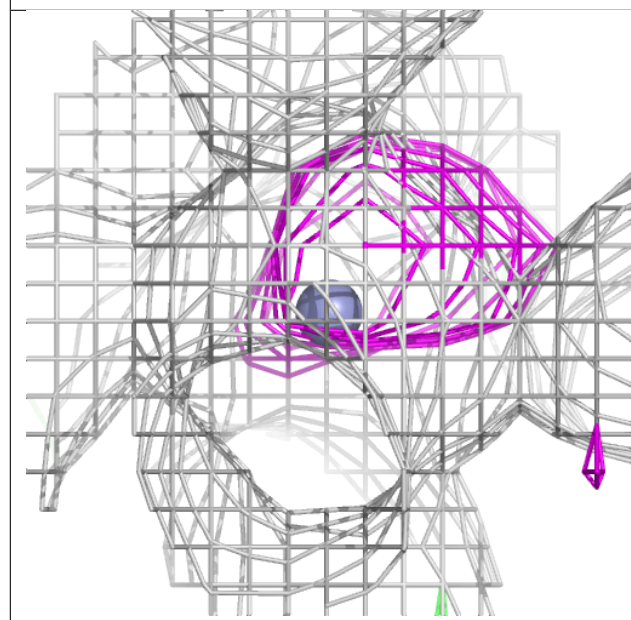
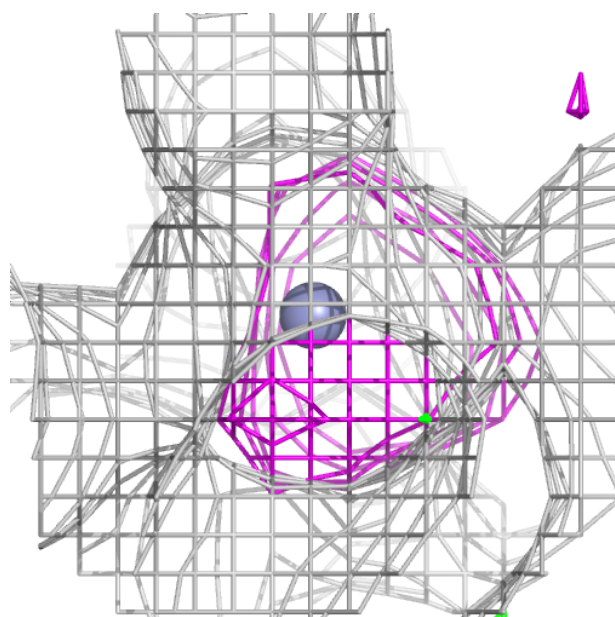
**Electron density around ZN B 508:**

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



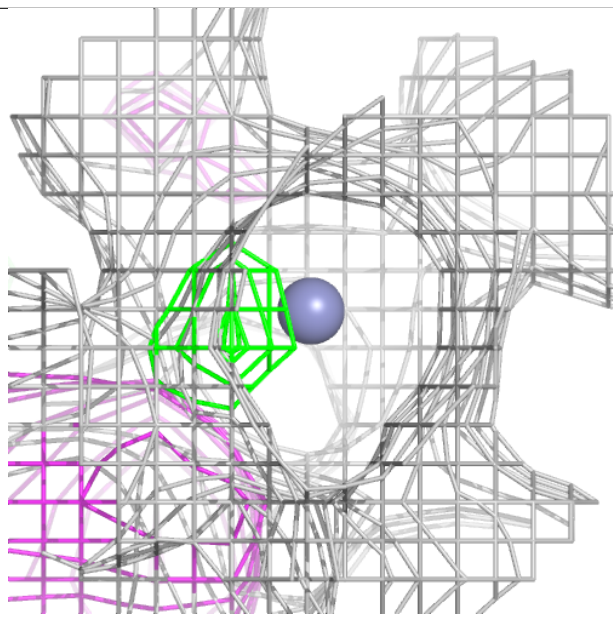
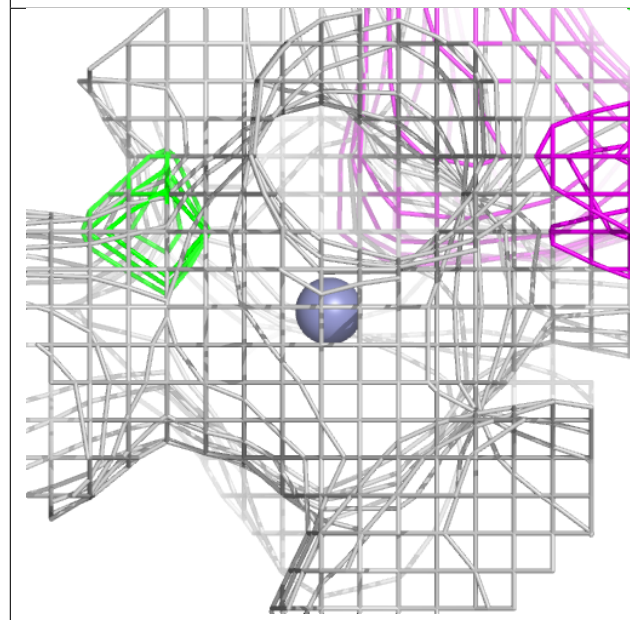
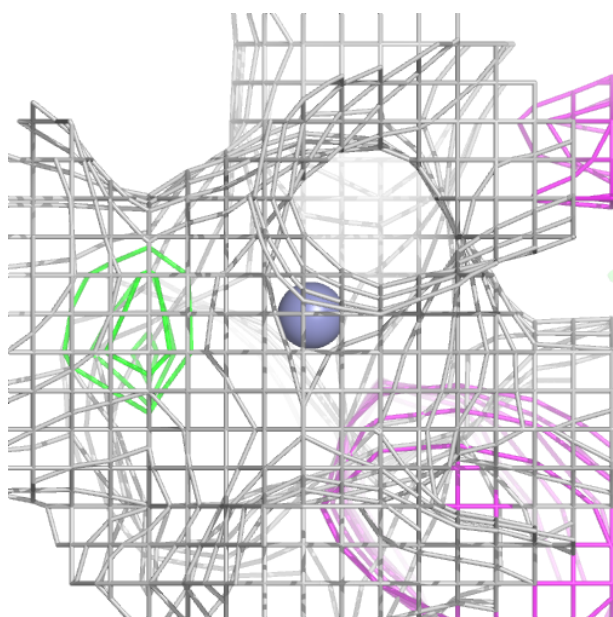
**Electron density around ZN A 504:**

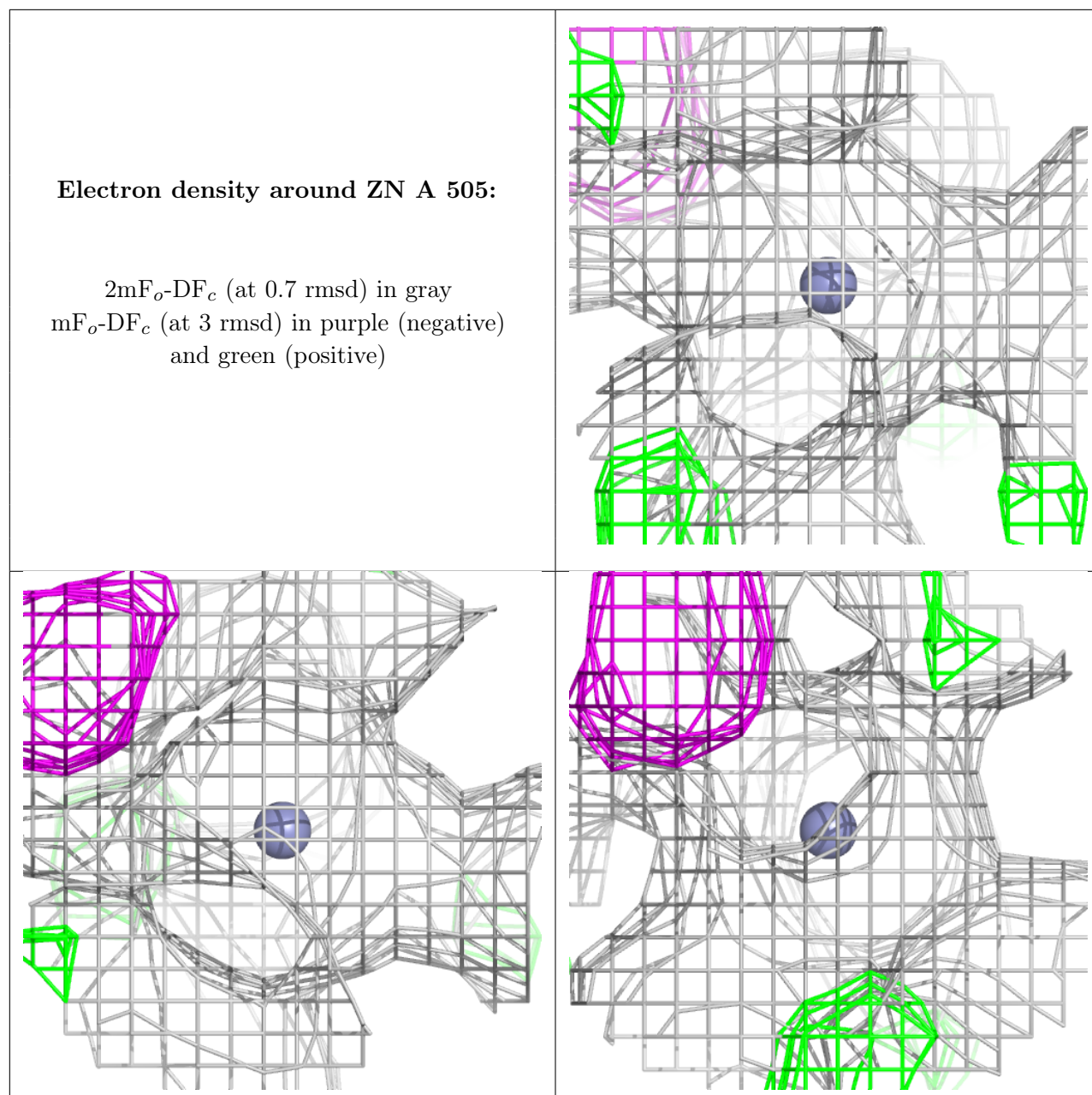
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ZN B 507:**

$2mF_o-DF_c$  (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.