



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2021 – 02:11 PM JST

PDB ID : 7EKG  
Title : Structure of SARS-CoV-2 Beta variant spike receptor-binding domain complexed with human ACE2  
Authors : Han, P.C.; Su, C.; Zhang, Y.F.; Qi, J.X.; Gao, G.F.  
Deposited on : 2021-04-05  
Resolution : 2.63 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.

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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 : 2.23.2  
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) : 2.23.2

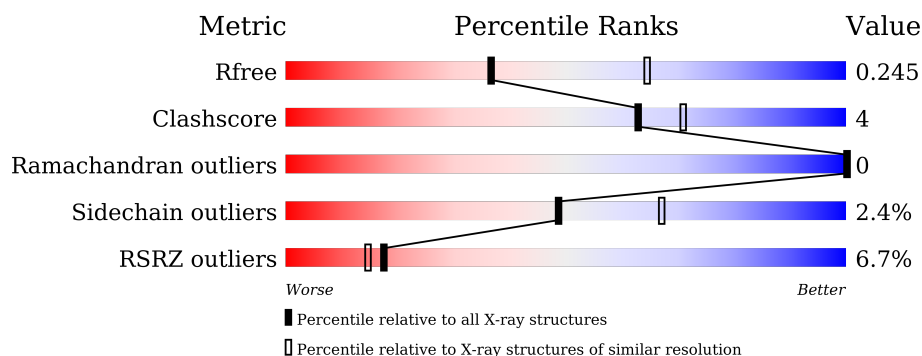
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.63 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	603	<div> <div>5%</div> <div>89%</div> <div>10%</div> </div>
2	B	229	<div> <div>10%</div> <div>72%</div> <div>13%</div> <div>15%</div> </div>
3	C	2	<div> <div>100%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6534 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			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	616	HIS	-	expression tag	UNP Q9BYF1
A	617	HIS	-	expression tag	UNP Q9BYF1
A	618	HIS	-	expression tag	UNP Q9BYF1
A	619	HIS	-	expression tag	UNP Q9BYF1
A	620	HIS	-	expression tag	UNP Q9BYF1
A	621	HIS	-	expression tag	UNP Q9BYF1

- 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	1	0
			1552	997	258	289	8			

There are 9 discrepancies between the modelled and reference sequences:

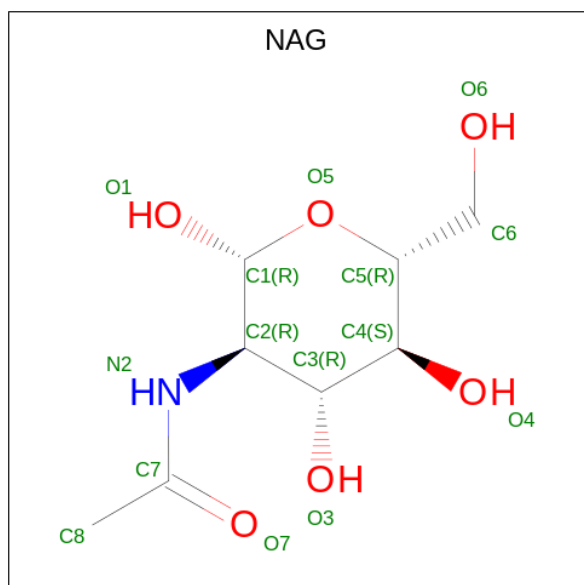
Chain	Residue	Modelled	Actual	Comment	Reference
B	417	ASN	LYS	engineered mutation	UNP P0DTC2
B	484	LYS	GLU	engineered mutation	UNP P0DTC2
B	501	TYR	ASN	engineered mutation	UNP P0DTC2
B	542	HIS	-	expression tag	UNP P0DTC2
B	543	HIS	-	expression tag	UNP P0DTC2
B	544	HIS	-	expression tag	UNP P0DTC2
B	545	HIS	-	expression tag	UNP P0DTC2
B	546	HIS	-	expression tag	UNP P0DTC2
B	547	HIS	-	expression tag	UNP P0DTC2

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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



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

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

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

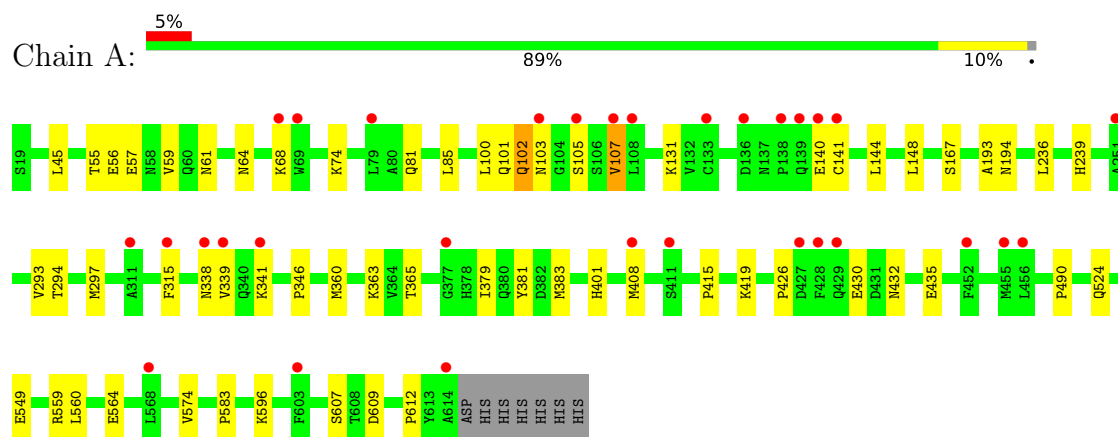
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	18	Total 18	O 18	0	0
6	B	3	Total 3	O 3	0	0

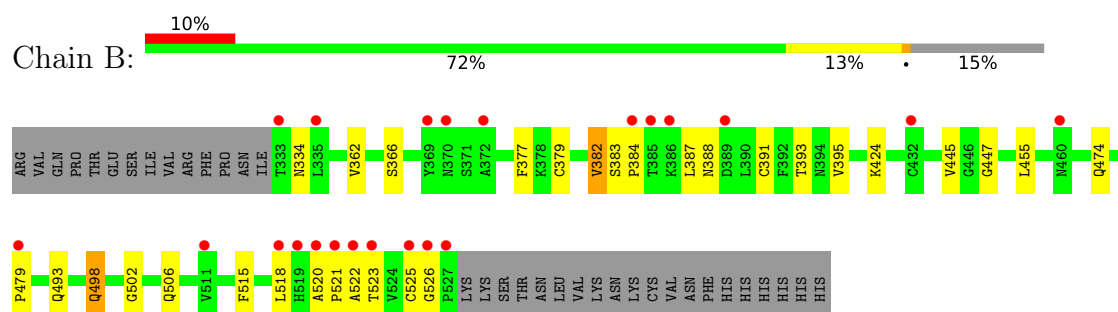
### 3 Residue-property plots [i](#)

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.

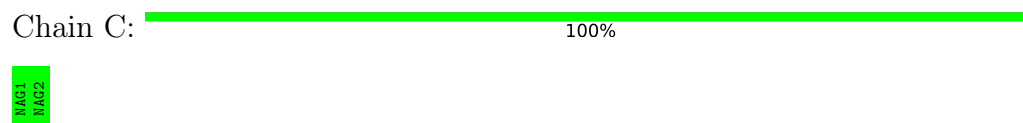
- Molecule 1: Angiotensin-converting enzyme 2



- Molecule 2: Spike protein S1



- 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	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.15Å 105.15Å 230.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.91 – 2.63 27.01 – 2.63	Depositor EDS
% Data completeness (in resolution range)	99.9 (26.91-2.63) 100.0 (27.01-2.63)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 2.64Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, $R_{free}$	0.214 , 0.248 0.214 , 0.245	Depositor DCC
$R_{free}$ test set	1944 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.8	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6534	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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, 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	0.27	0/4999	0.45	0/6792
2	B	0.47	4/1600 (0.2%)	0.55	2/2180 (0.1%)
All	All	0.33	4/6599 (0.1%)	0.48	2/8972 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	498[A]	GLN	C-N	8.39	1.50	1.34
2	B	498[B]	GLN	C-N	8.39	1.50	1.34
2	B	498[A]	GLN	C-O	6.22	1.35	1.23
2	B	498[B]	GLN	C-O	6.22	1.35	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	498[A]	GLN	O-C-N	-6.32	109.09	121.10
2	B	498[B]	GLN	O-C-N	-6.32	109.09	121.10

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	35	1
2	B	1552	0	1470	20	0
3	C	28	0	25	0	0
4	A	56	0	52	0	0
4	B	14	0	13	0	0
5	A	1	0	0	0	0
6	A	18	0	0	0	0
6	B	3	0	0	0	0
All	All	6534	0	6194	55	1

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

All (55) 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:107:VAL:HG11	1:A:194:ASN:ND2	1.66	1.10
1:A:107:VAL:HG11	1:A:194:ASN:HD21	1.28	0.89
1:A:107:VAL:CG1	1:A:194:ASN:HD21	2.00	0.73
1:A:490:PRO:HA	1:A:612:PRO:HG2	1.73	0.69
1:A:105:SER:O	1:A:105:SER:OG	2.16	0.64
2:B:520:ALA:HB1	2:B:521:PRO:HD2	1.79	0.64
1:A:607:SER:OG	1:A:609:ASP:OD1	2.20	0.60
2:B:366:SER:HB3	2:B:388:ASN:HD21	1.66	0.60
1:A:107:VAL:HG21	1:A:193:ALA:HB3	1.85	0.59
2:B:393:THR:HA	2:B:522:ALA:HA	1.84	0.58
1:A:560:LEU:HD22	1:A:564:GLU:HG3	1.84	0.57
1:A:432:ASN:HA	1:A:435:GLU:HG3	1.87	0.55
1:A:107:VAL:CG2	1:A:193:ALA:HB3	2.37	0.55
1:A:85:LEU:HG	1:A:101:GLN:HE22	1.72	0.54
1:A:131:LYS:HD3	1:A:141:CYS:HB2	1.90	0.52
2:B:521:PRO:HB2	2:B:523:THR:HG23	1.92	0.52
1:A:419:LYS:HE3	1:A:426:PRO:HA	1.92	0.52
2:B:379:CYS:HB2	2:B:384:PRO:HD3	1.91	0.51
2:B:393:THR:HG21	2:B:518:LEU:H	1.76	0.50
2:B:474:GLN:NE2	2:B:479:PRO:HA	2.27	0.50
2:B:334:ASN:O	2:B:362:VAL:N	2.39	0.50
1:A:55:THR:O	1:A:59:VAL:HG23	2.11	0.50
1:A:379:ILE:O	1:A:383:MET:HG3	2.12	0.49
2:B:383:SER:H	2:B:387:LEU:HD22	1.76	0.49
1:A:81:GLN:HG3	1:A:101:GLN:HG2	1.95	0.49
2:B:455:LEU:HD22	2:B:493:GLN:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:PRO:HB3	1:A:360:MET:HG3	1.94	0.48
1:A:144:LEU:HA	1:A:148:LEU:HB2	1.96	0.47
2:B:366:SER:HB3	2:B:388:ASN:ND2	2.30	0.47
1:A:140:GLU:HA	1:A:140:GLU:OE1	2.15	0.46
2:B:395:VAL:HG22	2:B:515:PHE:HD1	1.79	0.46
2:B:382:VAL:HG11	2:B:515:PHE:HE2	1.80	0.46
2:B:383:SER:O	2:B:387:LEU:HB2	2.16	0.46
1:A:107:VAL:HG21	1:A:193:ALA:CB	2.46	0.46
1:A:107:VAL:CG2	1:A:193:ALA:CB	2.94	0.46
1:A:239:HIS:CE1	1:A:596:LYS:HG2	2.51	0.45
2:B:447:GLY:HA2	2:B:498[A]:GLN:HG2	1.98	0.45
1:A:293:VAL:O	1:A:297:MET:HG3	2.17	0.45
1:A:294:THR:HG23	1:A:365:THR:HA	1.98	0.45
1:A:524:GLN:HG2	1:A:583:PRO:HG2	1.98	0.44
1:A:315:PHE:CZ	1:A:408:MET:HG3	2.52	0.44
1:A:131:LYS:HD3	1:A:141:CYS:CB	2.47	0.44
1:A:339:VAL:O	1:A:341:LYS:HG2	2.18	0.44
2:B:362:VAL:CG1	2:B:526:GLY:HA2	2.47	0.44
2:B:391:CYS:HA	2:B:525:CYS:HA	2.00	0.43
1:A:64:ASN:O	1:A:68:LYS:HG3	2.18	0.43
1:A:57:GLU:O	1:A:61:ASN:ND2	2.49	0.43
1:A:100:LEU:C	1:A:102:GLN:N	2.72	0.43
1:A:549:GLU:H	1:A:549:GLU:CD	2.23	0.42
2:B:502:GLY:O	2:B:506:GLN:HG3	2.20	0.41
2:B:362:VAL:HG13	2:B:526:GLY:HA2	2.01	0.41
1:A:74:LYS:HG2	1:A:105:SER:HB2	2.03	0.41
1:A:415:PRO:O	1:A:419:LYS:HG3	2.20	0.41
2:B:334:ASN:O	2:B:362:VAL:HG23	2.21	0.41
1:A:524:GLN:HB3	1:A:574:VAL:HG11	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:ASP:OD1	1:A:609:ASP:OD1[8_554]	2.16	0.04

## 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	594/603 (98%)	588 (99%)	6 (1%)	0	100	100
2	B	194/229 (85%)	184 (95%)	10 (5%)	0	100	100
All	All	788/832 (95%)	772 (98%)	16 (2%)	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	526/533 (99%)	513 (98%)	13 (2%)	47	66
2	B	169/202 (84%)	165 (98%)	4 (2%)	49	67
All	All	695/735 (95%)	678 (98%)	17 (2%)	49	67

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	56	GLU
1	A	102	GLN
1	A	103	ASN
1	A	107	VAL
1	A	167	SER
1	A	236	LEU
1	A	338	ASN

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Mol	Chain	Res	Type
1	A	363	LYS
1	A	381	TYR
1	A	401	HIS
1	A	430	GLU
1	A	559	ARG
2	B	377	PHE
2	B	382	VAL
2	B	424	LYS
2	B	445	VAL

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
1	A	194	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 ⓘ

2 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	0.28	0	17,19,21	0.56	0
3	NAG	C	2	3	14,14,15	0.32	0	17,19,21	0.43	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	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

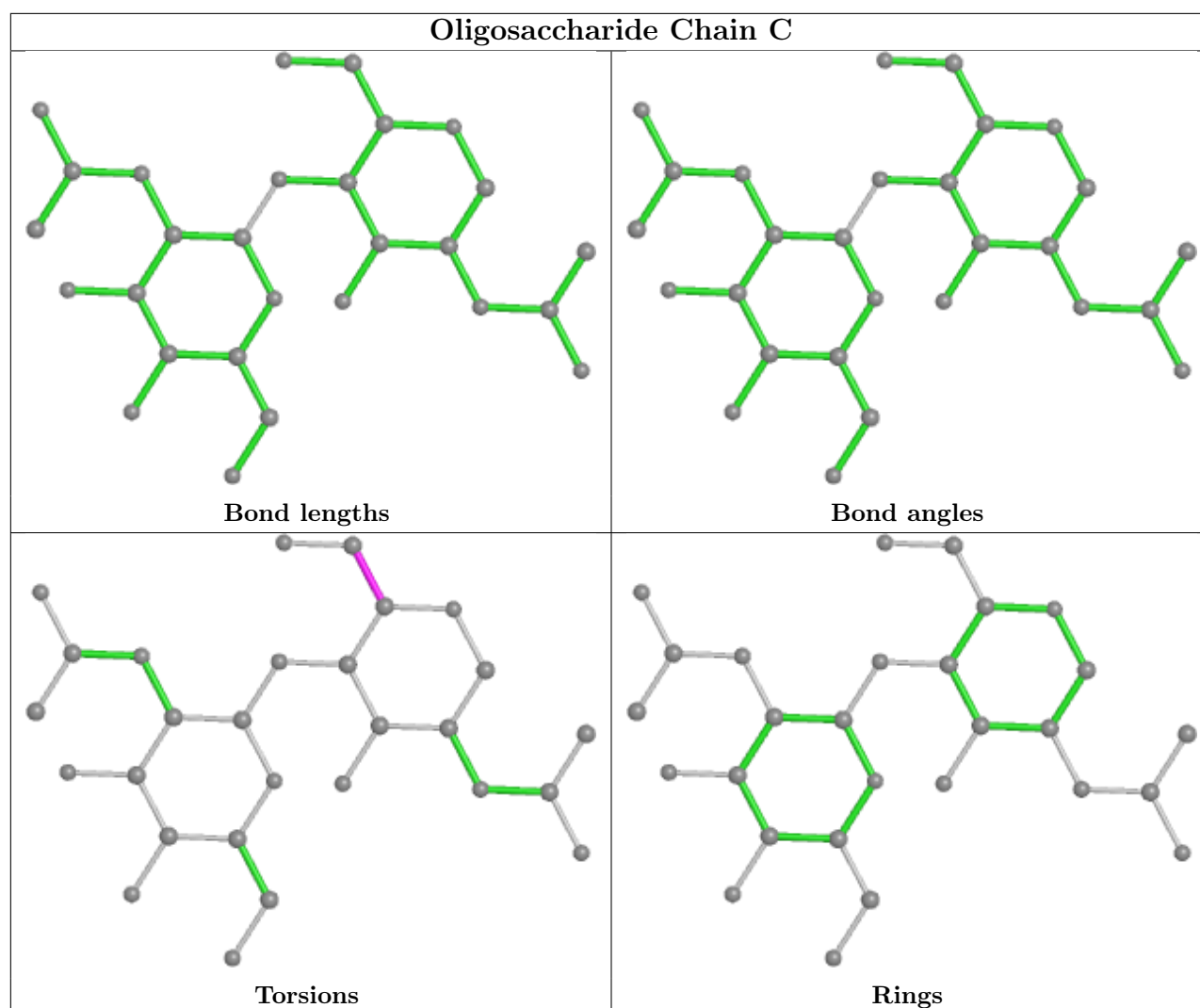
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-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 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\# Z  > 2$
4	NAG	B	601	2	14,14,15	0.28	0	17,19,21	0.48	0
4	NAG	A	702	1	14,14,15	0.28	0	17,19,21	0.46	0
4	NAG	A	704	1	14,14,15	0.28	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	701	1	14,14,15	0.40	0	17,19,21	0.61	1 (5%)
4	NAG	A	705	1	14,14,15	0.31	0	17,19,21	0.72	1 (5%)

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
4	NAG	B	601	2	-	0/6/23/26	0/1/1/1
4	NAG	A	702	1	-	0/6/23/26	0/1/1/1
4	NAG	A	704	1	-	2/6/23/26	0/1/1/1
4	NAG	A	701	1	-	0/6/23/26	0/1/1/1
4	NAG	A	705	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	705	NAG	C1-O5-C5	2.63	115.76	112.19
4	A	701	NAG	C1-O5-C5	2.08	115.01	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

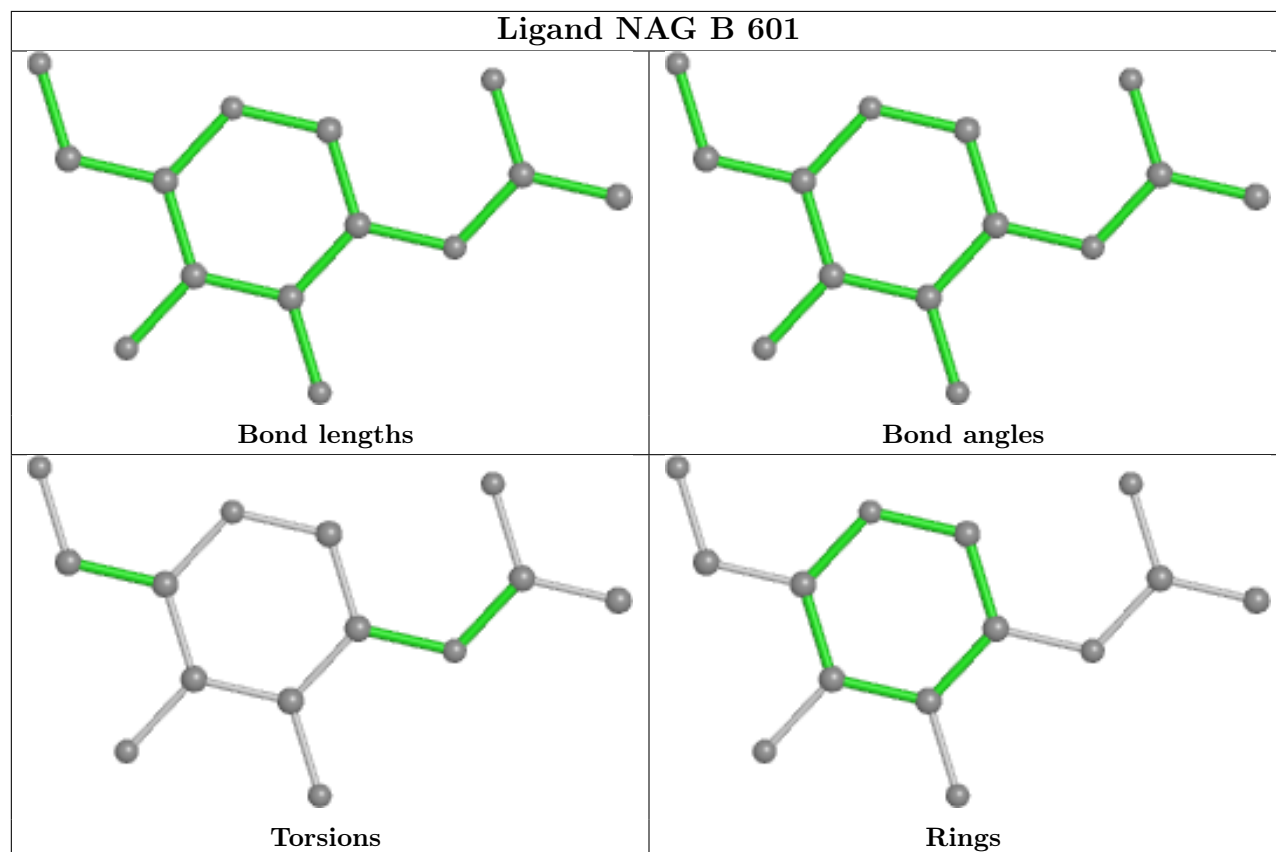
Mol	Chain	Res	Type	Atoms
4	A	704	NAG	C8-C7-N2-C2
4	A	704	NAG	O7-C7-N2-C2

There are no ring outliers.

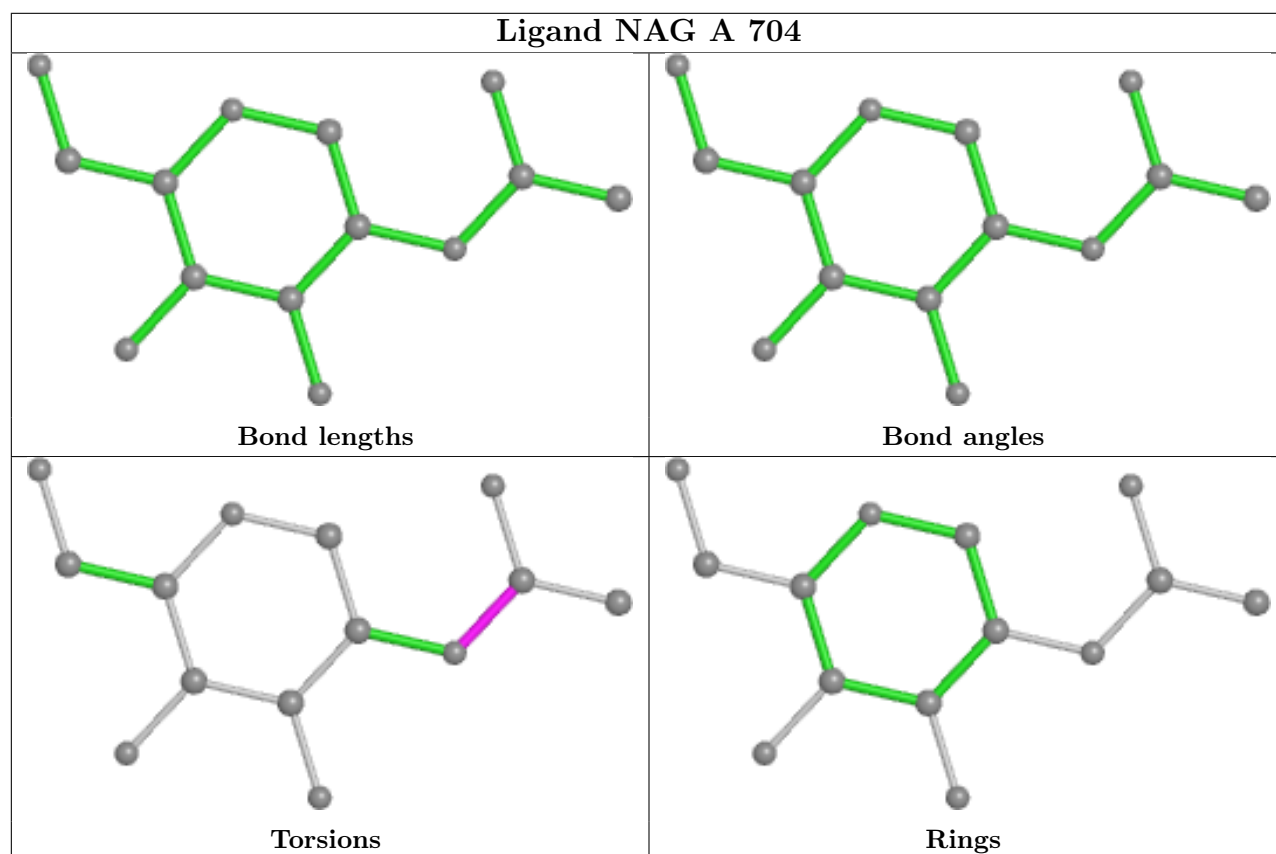
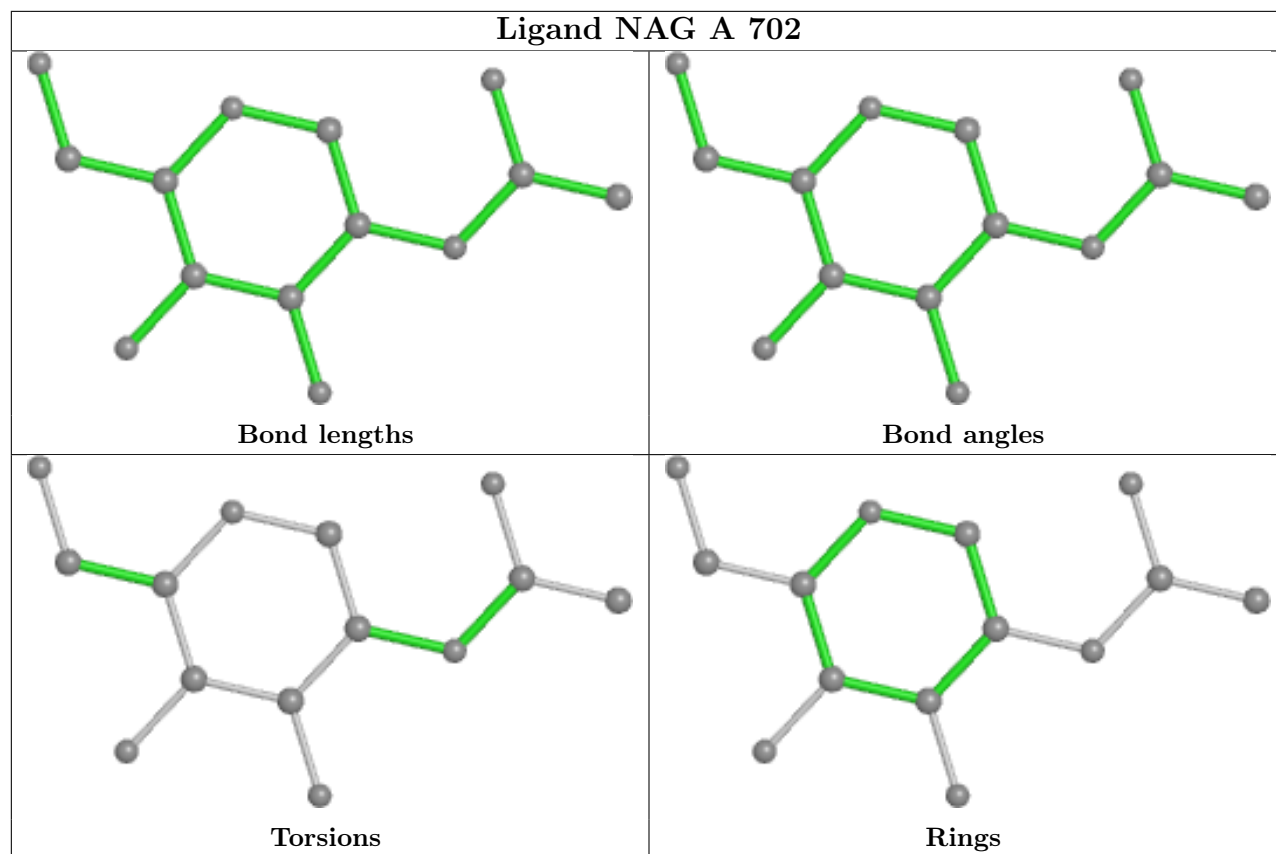
No monomer is involved in short contacts.

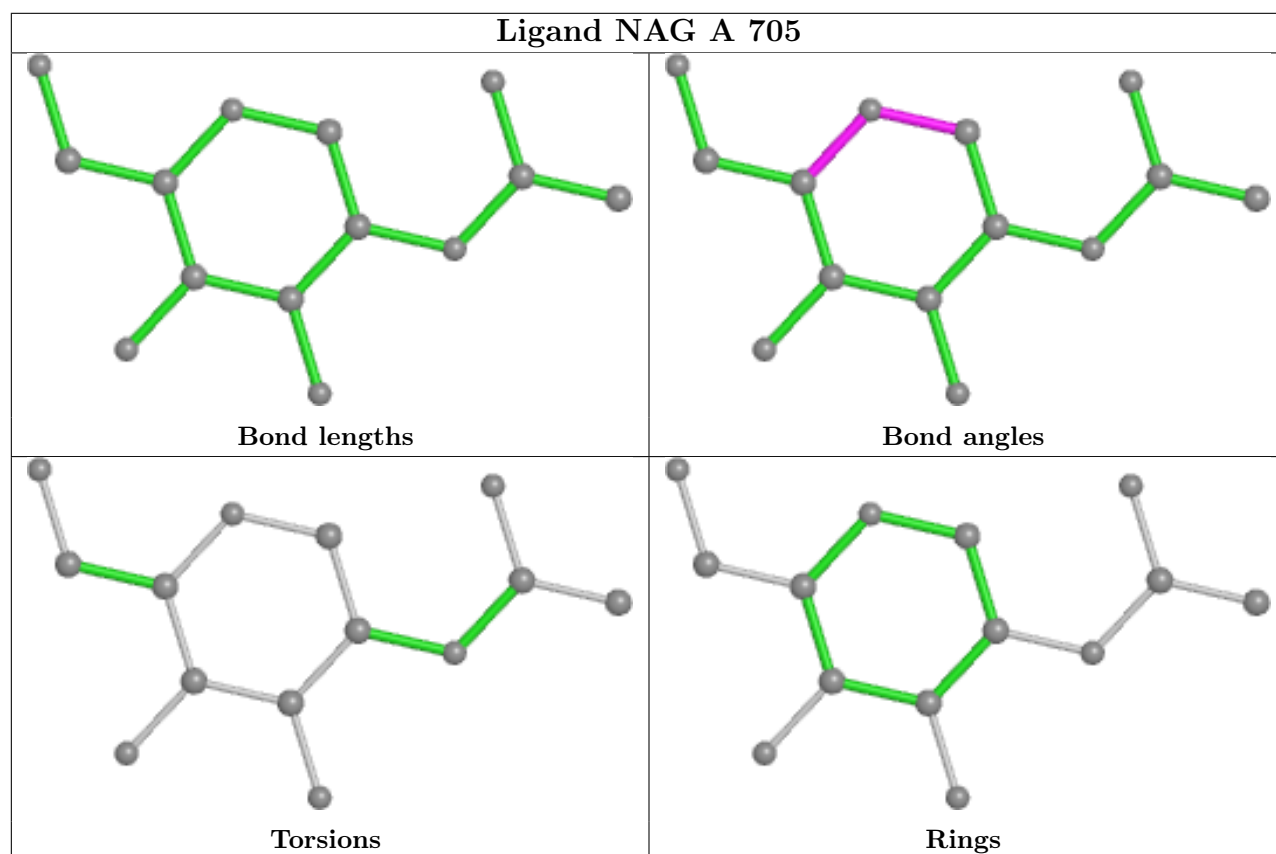
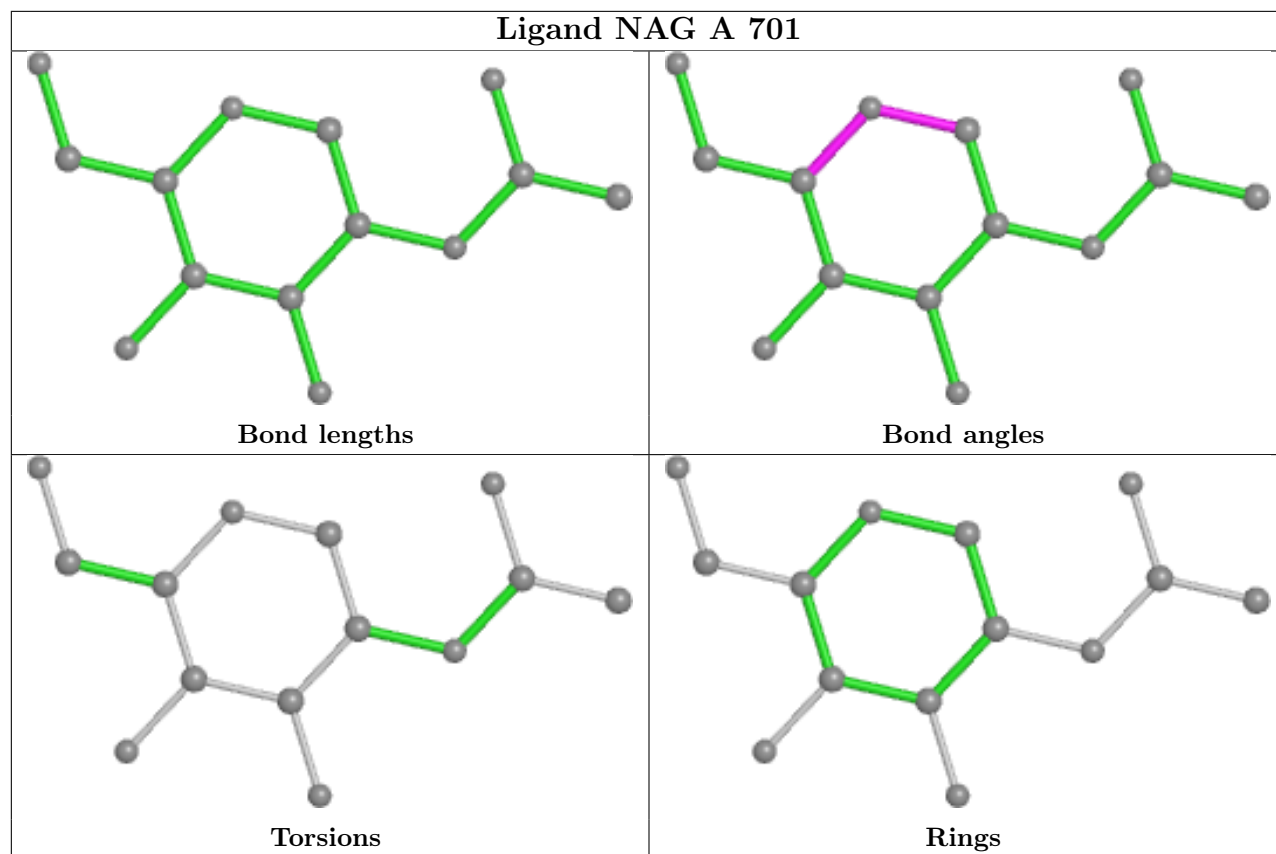
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	596/603 (98%)	0.08	31 (5%) 27 24	46, 63, 108, 183	0
2	B	195/229 (85%)	0.45	22 (11%) 5 3	52, 75, 149, 183	0
All	All	791/832 (95%)	0.17	53 (6%) 17 15	46, 66, 125, 183	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	519	HIS	7.0
2	B	333	THR	5.6
2	B	521	PRO	5.6
1	A	136	ASP	5.5
1	A	138	PRO	5.4
1	A	103	ASN	5.3
2	B	520	ALA	5.3
1	A	107	VAL	5.2
2	B	518	LEU	4.5
1	A	105	SER	4.4
1	A	338	ASN	4.1
2	B	385	THR	4.0
1	A	108	LEU	3.7
2	B	525	CYS	3.7
2	B	523	THR	3.6
2	B	372	ALA	3.6
1	A	455	MET	3.5
1	A	427	ASP	3.5
2	B	522	ALA	3.4
1	A	139	GLN	3.3
2	B	432	CYS	3.1
2	B	384	PRO	3.1
1	A	339	VAL	2.9
2	B	335	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	452	PHE	2.8
1	A	614	ALA	2.7
2	B	386	LYS	2.7
1	A	429	GLN	2.6
2	B	370	ASN	2.6
2	B	479	PRO	2.5
1	A	133	CYS	2.5
2	B	527	PRO	2.5
1	A	456	LEU	2.5
2	B	369	TYR	2.4
1	A	141	CYS	2.4
1	A	140	GLU	2.4
2	B	389	ASP	2.4
1	A	408	MET	2.3
1	A	341	LYS	2.3
1	A	315	PHE	2.3
1	A	68	LYS	2.3
1	A	377	GLY	2.3
1	A	79	LEU	2.3
2	B	460	ASN	2.2
1	A	428	PHE	2.2
2	B	511	VAL	2.2
1	A	311	ALA	2.2
1	A	411	SER	2.2
1	A	568	LEU	2.1
1	A	69	TRP	2.1
2	B	526	GLY	2.1
1	A	603	PHE	2.1
1	A	251	ALA	2.0

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

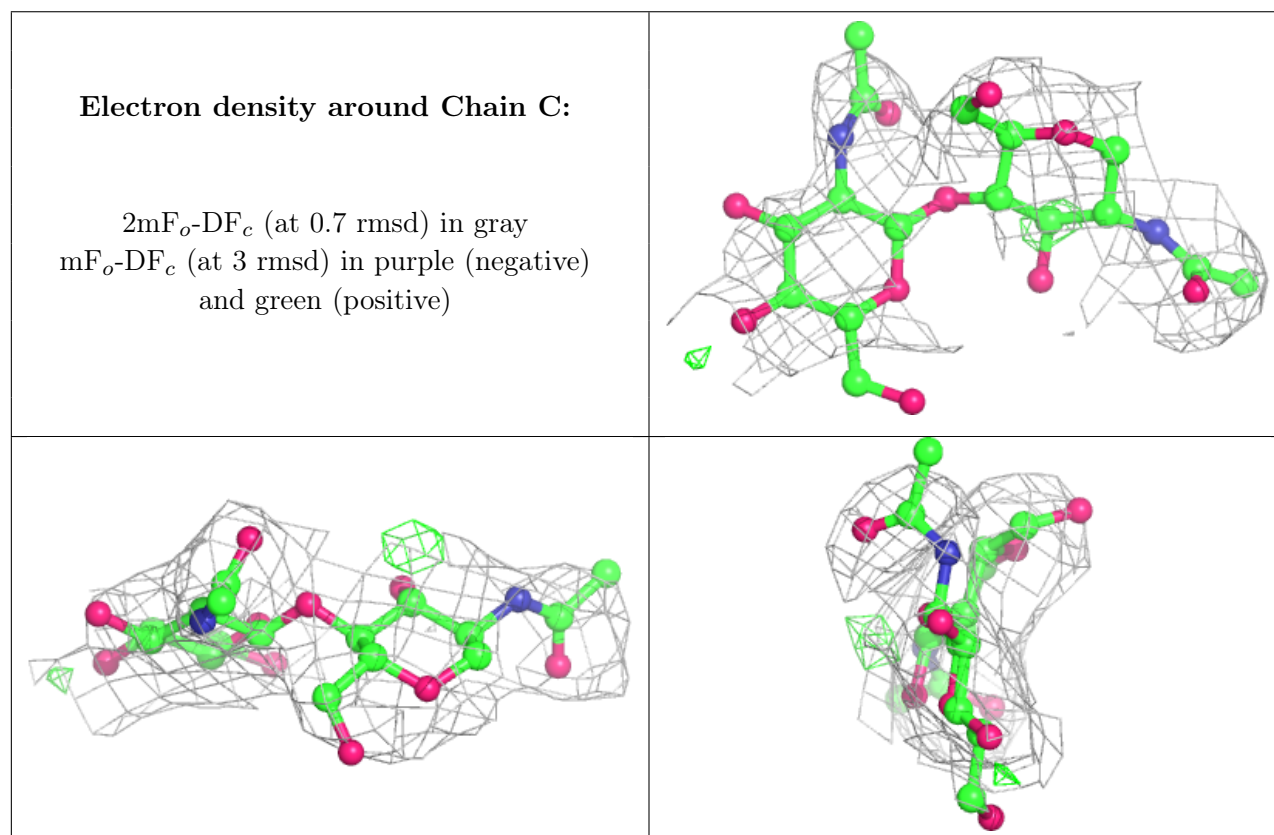
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	NAG	C	2	14/15	0.79	0.36	123,137,145,147	0
3	NAG	C	1	14/15	0.93	0.13	97,105,109,112	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.



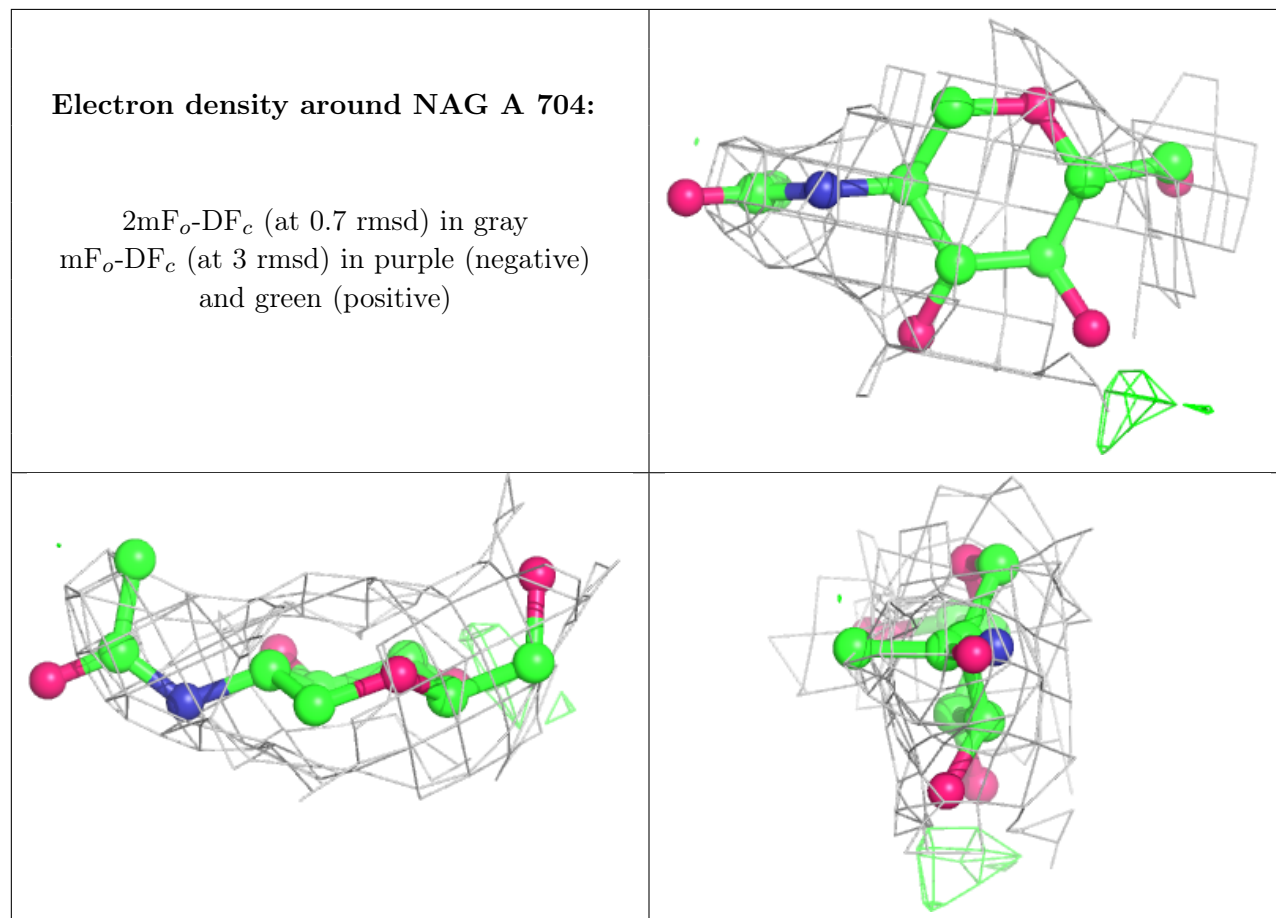
## 6.4 Ligands ⓘ

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	A	704	14/15	0.69	0.35	119,132,139,139	0
4	NAG	A	705	14/15	0.75	0.25	114,130,135,139	0
4	NAG	A	702	14/15	0.77	0.33	116,120,127,128	0
4	NAG	A	701	14/15	0.87	0.23	104,111,116,118	0
4	NAG	B	601	14/15	0.88	0.14	97,105,108,109	0
5	ZN	A	703	1/1	0.97	0.16	48,48,48,48	0

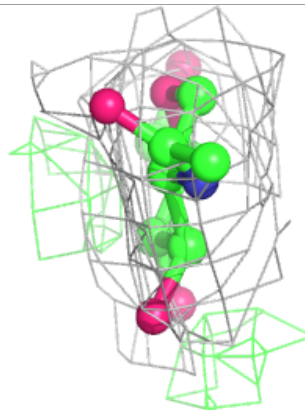
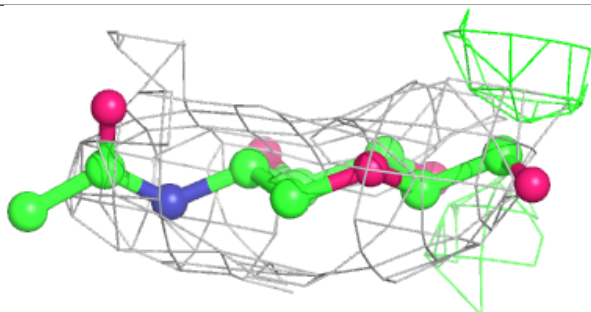
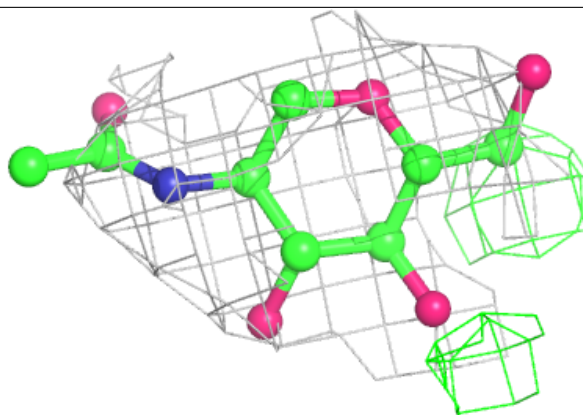
The following is a graphical depiction of the model fit to experimental electron density of all

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.

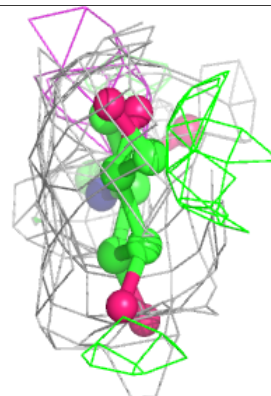
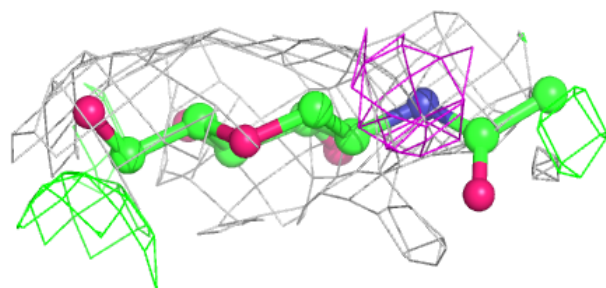
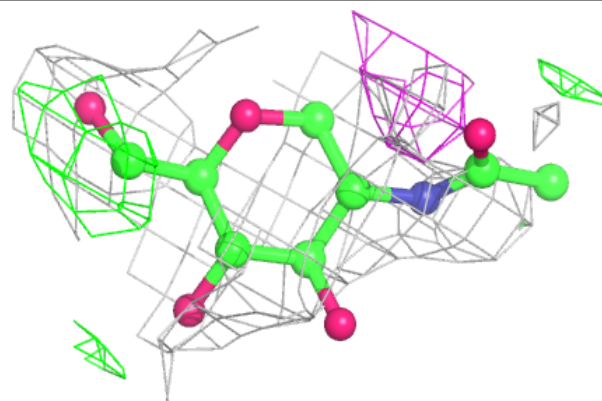


**Electron density around NAG A 705:**

$2mF_o-DF_c$  (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:**

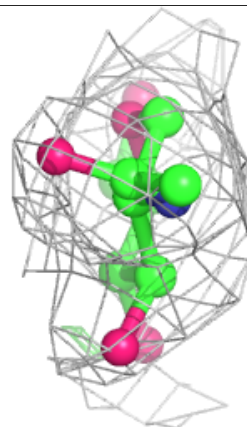
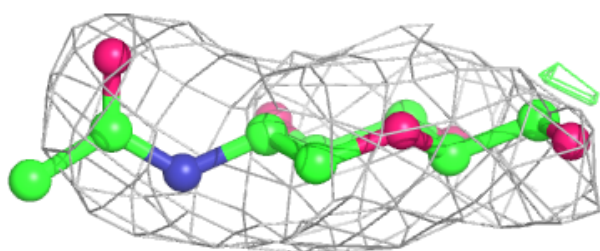
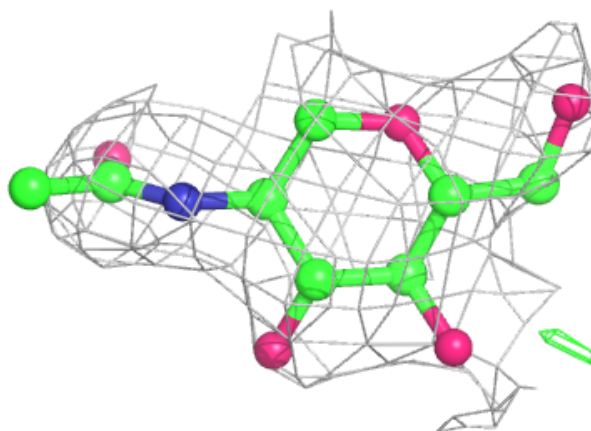
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



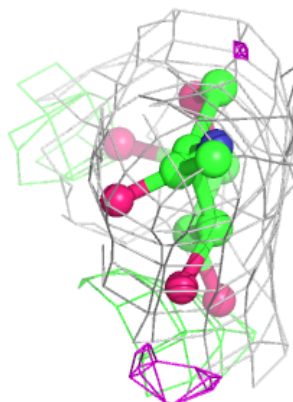
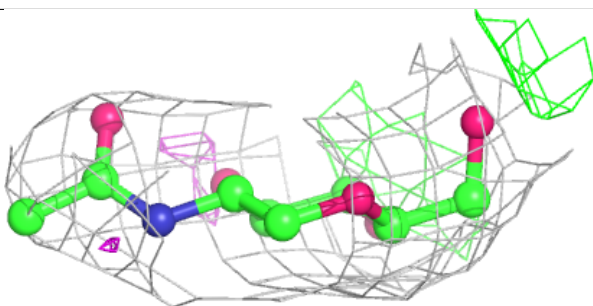
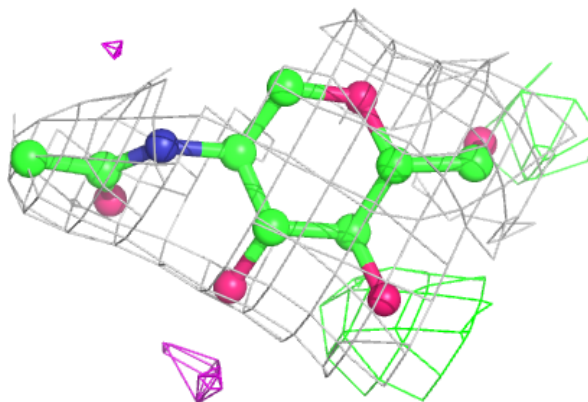


**Electron density around NAG A 701:**

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

**Electron density around NAG B 601:**

$2mF_o-DF_c$  (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.