



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 27, 2022 – 06:04 PM JST

PDB ID : 7XB0  
Title : Crystal structure of Omicron BA.2 RBD complexed with hACE2  
Authors : Li, L.; Liao, H.; Meng, Y.; Li, W.  
Deposited on : 2022-03-19  
Resolution : 2.90 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 : 2.29  
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) : 2.29

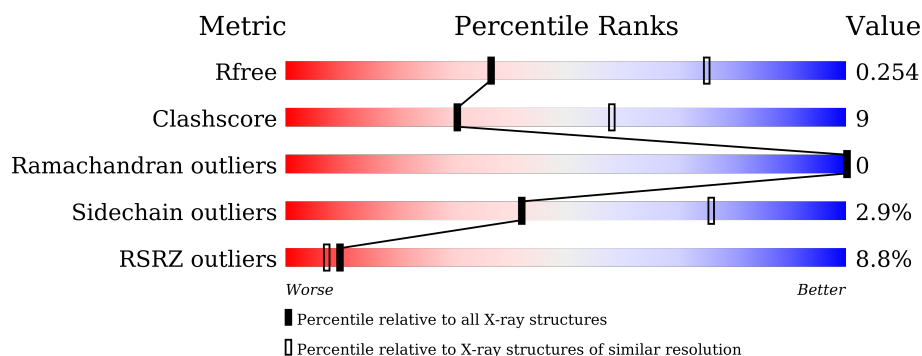
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	596	<div> <div>5%</div> <div>76%</div> <div>24%</div> <div>.</div> </div>
2	B	195	<div> <div>19%</div> <div>74%</div> <div>25%</div> <div>.</div> </div>
3	C	3	<div> <div>67%</div> <div>33%</div> </div>
4	D	2	<div> <div>100%</div> </div>
4	E	2	<div> <div>50%</div> <div>50%</div> </div>

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
4	NAG	D	1	-	-	-	X
4	NAG	D	2	-	-	-	X
4	NAG	E	2	-	-	-	X
6	NAG	A	702	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6557 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
1	A	596	Total	C	N	O	S	0	0	0
			4862	3111	805	917	29			

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	195	Total	C	N	O	S	0	0	0
			1557	1006	262	281	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	339	ASP	GLY	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	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2

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



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

- Molecule 4 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
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- 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).

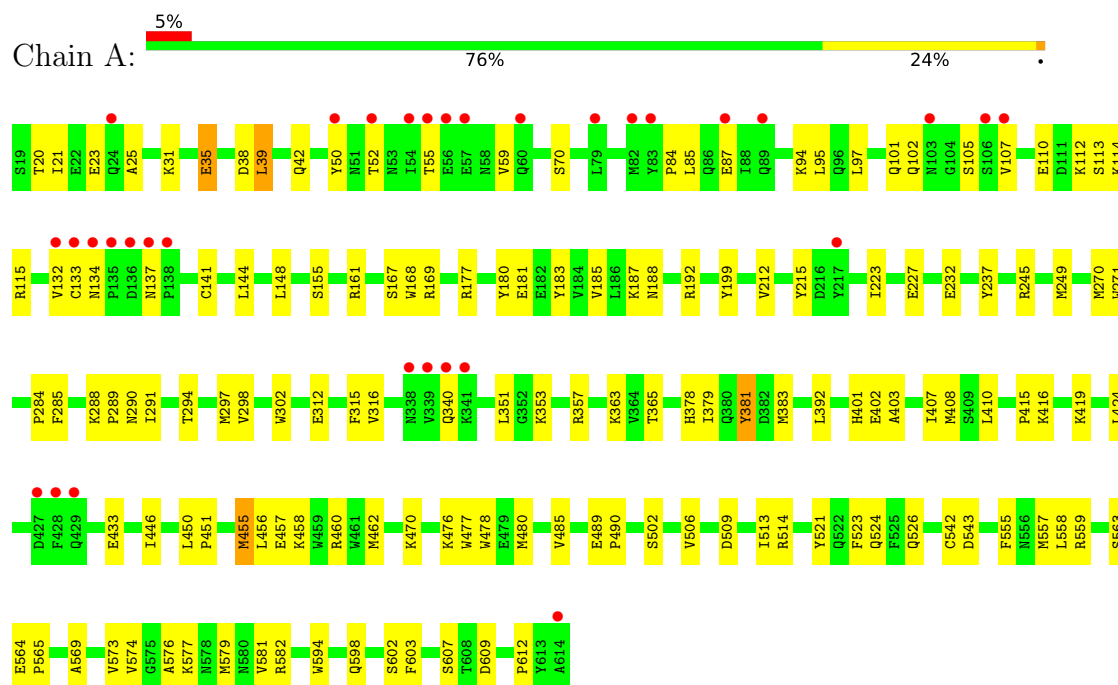


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

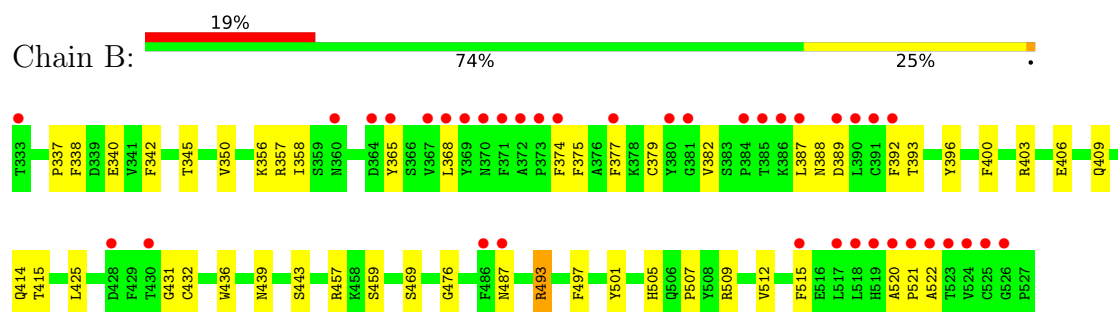
### 3 Residue-property plots

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

#### • Molecule 1: Angiotensin-converting enzyme 2



#### • Molecule 2: Spike protein S1



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





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

Chain D:  100%



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

Chain E:  50% 50%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.26Å 103.26Å 224.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.66 – 2.90 49.37 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.5 (19.66-2.90) 94.5 (49.37-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.216 , 0.255 0.215 , 0.254	Depositor DCC
$R_{free}$ test set	1306 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.1	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 27.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6557	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, 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	0.25	0/4999	0.43	0/6792
2	B	0.27	0/1605	0.51	0/2185
All	All	0.26	0/6604	0.45	0/8977

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	4634	85	0
2	B	1557	0	1479	34	0
3	C	39	0	34	1	0
4	D	28	0	25	0	0
4	E	28	0	25	3	0
5	A	1	0	0	0	0
6	A	42	0	39	1	0
All	All	6557	0	6236	117	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (117) 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:132:VAL:HG21	1:A:167:SER:HB3	1.60	0.83
1:A:25:ALA:HB1	1:A:97:LEU:HD11	1.66	0.78
2:B:403:ARG:HG3	2:B:406:GLU:HG3	1.70	0.74
2:B:365:TYR:HA	2:B:368:LEU:HD13	1.70	0.74
2:B:393:THR:HA	2:B:522:ALA:HA	1.76	0.68
2:B:374:PHE:HD1	2:B:436:TRP:HB3	1.59	0.67
1:A:38:ASP:O	1:A:42:GLN:HG3	1.97	0.64
2:B:409:GLN:HA	2:B:414:GLN:HG2	1.80	0.63
2:B:365:TYR:HD2	2:B:388:ASN:HB2	1.64	0.62
1:A:490:PRO:HA	1:A:612:PRO:HG2	1.81	0.62
1:A:134:ASN:OD1	1:A:137:ASN:HB3	2.00	0.61
1:A:31:LYS:HG2	1:A:35:GLU:OE1	2.00	0.60
1:A:457:GLU:HG2	1:A:513:ILE:HB	1.84	0.60
1:A:607:SER:OG	1:A:609:ASP:OD1	2.19	0.59
1:A:476:LYS:O	1:A:480:MET:HG3	2.03	0.59
1:A:84:PRO:HG2	1:A:87:GLU:OE1	2.03	0.58
1:A:379:ILE:O	1:A:383:MET:HG3	2.03	0.58
2:B:425:LEU:HD21	2:B:512:VAL:HG11	1.84	0.58
1:A:181:GLU:O	1:A:185:VAL:HG23	2.05	0.57
1:A:35:GLU:O	1:A:39:LEU:HD12	2.04	0.57
2:B:345:THR:O	2:B:509:ARG:NH2	2.39	0.56
2:B:457:ARG:NH1	2:B:459:SER:O	2.39	0.56
1:A:50:TYR:CE1	1:A:59:VAL:HG22	2.40	0.56
1:A:312:GLU:O	1:A:316:VAL:HG23	2.05	0.55
2:B:340:GLU:OE1	2:B:356:LYS:NZ	2.38	0.55
1:A:85:LEU:HD22	1:A:94:LYS:HG3	1.89	0.54
1:A:133:CYS:HA	1:A:141:CYS:HA	1.89	0.54
2:B:415:THR:HG21	3:C:3:BMA:H4	1.90	0.54
1:A:407:ILE:HB	1:A:526:GLN:HG2	1.90	0.53
1:A:212:VAL:HG12	1:A:215:TYR:HB2	1.92	0.52
1:A:177:ARG:NH2	1:A:470:LYS:O	2.44	0.51
1:A:112:LYS:HG2	1:A:115:ARG:HH21	1.76	0.51
1:A:245:ARG:NH2	1:A:603:PHE:O	2.44	0.50
1:A:237:TYR:OH	1:A:485:VAL:O	2.21	0.50
2:B:338:PHE:CD2	2:B:368:LEU:HD11	2.47	0.50
1:A:294:THR:HG23	1:A:365:THR:HA	1.94	0.50
1:A:446:ILE:HD13	1:A:523:PHE:HZ	1.76	0.50
1:A:290:ASN:OD1	1:A:291:ILE:N	2.44	0.50
1:A:284:PRO:HB3	1:A:594:TRP:CZ2	2.47	0.49
1:A:564:GLU:HG3	1:A:565:PRO:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:TYR:HE1	1:A:59:VAL:HG22	1.76	0.49
1:A:289:PRO:O	1:A:290:ASN:HB3	2.13	0.49
1:A:455:MET:HE2	1:A:480:MET:HB2	1.94	0.49
1:A:20:THR:HG23	1:A:23:GLU:H	1.78	0.48
1:A:458:LYS:O	1:A:462:MET:HG3	2.13	0.48
2:B:338:PHE:CG	2:B:368:LEU:HD11	2.49	0.48
2:B:342:PHE:HB2	4:E:1:NAG:H82	1.94	0.48
2:B:520:ALA:HB1	2:B:521:PRO:HD2	1.95	0.48
1:A:85:LEU:HD13	1:A:94:LYS:HE3	1.96	0.48
1:A:524:GLN:HB3	1:A:574:VAL:HG11	1.96	0.48
1:A:555:PHE:O	1:A:559:ARG:HG2	2.14	0.47
1:A:168:TRP:CD1	1:A:502:SER:HB2	2.50	0.47
1:A:594:TRP:CZ2	1:A:598:GLN:HG3	2.50	0.47
1:A:105:SER:HA	1:A:107:VAL:HG12	1.95	0.47
2:B:431:GLY:HA2	2:B:515:PHE:CD2	2.50	0.47
1:A:97:LEU:O	1:A:101:GLN:HG3	2.15	0.47
1:A:212:VAL:CG1	1:A:215:TYR:HB2	2.45	0.47
1:A:35:GLU:OE1	2:B:493:ARG:NH1	2.48	0.46
1:A:353:LYS:HD2	2:B:505:HIS:ND1	2.29	0.46
1:A:381:TYR:CE1	1:A:558:LEU:HA	2.50	0.46
2:B:382:VAL:HG23	2:B:387:LEU:HD23	1.98	0.46
1:A:180:TYR:HA	1:A:183:TYR:HB3	1.97	0.46
1:A:297:MET:HG2	1:A:302:TRP:CE3	2.49	0.46
1:A:521:TYR:HE1	1:A:579:MET:HB2	1.80	0.46
2:B:368:LEU:HA	4:E:1:NAG:H83	1.97	0.46
1:A:188:ASN:O	1:A:192:ARG:HD2	2.15	0.46
1:A:223:ILE:O	1:A:227:GLU:HG3	2.15	0.46
1:A:288:LYS:HE3	1:A:433:GLU:OE1	2.15	0.45
1:A:52:THR:O	1:A:340:GLN:NE2	2.46	0.45
1:A:363:LYS:HB2	1:A:365:THR:HG23	1.97	0.45
1:A:456:LEU:HD12	1:A:477:TRP:HH2	1.82	0.45
1:A:232:GLU:HB2	1:A:581:VAL:HG11	1.98	0.45
1:A:574:VAL:HG23	1:A:576:ALA:H	1.82	0.45
1:A:415:PRO:O	1:A:419:LYS:HG3	2.17	0.44
1:A:557:MET:HG2	1:A:569:ALA:HB1	1.99	0.44
1:A:351:LEU:HD12	1:A:351:LEU:H	1.81	0.44
2:B:493:ARG:HD3	2:B:493:ARG:HA	1.40	0.44
2:B:392:PHE:CD2	2:B:515:PHE:HB3	2.52	0.44
2:B:439:ASN:O	2:B:443:SER:HB2	2.17	0.44
1:A:416:LYS:HD2	1:A:543:ASP:HB3	2.00	0.44
1:A:478:TRP:CD2	1:A:489:GLU:HB3	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LEU:HD23	1:A:85:LEU:HA	1.87	0.43
1:A:450:LEU:HB2	1:A:451:PRO:HD3	2.01	0.43
2:B:337:PRO:HD2	2:B:358:ILE:HD13	2.00	0.43
2:B:350:VAL:HG23	2:B:400:PHE:CD1	2.54	0.43
2:B:497:PHE:CD2	2:B:507:PRO:HB3	2.53	0.43
1:A:187:LYS:HB3	1:A:199:TYR:CG	2.54	0.43
1:A:378:HIS:HE1	1:A:402:GLU:HA	1.84	0.43
2:B:357:ARG:HG3	2:B:396:TYR:CE1	2.54	0.43
1:A:353:LYS:HG3	2:B:501:TYR:CZ	2.53	0.42
1:A:458:LYS:HG2	1:A:480:MET:HE1	2.01	0.42
6:A:703:NAG:O7	6:A:703:NAG:H3	2.20	0.42
2:B:374:PHE:CD1	2:B:436:TRP:HB3	2.46	0.42
1:A:215:TYR:CE1	1:A:577:LYS:HE3	2.54	0.42
2:B:342:PHE:CB	4:E:1:NAG:H82	2.50	0.42
1:A:460:ARG:NH1	1:A:506:VAL:HA	2.34	0.42
1:A:410:LEU:HD12	1:A:526:GLN:HG3	2.00	0.42
1:A:315:PHE:CZ	1:A:408:MET:HG3	2.55	0.42
1:A:285:PHE:CE2	1:A:433:GLU:HG2	2.54	0.41
1:A:144:LEU:HA	1:A:148:LEU:HB2	2.02	0.41
1:A:294:THR:O	1:A:298:VAL:HG23	2.20	0.41
1:A:183:TYR:OH	1:A:509:ASP:OD1	2.24	0.41
1:A:403:ALA:O	1:A:407:ILE:HG23	2.21	0.41
2:B:476:GLY:H	2:B:487:ASN:HB3	1.86	0.41
1:A:95:LEU:HD12	1:A:95:LEU:HA	1.85	0.41
1:A:351:LEU:HD11	1:A:357:ARG:HG3	2.02	0.41
1:A:155:SER:O	1:A:161:ARG:HD2	2.21	0.41
1:A:21:ILE:O	1:A:21:ILE:HG13	2.21	0.41
1:A:55:THR:O	1:A:59:VAL:HG23	2.21	0.41
1:A:169:ARG:NH2	1:A:270:MET:O	2.49	0.41
1:A:392:LEU:HD13	1:A:563:SER:HA	2.01	0.41
2:B:476:GLY:N	2:B:487:ASN:HB3	2.36	0.41
2:B:379:CYS:HA	2:B:432:CYS:HA	2.02	0.40
2:B:431:GLY:HA2	2:B:515:PHE:HD2	1.85	0.40
1:A:237:TYR:CD1	1:A:451:PRO:HG2	2.56	0.40
1:A:419:LYS:HG2	1:A:424:LEU:HB3	2.03	0.40
1:A:110:GLU:O	1:A:114:LYS:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	594/596 (100%)	584 (98%)	10 (2%)	0	100	100
2	B	193/195 (99%)	179 (93%)	14 (7%)	0	100	100
All	All	787/791 (100%)	763 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	526/526 (100%)	511 (97%)	15 (3%)	42	76
2	B	167/167 (100%)	162 (97%)	5 (3%)	41	75
All	All	693/693 (100%)	673 (97%)	20 (3%)	42	76

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	39	LEU
1	A	70	SER
1	A	102	GLN
1	A	113	SER
1	A	249	MET
1	A	271	TRP
1	A	381	TYR

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Mol	Chain	Res	Type
1	A	401	HIS
1	A	455	MET
1	A	514	ARG
1	A	542	CYS
1	A	573	VAL
1	A	582	ARG
1	A	602	SER
2	B	375	PHE
2	B	377	PHE
2	B	389	ASP
2	B	469	SER
2	B	493	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
2	B	405	ASN
2	B	474	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

7 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	C	1	3,1	14,14,15	0.33	0	17,19,21	0.53	0
3	NAG	C	2	3	14,14,15	0.30	0	17,19,21	0.52	0
3	BMA	C	3	3	11,11,12	0.61	0	15,15,17	0.72	0
4	NAG	D	1	4,1	14,14,15	0.44	0	17,19,21	0.51	0
4	NAG	D	2	4	14,14,15	0.25	0	17,19,21	0.41	0
4	NAG	E	1	4,2	14,14,15	0.21	0	17,19,21	0.56	0
4	NAG	E	2	4	14,14,15	0.23	0	17,19,21	0.40	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	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3	BMA	1	0

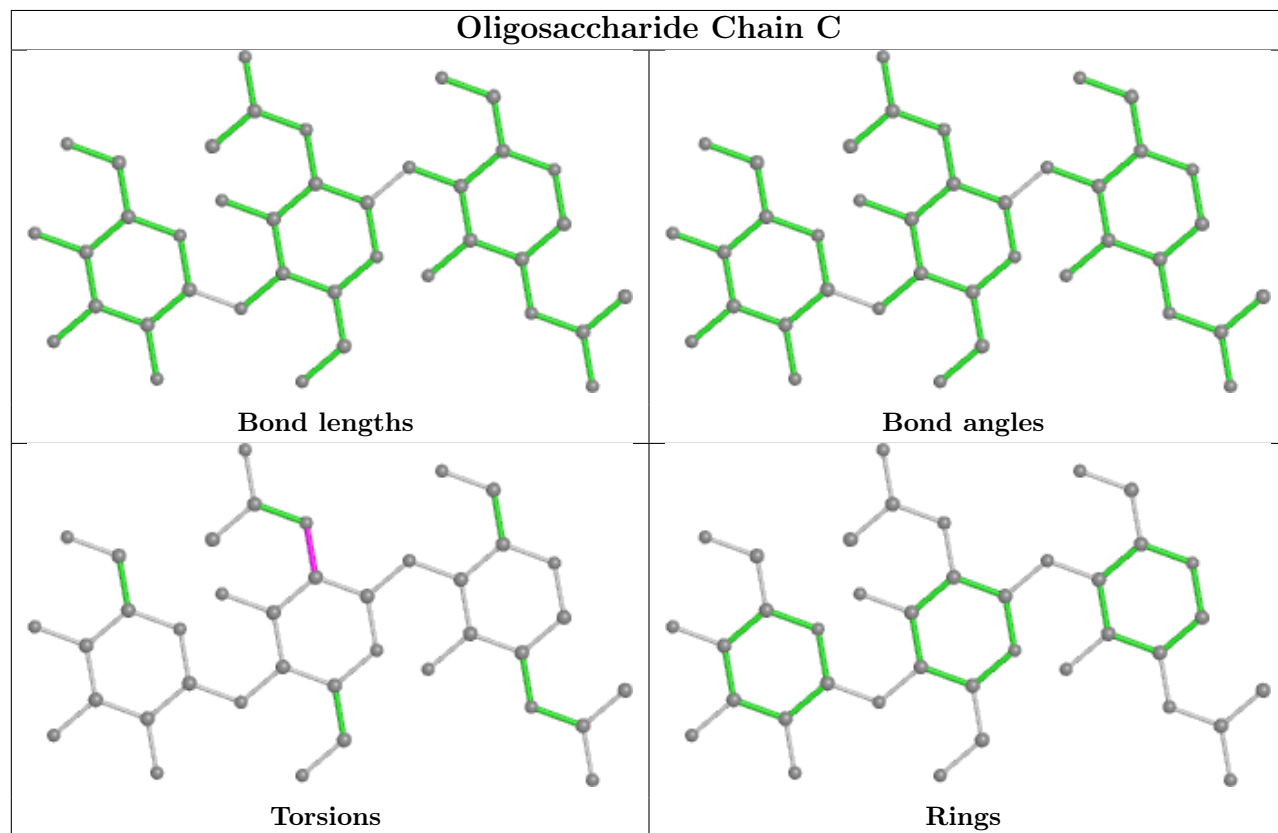
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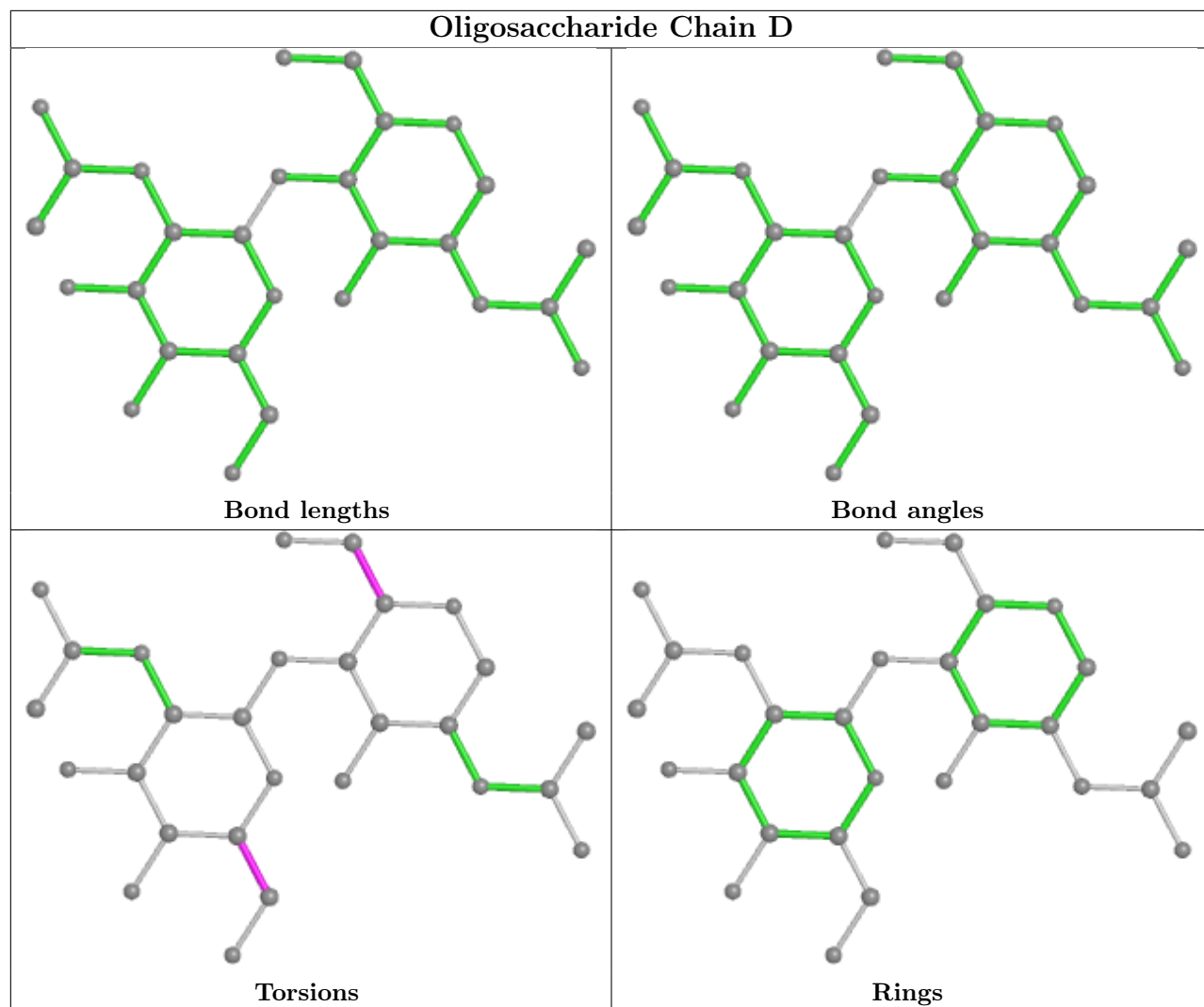


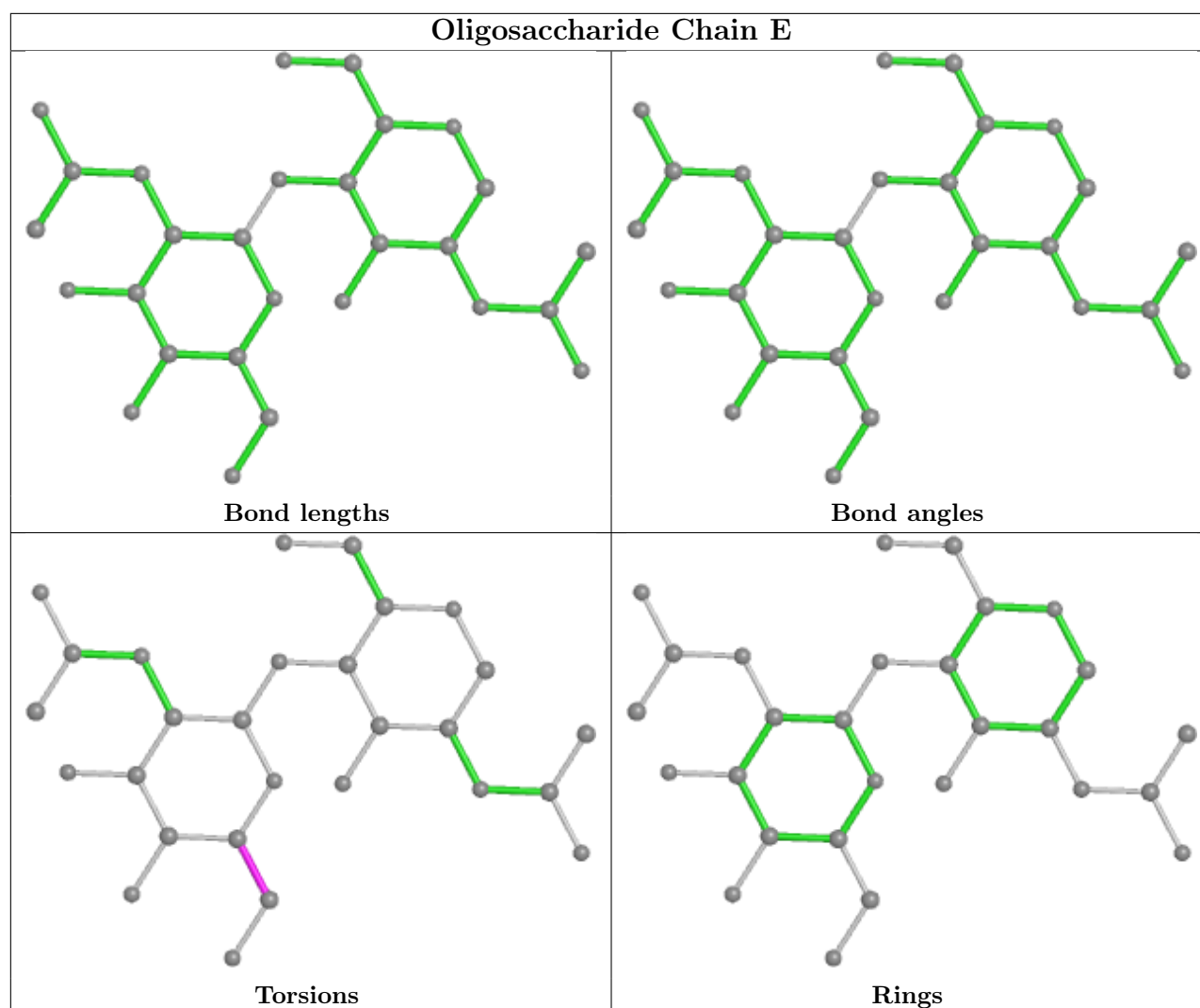
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	3	0

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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	702	1	14,14,15	0.42	0	17,19,21	0.43	0
6	NAG	A	703	1	14,14,15	0.24	0	17,19,21	0.99	1 (5%)
6	NAG	A	704	1	14,14,15	0.32	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
6	NAG	A	702	1	-	2/6/23/26	0/1/1/1
6	NAG	A	703	1	-	2/6/23/26	0/1/1/1
6	NAG	A	704	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	703	NAG	C2-N2-C7	3.47	127.84	122.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

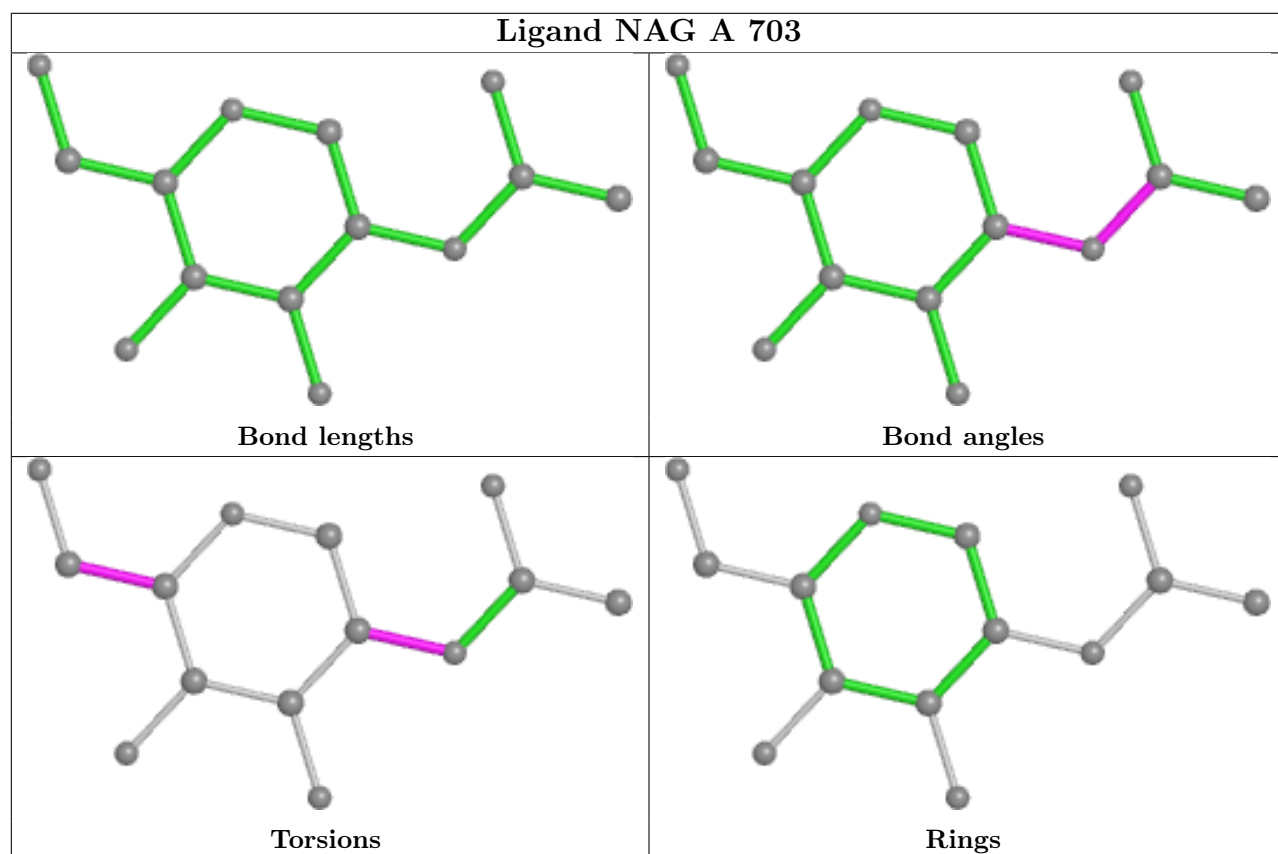
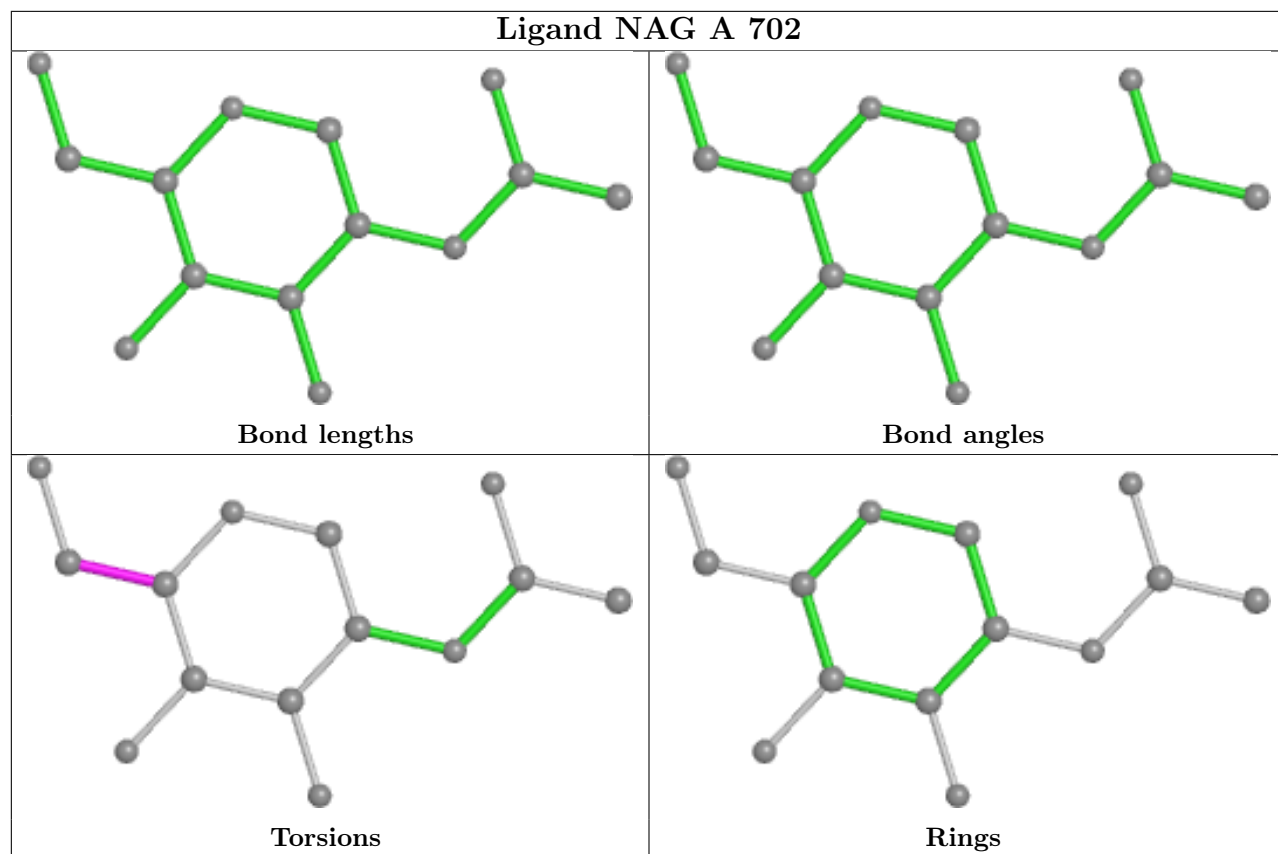
Mol	Chain	Res	Type	Atoms
6	A	703	NAG	C3-C2-N2-C7
6	A	702	NAG	O5-C5-C6-O6
6	A	702	NAG	C4-C5-C6-O6
6	A	703	NAG	O5-C5-C6-O6

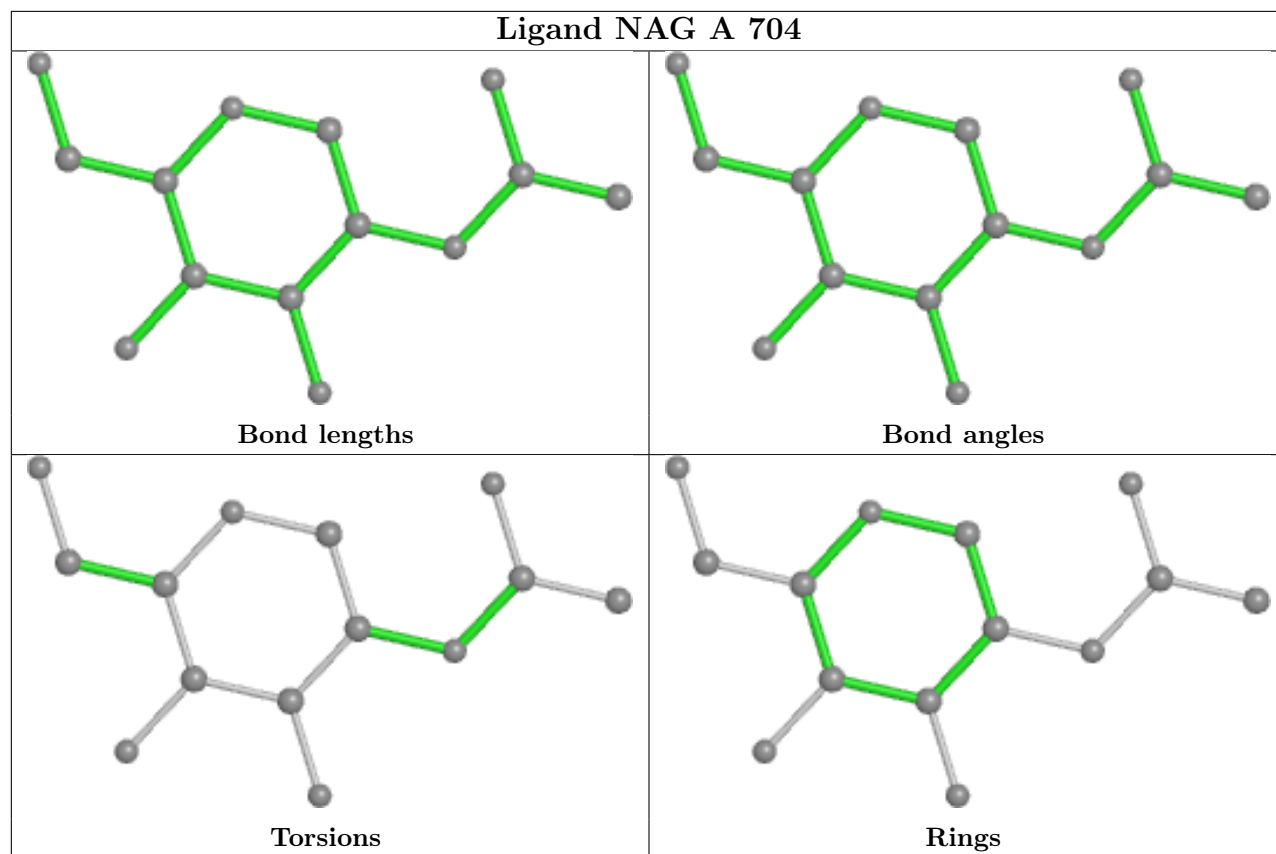
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	703	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 ⓘ

### 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	596/596 (100%)	0.45	32 (5%)	25 22	25, 48, 90, 179	0
2	B	195/195 (100%)	1.04	38 (19%)	1 0	34, 61, 143, 166	0
All	All	791/791 (100%)	0.60	70 (8%)	10 7	25, 50, 108, 179	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	136	ASP	10.1
2	B	333	THR	8.3
2	B	371	PHE	7.4
1	A	339	VAL	6.7
2	B	368	LEU	6.0
2	B	517	LEU	5.9
2	B	518	LEU	5.1
2	B	521	PRO	4.9
1	A	106	SER	4.6
1	A	107	VAL	4.6
2	B	370	ASN	4.5
1	A	137	ASN	4.4
2	B	391	CYS	4.2
1	A	338	ASN	4.1
2	B	525	CYS	4.0
2	B	367	VAL	4.0
2	B	369	TYR	3.8
2	B	373	PRO	3.8
2	B	519	HIS	3.8
1	A	427	ASP	3.8
2	B	523	THR	3.8
1	A	341	LYS	3.7
2	B	381	GLY	3.6
2	B	522	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	56	GLU	3.4
2	B	387	LEU	3.3
2	B	389	ASP	3.2
1	A	50	TYR	3.1
2	B	390	LEU	3.0
2	B	515	PHE	2.9
2	B	386	LYS	2.9
2	B	372	ALA	2.9
1	A	55	THR	2.9
1	A	135	PRO	2.9
1	A	134	ASN	2.9
2	B	486	PHE	2.8
1	A	133	CYS	2.8
1	A	83	TYR	2.8
2	B	392	PHE	2.7
2	B	364	ASP	2.7
2	B	428	ASP	2.7
2	B	377	PHE	2.7
2	B	524	VAL	2.7
2	B	384	PRO	2.7
2	B	520	ALA	2.6
1	A	217	TYR	2.5
1	A	79	LEU	2.5
2	B	374	PHE	2.5
2	B	430	THR	2.5
2	B	380	TYR	2.4
1	A	52	THR	2.4
1	A	614	ALA	2.4
1	A	103	ASN	2.4
1	A	82	MET	2.3
1	A	24	GLN	2.3
2	B	360	ASN	2.2
1	A	54	ILE	2.2
1	A	89	GLN	2.2
2	B	365	TYR	2.1
1	A	428	PHE	2.1
2	B	385	THR	2.1
2	B	526	GLY	2.1
1	A	429	GLN	2.1
1	A	60	GLN	2.1
1	A	340	GLN	2.1
1	A	87	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	57	GLU	2.1
2	B	487	ASN	2.1
1	A	132	VAL	2.0
1	A	138	PRO	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](#)

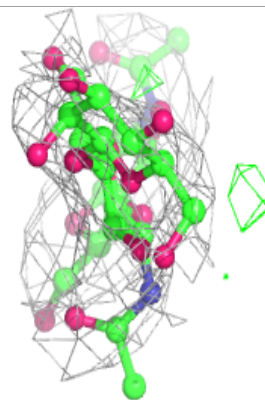
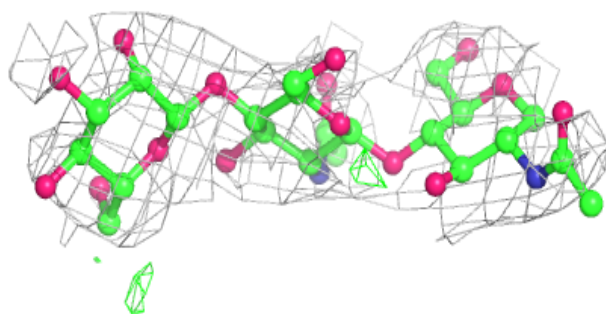
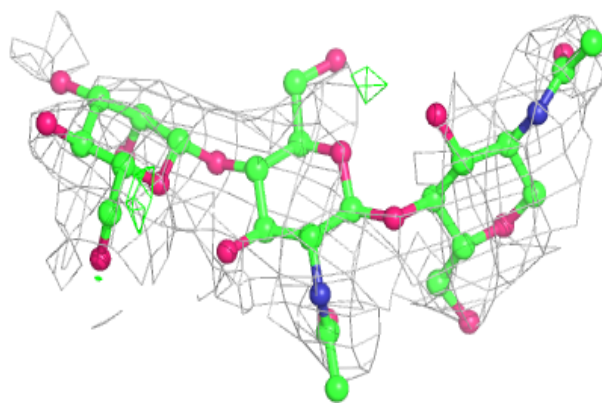
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	E	2	14/15	0.51	0.67	166,177,184,185	0
4	NAG	D	2	14/15	0.62	0.49	131,146,150,151	0
3	BMA	C	3	11/12	0.66	0.32	94,114,121,124	0
4	NAG	E	1	14/15	0.68	0.36	133,151,164,170	0
4	NAG	D	1	14/15	0.70	0.42	91,129,142,147	0
3	NAG	C	2	14/15	0.83	0.23	112,123,129,131	0
3	NAG	C	1	14/15	0.87	0.18	79,85,90,95	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.

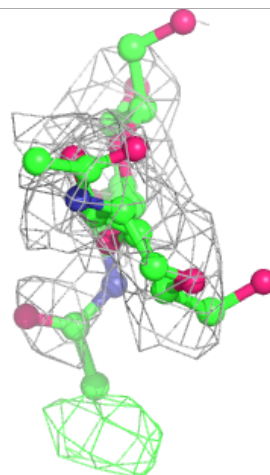
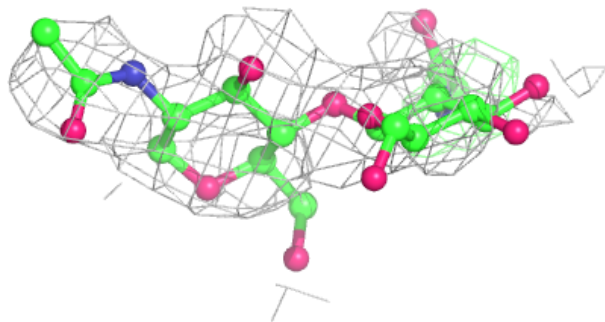
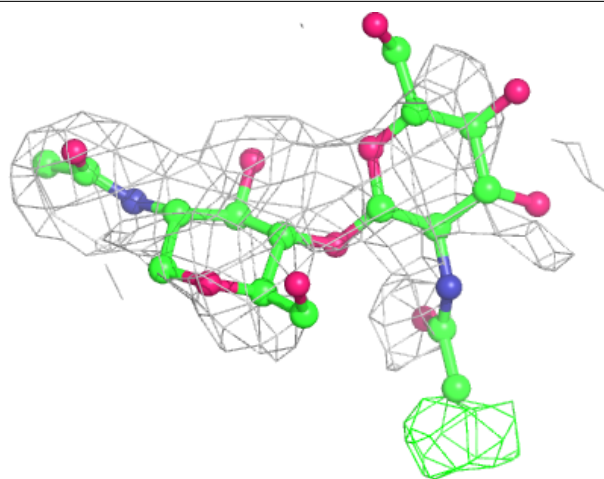
**Electron density around Chain C:**

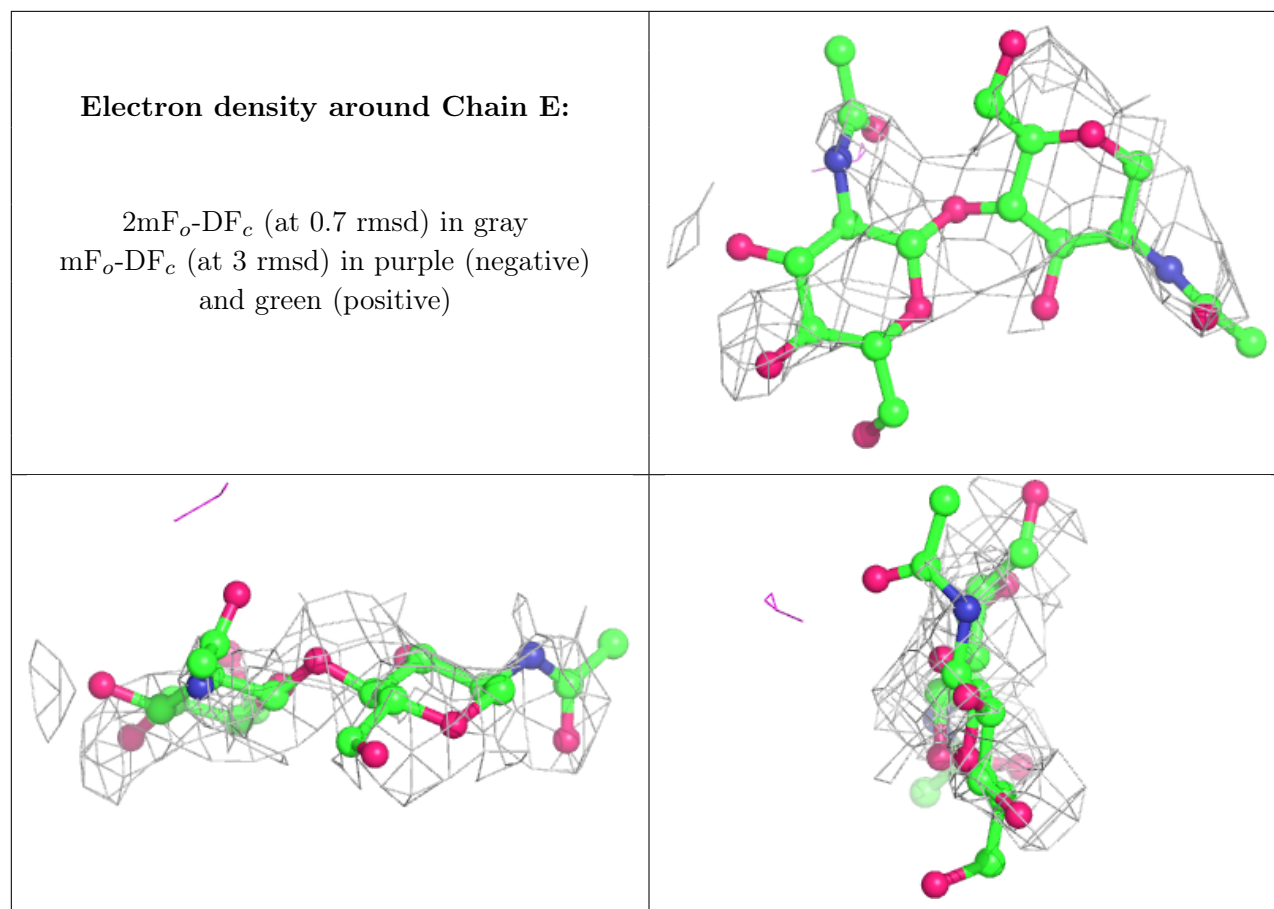
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain 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](#)

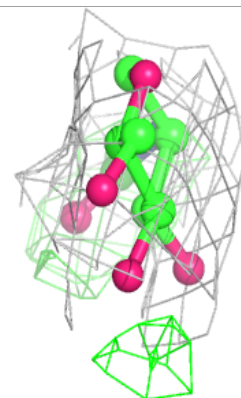
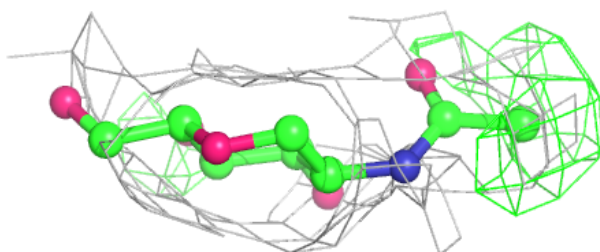
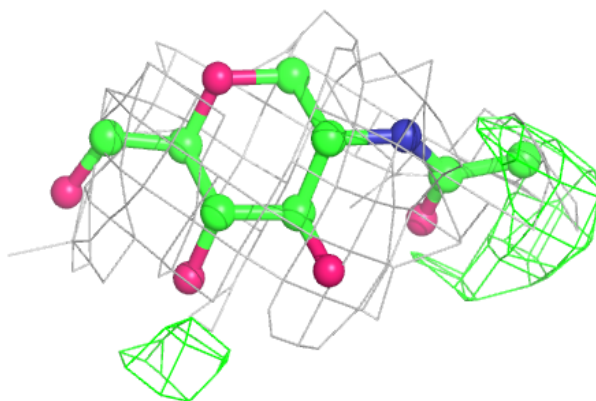
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	A	703	14/15	0.66	0.23	97,118,123,124	0
6	NAG	A	704	14/15	0.72	0.39	67,84,103,106	0
6	NAG	A	702	14/15	0.75	0.50	94,114,126,130	0
5	ZN	A	701	1/1	0.92	0.16	66,66,66,66	0

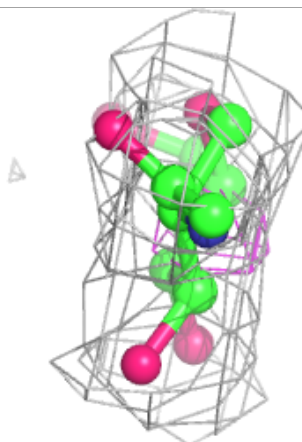
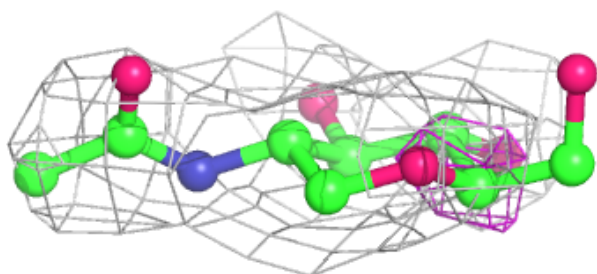
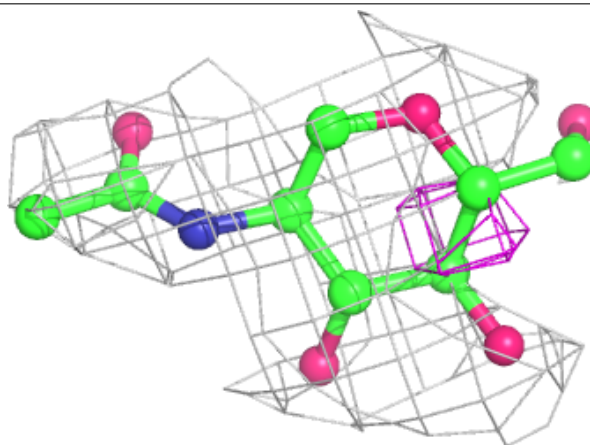
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAG A 703:**

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

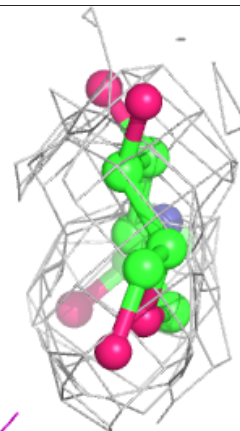
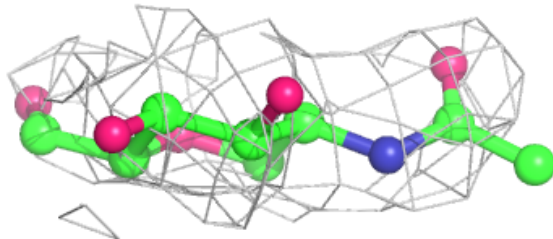
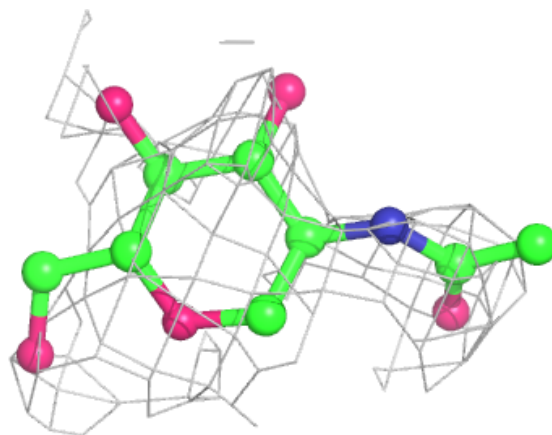
**Electron density around NAG A 704:**

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



**Electron density around NAG A 702:**

$2mF_o-DF_c$  (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.