



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2021 – 12:42 PM EDT

PDB ID : 7MWW  
Title : Structure of hepatitis C virus envelope full-length glycoprotein 2 (eE2) from J6 genotype  
Authors : Kumar, A.; Hossain, R.A.; Yost, S.A.; Bu, W.; Wang, Y.; Dearborn, A.D.; Grakoui, A.; Cohen, J.I.; Marcotrigiano, J.  
Deposited on : 2021-05-17  
Resolution : 2.71 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 : 2.23.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.1

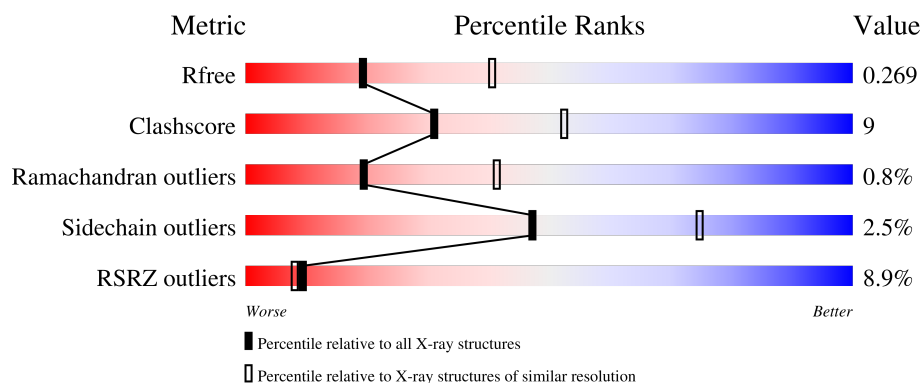
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	E	272	<div> <div>19%</div> <div>38% 21% .. 38%</div> </div>
2	H	221	<div> <div>%</div> <div>89% 10% .</div> </div>
3	L	240	<div> <div>82% 8% 9%</div> </div>
4	A	3	<div> <div>100%</div> </div>
5	B	2	<div> <div>100%</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	A	2	-	-	-	X
4	BMA	A	3	-	-	-	X
5	NAG	B	2	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4802 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 Core protein precursor eE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	169	Total	C	N	O	S	0	0	0
			1295	832	215	234	14			

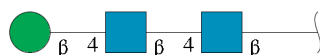
- Molecule 2 is a protein called 2A12 Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1636	1025	268	338	5			

- Molecule 3 is a protein called 2A12 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	218	Total	C	N	O	S	0	0	0
			1674	1040	280	346	8			

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



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

- Molecule 5 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
5	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 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
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	4	Total	O	0	0
			4	4		
7	H	47	Total	O	0	0
			47	47		
7	L	51	Total	O	0	0
			51	51		



MAG1  
MAG2  
B/A3

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

100%

MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.84Å 155.56Å 129.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.33 – 2.71 33.33 – 2.71	Depositor EDS
% Data completeness (in resolution range)	98.4 (33.33-2.71) 99.0 (33.33-2.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 2.72Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.218 , 0.270 0.216 , 0.269	Depositor DCC
$R_{free}$ test set	1314 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.7	Xtriage
Anisotropy	0.644	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 61.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	4802	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: NAG, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	E	0.45	2/1341 (0.1%)	0.69	2/1841 (0.1%)
2	H	0.32	0/1676	0.49	0/2297
3	L	0.31	0/1711	0.48	0/2326
All	All	0.36	2/4728 (0.0%)	0.55	2/6464 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	452	CYS	C-N	8.48	1.50	1.34
1	E	533	GLU	CD-OE2	-5.01	1.20	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	452	CYS	O-C-N	8.67	137.57	121.10
1	E	452	CYS	C-N-CD	8.03	145.25	128.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	434	HIS	Peptide
1	E	511	PHE	Peptide

## 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	E	1295	0	1193	66	0
2	H	1636	0	1578	11	0
3	L	1674	0	1578	8	0
4	A	39	0	34	0	0
5	B	28	0	25	0	0
6	E	28	0	26	1	0
7	E	4	0	0	0	0
7	H	47	0	0	0	0
7	L	51	0	0	0	0
All	All	4802	0	4434	83	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 (83) 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:E:452:CYS:H	1:E:453:PRO:HD3	1.38	0.88
1:E:520:THR:HA	1:E:538:VAL:HB	1.55	0.87
1:E:452:CYS:N	1:E:453:PRO:CD	2.41	0.84
1:E:452:CYS:H	1:E:453:PRO:CD	1.91	0.80
1:E:534:ASN:H	1:E:536:THR:HG23	1.49	0.77
1:E:521:THR:HA	1:E:527:PRO:HA	1.74	0.69
1:E:539:PHE:HB3	1:E:541:LEU:HD21	1.75	0.69
1:E:521:THR:O	1:E:538:VAL:HG12	1.92	0.69
1:E:435:THR:HG21	1:E:561:GLY:HA3	1.73	0.69
1:E:508:VAL:HG13	1:E:556:TRP:HB3	1.74	0.69
1:E:424:ARG:HB2	1:E:520:THR:OG1	1.93	0.69
1:E:608:THR:HG22	1:E:611:CYS:HB2	1.75	0.69
2:H:124:PRO:HB3	2:H:150:TYR:HB3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:428:ASN:ND2	1:E:501:ALA:O	2.28	0.67
1:E:566:CYS:SG	1:E:567:GLY:N	2.69	0.65
1:E:545:ARG:O	1:E:549:GLY:N	2.31	0.62
1:E:433:LEU:HD12	1:E:433:LEU:H	1.66	0.61
1:E:431:ASP:O	1:E:434:HIS:NE2	2.34	0.60
1:E:544:THR:HG23	1:E:545:ARG:H	1.67	0.60
1:E:545:ARG:NH1	1:E:600:LYS:O	2.34	0.60
1:E:608:THR:HG23	1:E:610:ARG:H	1.66	0.60
2:H:38:ASN:HB2	2:H:48:ILE:HD11	1.83	0.60
1:E:520:THR:HB	1:E:528:THR:HB	1.84	0.59
1:E:533:GLU:H	1:E:536:THR:HG21	1.67	0.59
1:E:536:THR:HB	1:E:538:VAL:HG13	1.85	0.59
1:E:500:SER:O	1:E:503:THR:HG22	2.03	0.58
3:L:43:GLN:HB2	3:L:53:LEU:HD11	1.85	0.58
1:E:527:PRO:HB2	1:E:529:TYR:CE2	2.39	0.58
1:E:562:TYR:HD2	1:E:563:THR:H	1.53	0.56
1:E:431:ASP:HB3	1:E:437:PHE:CD2	2.40	0.56
1:E:431:ASP:HB3	1:E:437:PHE:CE2	2.40	0.55
1:E:545:ARG:HG2	1:E:552:PHE:CD2	2.41	0.55
1:E:557:MET:HA	1:E:563:THR:HB	1.89	0.55
2:H:93:VAL:HG22	2:H:113:SER:HB2	1.89	0.54
1:E:437:PHE:CG	1:E:561:GLY:HA2	2.43	0.54
1:E:536:THR:O	1:E:538:VAL:HG22	2.08	0.54
1:E:614:ASP:HA	1:E:618:ARG:HD3	1.88	0.54
1:E:532:GLY:O	1:E:533:GLU:HG3	2.08	0.54
1:E:565:THR:OG1	1:E:566:CYS:N	2.41	0.53
1:E:521:THR:HG22	1:E:538:VAL:O	2.08	0.53
1:E:528:THR:HG22	1:E:530:THR:H	1.74	0.53
1:E:556:TRP:O	1:E:563:THR:OG1	2.11	0.52
2:H:106:ASP:HA	3:L:52:LEU:HD22	1.92	0.51
1:E:512:THR:HG22	1:E:513:PRO:HD2	1.93	0.50
1:E:557:MET:HB2	1:E:621:HIS:CD2	2.46	0.50
1:E:567:GLY:HA3	1:E:603:SER:HB3	1.93	0.50
1:E:424:ARG:NH1	1:E:527:PRO:HB3	2.27	0.49
1:E:599:LEU:H	1:E:599:LEU:HD23	1.79	0.48
3:L:41:TRP:CZ3	3:L:94:CYS:HB3	2.48	0.48
1:E:536:THR:O	1:E:538:VAL:N	2.46	0.48
1:E:619:LEU:HD12	1:E:626:VAL:HG12	1.96	0.48
1:E:431:ASP:CG	1:E:434:HIS:CD2	2.88	0.47
2:H:40:ARG:HG2	2:H:92:ALA:HB2	1.96	0.47
1:E:431:ASP:O	1:E:434:HIS:CD2	2.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:500:SER:HB2	1:E:537:ASP:HA	1.97	0.46
1:E:521:THR:H	1:E:538:VAL:HG12	1.81	0.45
1:E:443:TYR:C	1:E:445:HIS:H	2.20	0.45
1:E:512:THR:O	1:E:513:PRO:C	2.54	0.45
1:E:431:ASP:HB2	1:E:435:THR:OG1	2.16	0.45
1:E:569:PRO:HA	1:E:570:PRO:HD3	1.86	0.45
2:H:120:LYS:HD3	2:H:120:LYS:HA	1.75	0.45
2:H:20:LEU:HD12	2:H:81:LEU:HD23	1.98	0.44
1:E:501:ALA:O	1:E:504:VAL:HG12	2.17	0.44
3:L:81:ILE:HB	3:L:84:VAL:HG12	2.00	0.44
3:L:201:GLU:HG3	3:L:212:VAL:HG12	2.00	0.44
3:L:125:PRO:HB3	3:L:215:PHE:CZ	2.53	0.43
1:E:431:ASP:OD2	1:E:431:ASP:N	2.51	0.43
1:E:424:ARG:HB3	1:E:529:TYR:HA	2.00	0.43
1:E:522:ASP:OD1	1:E:522:ASP:N	2.50	0.43
1:E:440:SER:HA	1:E:446:SER:HB2	2.00	0.43
1:E:536:THR:HB	1:E:538:VAL:CG1	2.48	0.43
1:E:557:MET:HA	1:E:563:THR:CB	2.47	0.43
1:E:610:ARG:HH22	6:E:701:NAG:H2	1.84	0.43
1:E:512:THR:CG2	1:E:513:PRO:HD2	2.49	0.42
1:E:431:ASP:OD1	1:E:434:HIS:HD2	2.02	0.42
2:H:175:LEU:HD12	2:H:180:TYR:CZ	2.55	0.42
3:L:39:LEU:HG	3:L:40:ALA:N	2.35	0.42
1:E:632:LYS:NZ	2:H:30:LYS:O	2.53	0.41
2:H:91:THR:HG23	2:H:115:THR:HA	2.01	0.41
3:L:143:ASN:HB3	3:L:144:ASN:OD1	2.21	0.41
1:E:533:GLU:H	1:E:536:THR:CG2	2.34	0.41
1:E:521:THR:H	1:E:538:VAL:CB	2.33	0.41
2:H:1:GLU:HA	2:H:107:SER:OG	2.21	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	E	163/272 (60%)	133 (82%)	25 (15%)	5 (3%)	4	9
2	H	217/221 (98%)	208 (96%)	9 (4%)	0	100	100
3	L	216/240 (90%)	208 (96%)	8 (4%)	0	100	100
All	All	596/733 (81%)	549 (92%)	42 (7%)	5 (1%)	19	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	435	THR
1	E	493	PRO
1	E	532	GLY
1	E	533	GLU
1	E	452	CYS

### 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	E	142/235 (60%)	137 (96%)	5 (4%)	36	63
2	H	187/189 (99%)	184 (98%)	3 (2%)	62	83
3	L	191/214 (89%)	186 (97%)	5 (3%)	46	73
All	All	520/638 (82%)	507 (98%)	13 (2%)	47	75

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	551	TRP
1	E	557	MET
1	E	562	TYR
1	E	564	LYS
1	E	566	CYS
2	H	50	ARG
2	H	85	SER
2	H	210	LYS

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Mol	Chain	Res	Type
3	L	22	SER
3	L	71	SER
3	L	83	SER
3	L	159	SER
3	L	161	ARG

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

### 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 ⓘ

5 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	$\# Z  > 2$
4	NAG	A	1	1,4	14,14,15	0.26	0	17,19,21	0.45	0
4	NAG	A	2	4	14,14,15	0.28	0	17,19,21	0.52	0
4	BMA	A	3	4	11,11,12	0.73	0	15,15,17	0.70	0
5	NAG	B	1	1,5	14,14,15	0.26	0	17,19,21	0.47	0
5	NAG	B	2	5	14,14,15	0.25	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
4	NAG	A	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	A	2	4	-	3/6/23/26	0/1/1/1
4	BMA	A	3	4	-	2/2/19/22	0/1/1/1
5	NAG	B	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	B	2	5	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

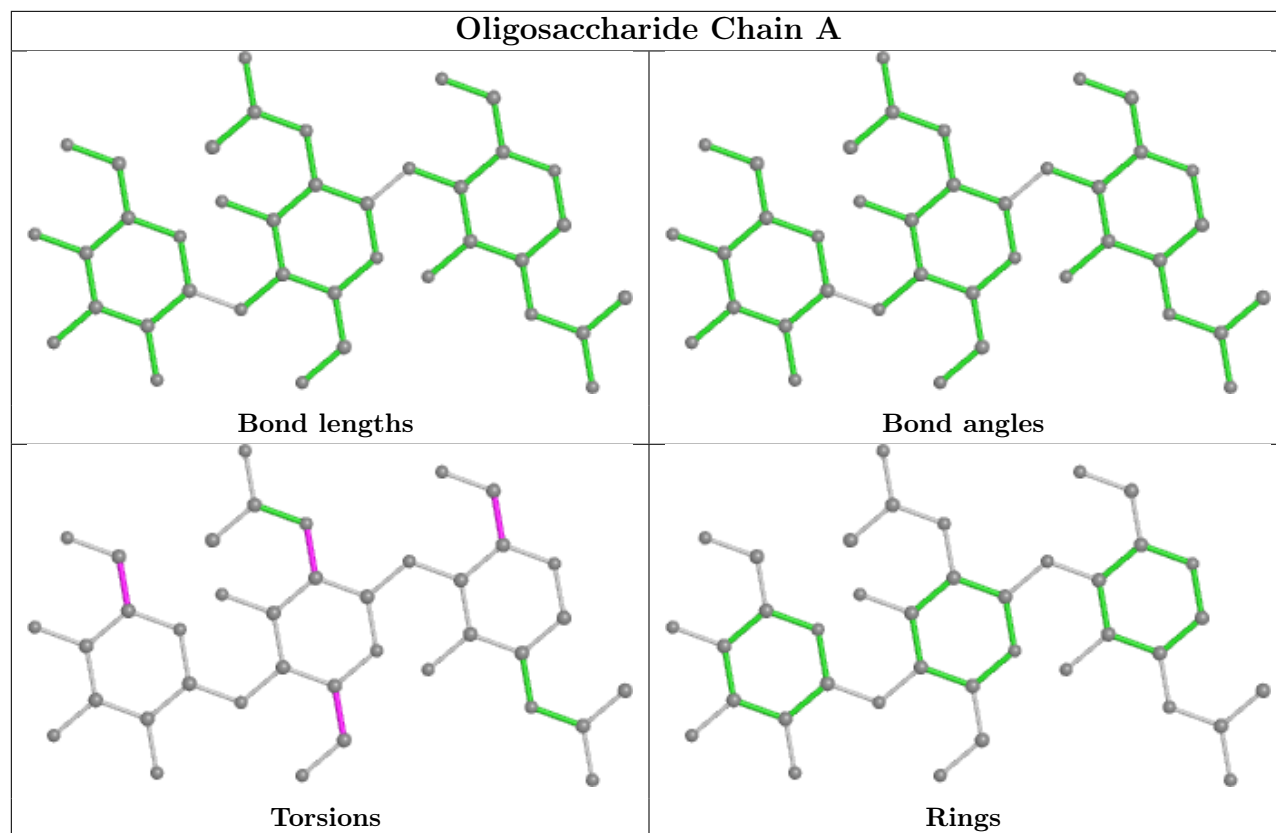
All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1	NAG	O5-C5-C6-O6
5	B	2	NAG	O5-C5-C6-O6
5	B	2	NAG	C4-C5-C6-O6
5	B	2	NAG	C8-C7-N2-C2
5	B	2	NAG	O7-C7-N2-C2
4	A	1	NAG	C4-C5-C6-O6
4	A	2	NAG	O5-C5-C6-O6
5	B	1	NAG	C4-C5-C6-O6
4	A	1	NAG	O5-C5-C6-O6
4	A	2	NAG	C4-C5-C6-O6
4	A	3	BMA	C4-C5-C6-O6
4	A	3	BMA	O5-C5-C6-O6
4	A	2	NAG	C3-C2-N2-C7

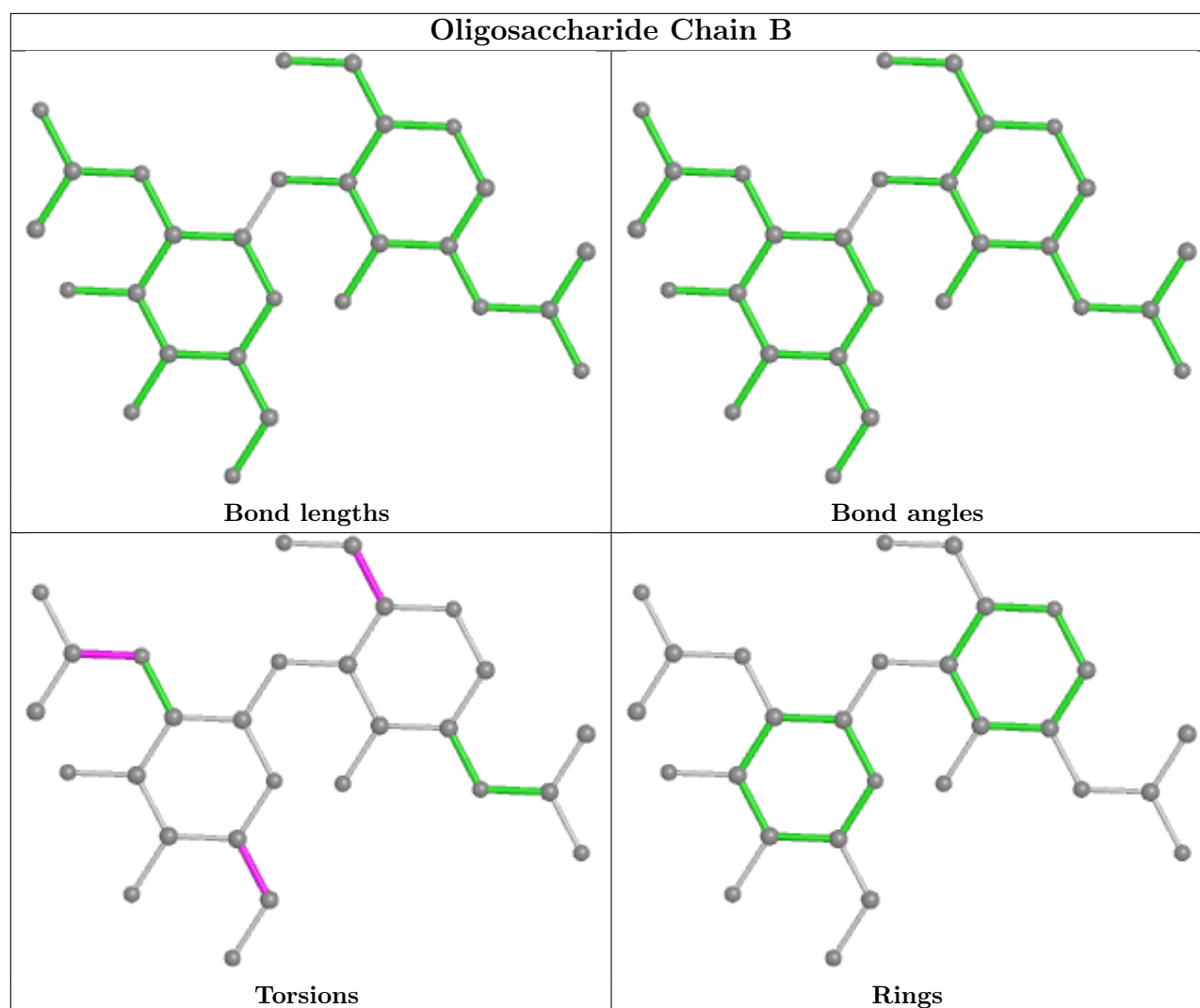
There are no ring outliers.

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](#)

2 ligands 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	$\# Z  > 2$
6	NAG	E	701	1	14,14,15	0.23	0	17,19,21	0.46	0
6	NAG	E	702	1	14,14,15	1.12	2 (14%)	17,19,21	0.84	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	E	701	1	-	0/6/23/26	0/1/1/1
6	NAG	E	702	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	702	NAG	C1-C2	3.13	1.57	1.52
6	E	702	NAG	O5-C1	2.50	1.47	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

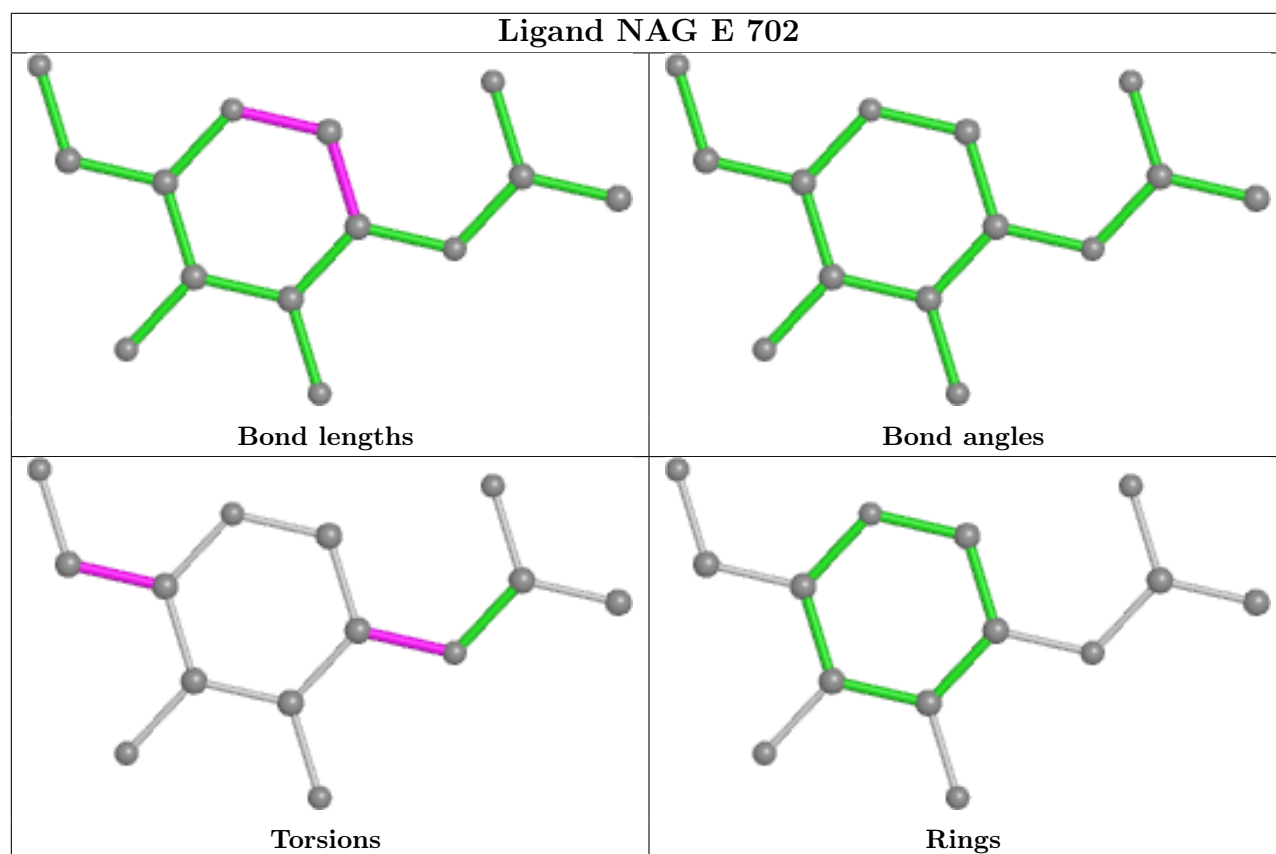
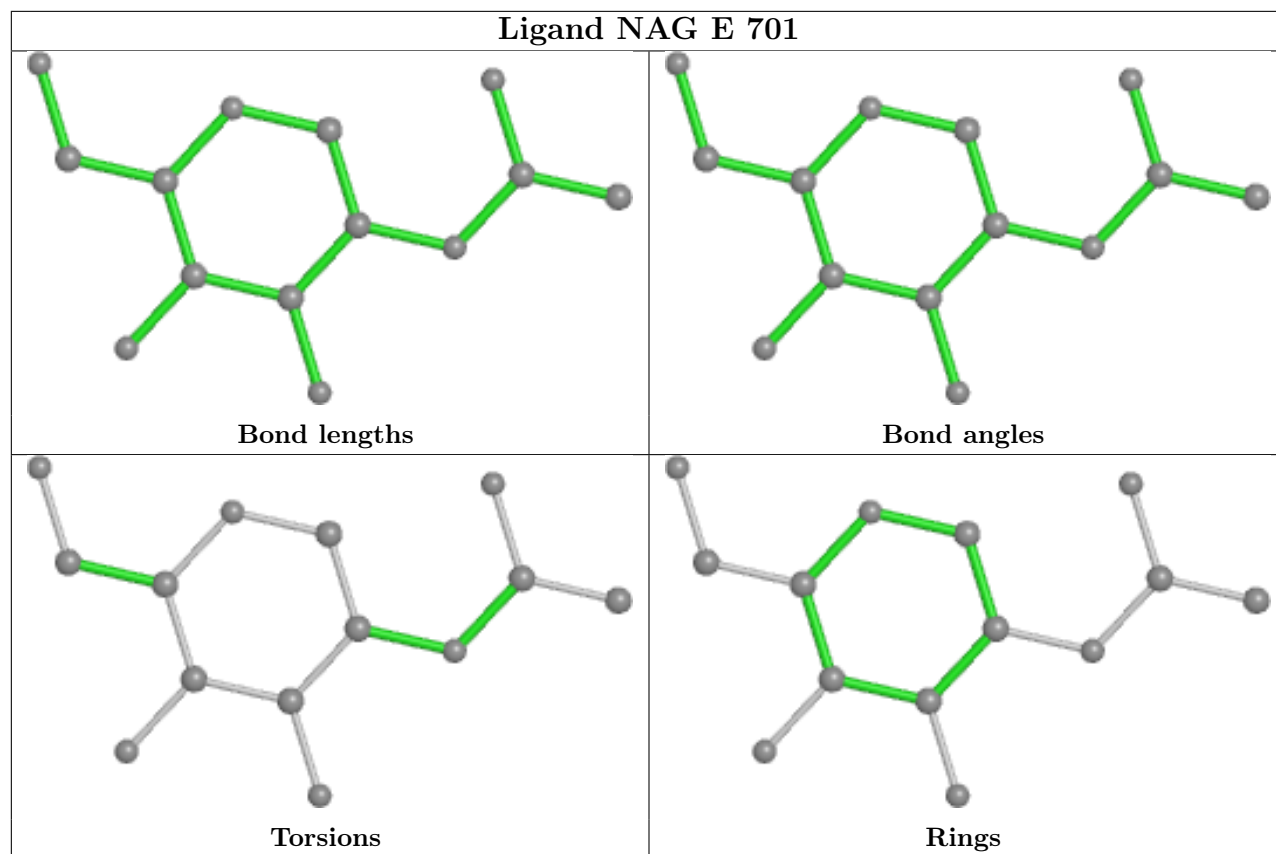
Mol	Chain	Res	Type	Atoms
6	E	702	NAG	C3-C2-N2-C7
6	E	702	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	701	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	E	169/272 (62%)	1.47	52 (30%) <b>0</b> <b>0</b>	37, 108, 145, 166	0
2	H	219/221 (99%)	-0.11	2 (0%) <b>84</b> <b>85</b>	16, 33, 66, 89	0
3	L	218/240 (90%)	-0.22	0 <b>100</b> <b>100</b>	17, 36, 69, 93	0
All	All	606/733 (82%)	0.29	54 (8%) <b>9</b> <b>8</b>	16, 42, 124, 166	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	444	THR	6.4
1	E	432	SER	6.4
1	E	445	HIS	6.0
1	E	443	TYR	6.0
1	E	447	PHE	5.9
1	E	450	SER	5.8
1	E	650	PHE	5.7
1	E	434	HIS	5.6
1	E	491	TYR	5.5
1	E	529	TYR	5.3
1	E	449	SER	4.4
1	E	537	ASP	4.1
1	E	525	GLY	4.0
1	E	533	GLU	4.0
1	E	451	GLY	4.0
1	E	452	CYS	4.0
1	E	433	LEU	3.9
1	E	527	PRO	3.9
1	E	453	PRO	3.9
1	E	498	VAL	3.7
1	E	519	GLY	3.7
1	E	571	CYS	3.6
1	E	561	GLY	3.6

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	E	422	ILE	3.5
1	E	600	LYS	3.4
1	E	423	ASN	3.2
1	E	538	VAL	3.1
1	E	448	ASN	3.1
1	E	526	ALA	3.0
1	E	548	LEU	2.9
1	E	562	TYR	2.8
1	E	536	THR	2.8
1	E	439	ALA	2.6
1	E	555	THR	2.5
1	E	531	TRP	2.5
1	E	649	ASN	2.4
2	H	219	GLY	2.4
1	E	569	PRO	2.4
1	E	426	ALA	2.3
1	E	490	HIS	2.3
1	E	492	PRO	2.3
1	E	596	THR	2.3
1	E	499	VAL	2.3
1	E	599	LEU	2.3
1	E	522	ASP	2.2
1	E	446	SER	2.2
2	H	75	SER	2.1
1	E	436	GLY	2.1
1	E	435	THR	2.1
1	E	560	SER	2.1
1	E	441	LEU	2.1
1	E	539	PHE	2.0
1	E	497	GLY	2.0
1	E	563	THR	2.0

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

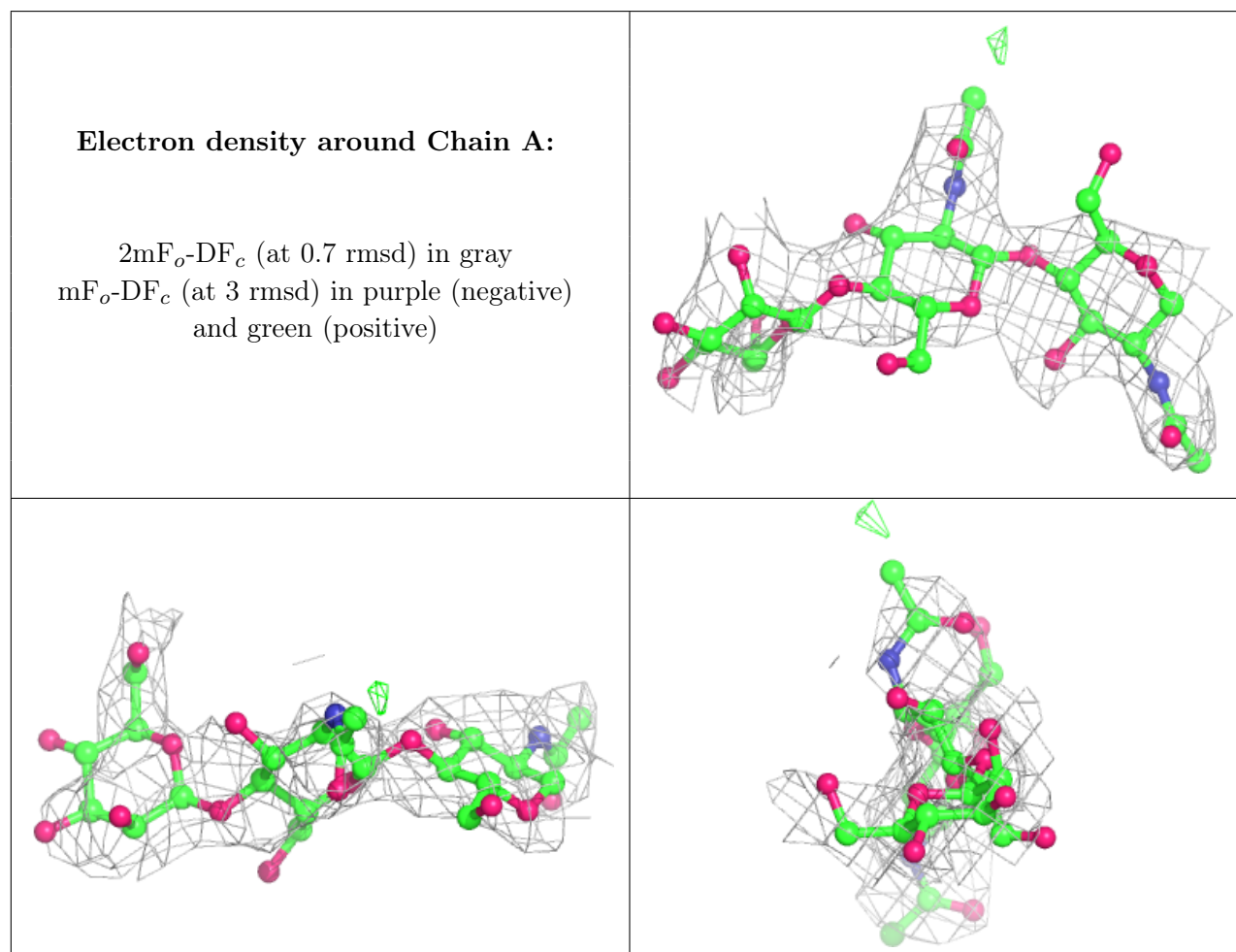
There are no non-standard protein/DNA/RNA residues in this entry.

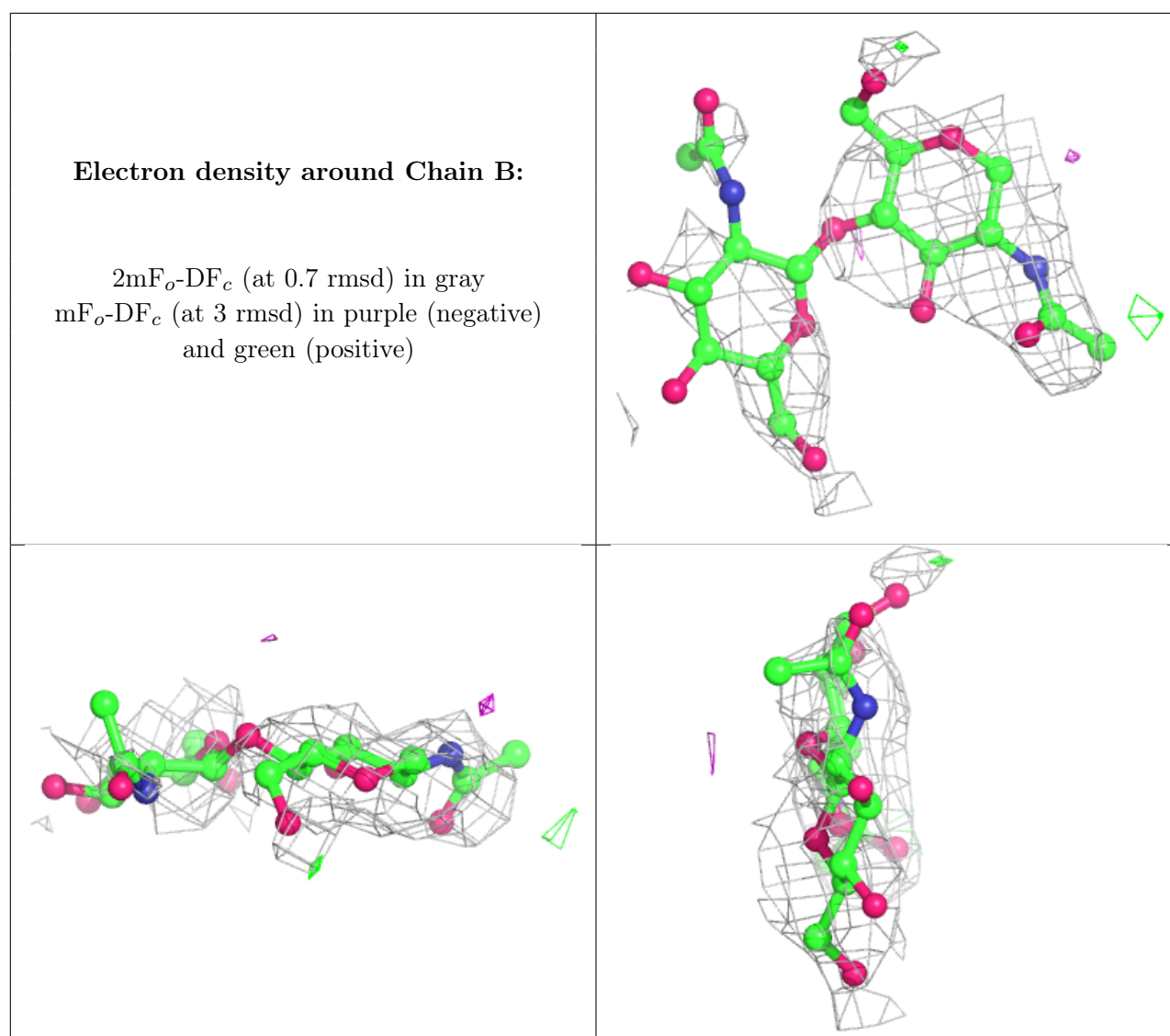
## 6.3 Carbohydrates [i](#)

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
5	NAG	B	2	14/15	0.55	0.61	137,167,178,184	0
4	BMA	A	3	11/12	0.64	0.44	118,131,142,151	0
4	NAG	A	2	14/15	0.75	0.40	111,132,138,143	0
5	NAG	B	1	14/15	0.83	0.36	99,128,139,152	0
4	NAG	A	1	14/15	0.87	0.43	90,101,124,124	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.

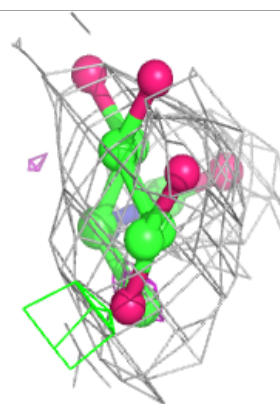
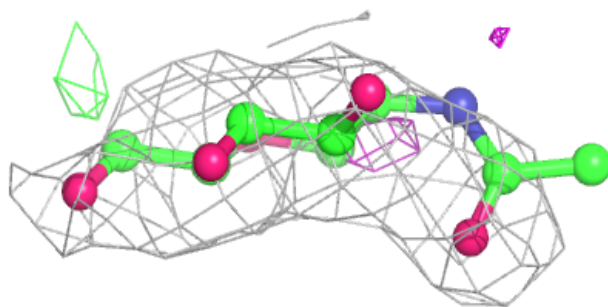
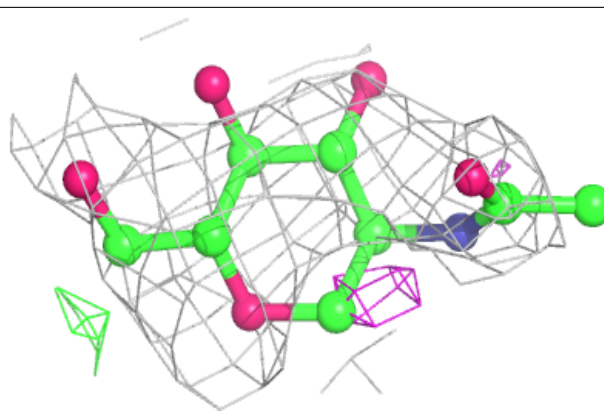
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	E	702	14/15	0.63	0.34	104,120,130,130	0
6	NAG	E	701	14/15	0.83	0.40	91,119,122,124	0

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.

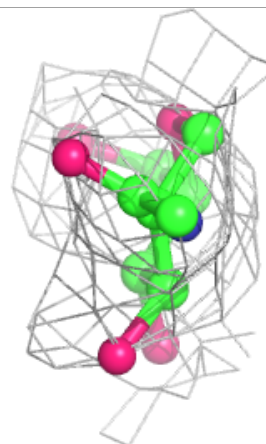
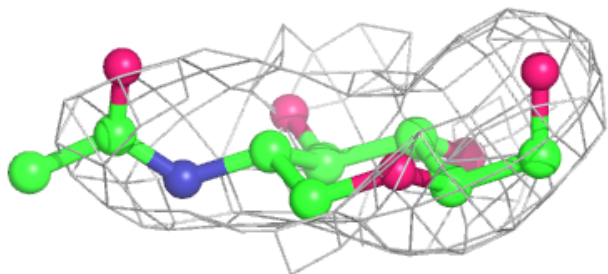
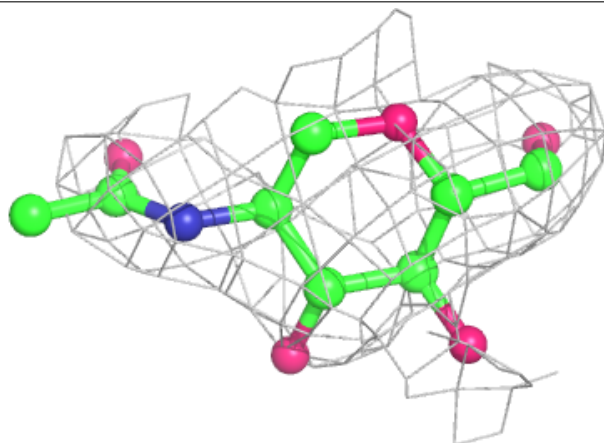


**Electron density around NAG E 702:**

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

**Electron density around NAG E 701:**

$2mF_o-DF_c$  (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.