



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2026 – 04:20 am BST

PDB ID : 30CP / pdb_000030cp
Title : Structure of the Hepatitis C Virus E2 Core from Genotype 6a in Complex with Germline Reverted Variants of the Broadly Neutralizing Antibody AR3C
Authors : Yechezkel, I.; Tzarum, N.
Deposited on : 2026-04-21
Resolution : 1.93 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

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>.

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

MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

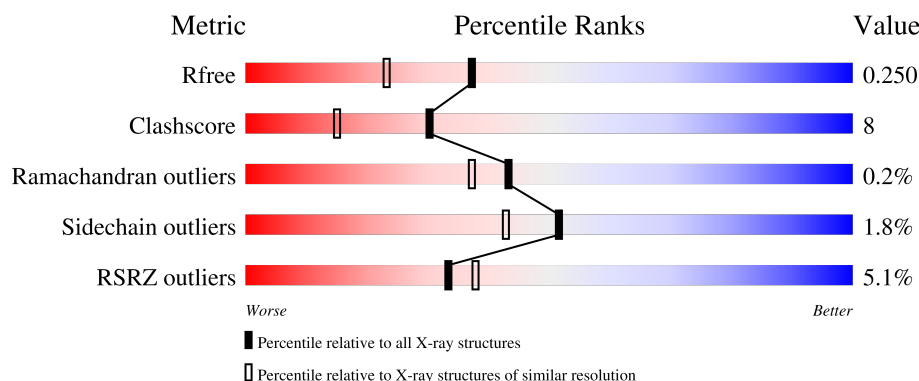
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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 ≥ 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	H	232	3% 87% 12% .
2	L	233	5% 76% 15% . 9%
3	D0A0	189	7% 87% .. 12%
4	E	2	50% 50%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9778 atoms, of which 4677 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 Fab AR3C GL heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	H	229	Total	C	H	N	O	S	0	9	0
			3412	1084	1693	285	342	8			

- Molecule 2 is a protein called Fab AR3C GL light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	212	Total	C	H	N	O	S	0	4	0
			3225	1016	1596	279	329	5			

- Molecule 3 is a protein called HCV E2 envelope protein.

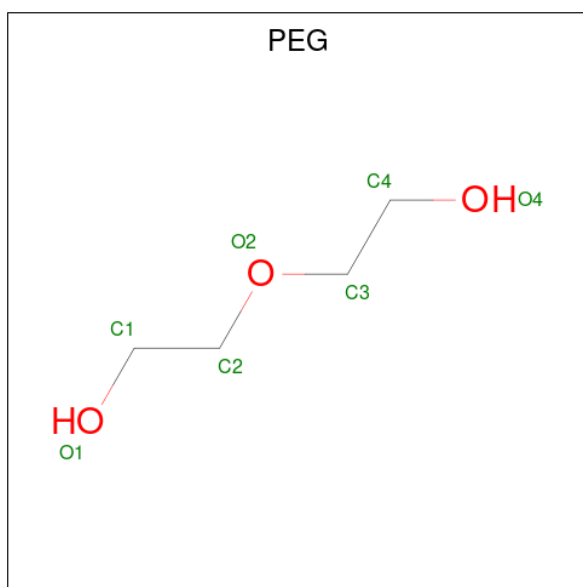
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D0A0	167	Total	C	H	N	O	S	0	7	0
			2545	835	1232	224	241	13			

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



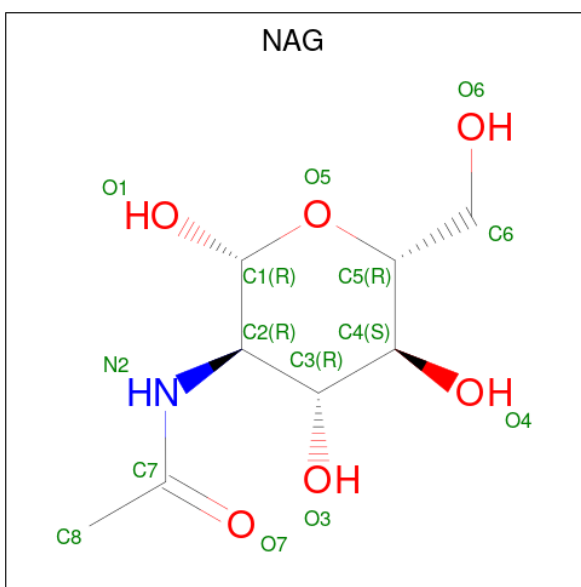
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	E	2	Total	C	H	N	O		0	0	0
			56	16	28	2	10				

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	H	O	0	0
			17	4	10	3		
5	H	1	Total	C	H	O	0	0
			17	4	10	3		
5	H	1	Total	C	H	O	0	0
			17	4	10	3		
5	H	1	Total	C	H	O	0	0
			17	4	10	3		
5	H	1	Total	C	H	O	0	0
			17	4	10	3		
5	L	1	Total	C	H	O	0	0
			17	4	10	3		
5	D0A0	1	Total	C	H	O	0	0
			17	4	10	3		
5	D0A0	1	Total	C	H	O	0	0
			17	4	10	3		
5	D0A0	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D0A0	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
6	D0A0	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

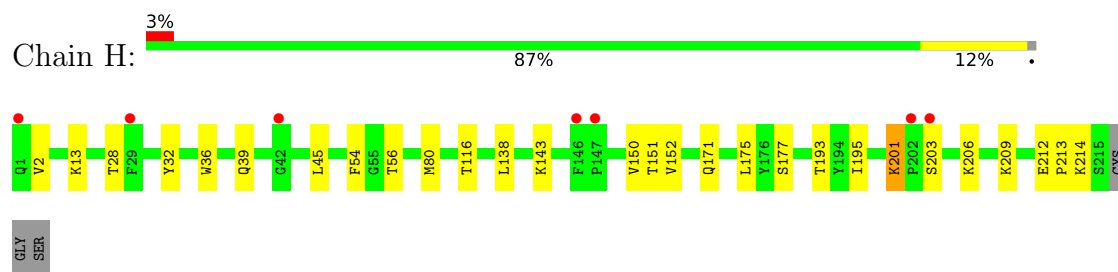
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	115	Total	O	0	0
			115	115		
7	L	106	Total	O	0	0
			106	106		
7	D0A0	93	Total	O	0	0
			93	93		

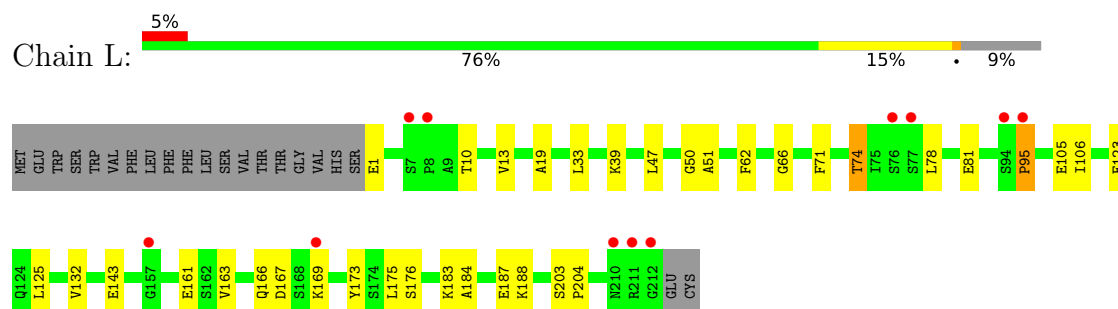
3 Residue-property plots [i](#)

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.

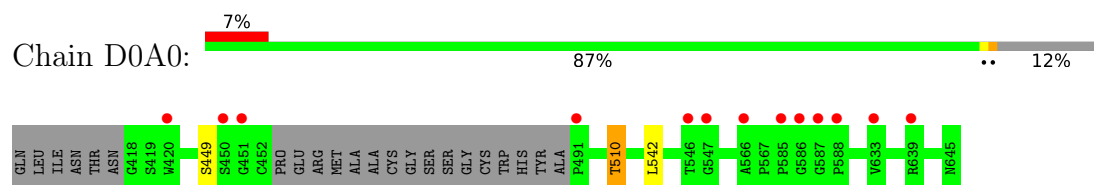
- Molecule 1: Fab AR3C GL heavy chain



- Molecule 2: Fab AR3C GL light chain



- Molecule 3: HCV E2 envelope protein



- Molecule 4: 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 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.33Å 64.45Å 183.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.05 – 1.93 44.05 – 1.93	Depositor EDS
% Data completeness (in resolution range)	98.2 (44.05-1.93) 98.2 (44.05-1.93)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.202 , 0.245 0.206 , 0.250	Depositor DCC
R_{free} test set	2809 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9778	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PEG, 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	H	0.46	2/1797 (0.1%)	0.69	2/2446 (0.1%)
2	L	0.46	0/1677	0.72	1/2278 (0.0%)
3	D0A0	0.37	0/1379	0.57	1/1888 (0.1%)
All	All	0.44	2/4853 (0.0%)	0.67	4/6612 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	152[A]	VAL	N-CA	6.43	1.53	1.46
1	H	152[B]	VAL	N-CA	6.43	1.53	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	151	THR	CA-C-N	-8.24	111.53	122.99
1	H	151	THR	C-N-CA	-8.24	111.53	122.99
3	D0A0	510	THR	CA-C-O	-5.49	112.64	120.16
2	L	95	PRO	N-CA-C	-5.01	102.15	112.47

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	H	1719	1693	1646	19	0
2	L	1629	1596	1578	31	0
3	D0A0	1313	1232	0	0	0
4	E	28	28	25	0	0
5	D0A0	28	40	0	0	0
5	H	35	50	50	0	0
5	L	7	10	10	0	0
6	D0A0	28	28	0	0	0
7	D0A0	93	0	0	0	1
7	H	115	0	0	6	0
7	L	106	0	0	3	0
All	All	5101	4677	3309	50	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 8.

All (50) 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)
2:L:10[B]:THR:HG23	7:L:413:HOH:O	1.75	0.86
1:H:212:GLU:HG3	1:H:213:PRO:HD2	1.64	0.78
2:L:10[B]:THR:HG22	2:L:143:GLU:OE1	1.82	0.78
2:L:161:GLU:HG2	2:L:175:LEU:HD21	1.69	0.75
7:H:404:HOH:O	2:L:123:GLU:HG2	1.86	0.75
1:H:171:GLN:HG3	1:H:175:LEU:O	1.95	0.65
1:H:116:THR:HG22	1:H:203:SER:HB3	1.83	0.60
2:L:10[B]:THR:CG2	2:L:143:GLU:OE1	2.49	0.60
1:H:54:PHE:HB2	1:H:56:THR:HG22	1.83	0.60
2:L:167:ASP:OD1	2:L:169:LYS:HG2	2.01	0.60
1:H:39:GLN:HB2	1:H:45:LEU:HD23	1.86	0.57
1:H:212:GLU:HG3	1:H:213:PRO:CD	2.33	0.57
2:L:1:GLU:HA	2:L:1:GLU:OE1	2.04	0.57
2:L:166:GLN:HG3	2:L:173:TYR:CZ	2.40	0.56
2:L:183:LYS:O	2:L:187:GLU:HG3	2.06	0.56
2:L:125:LEU:O	2:L:183:LYS:HD2	2.08	0.54
2:L:105:GLU:OE1	2:L:173:TYR:OH	2.17	0.54
2:L:163[B]:VAL:HG22	2:L:175:LEU:HD12	1.91	0.53
2:L:81:GLU:H	2:L:81:GLU:CD	2.18	0.52
2:L:66:GLY:HA3	2:L:71:PHE:CD2	2.46	0.51
1:H:36:TRP:CE2	1:H:80:MET:HB2	2.46	0.50
1:H:28:THR:HG23	1:H:32:TYR:CE1	2.47	0.50
1:H:209:LYS:NZ	7:H:404:HOH:O	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:213:PRO:O	1:H:214:LYS:HG2	2.12	0.50
1:H:171:GLN:NE2	7:H:405:HOH:O	2.44	0.50
2:L:106:ILE:HG22	2:L:166:GLN:OE1	2.12	0.50
2:L:10[B]:THR:OG1	2:L:105:GLU:CD	2.55	0.50
2:L:1:GLU:H1	2:L:95:PRO:HG2	1.78	0.49
2:L:184:ALA:O	2:L:188:LYS:HG2	2.14	0.47
2:L:10[B]:THR:HG21	2:L:143:GLU:OE2	2.13	0.47
2:L:39:LYS:NZ	7:L:404:HOH:O	2.43	0.47
7:H:404:HOH:O	2:L:123:GLU:CG	2.54	0.47
2:L:13:VAL:HG21	2:L:19:ALA:HB2	1.97	0.46
1:H:193:THR:HG22	1:H:195:ILE:HG13	1.97	0.45
1:H:213:PRO:C	1:H:214:LYS:HG2	2.42	0.45
1:H:138:LEU:C	1:H:138:LEU:HD12	2.42	0.44
2:L:19:ALA:O	2:L:74:THR:HA	2.18	0.44
2:L:39:LYS:CE	7:L:404:HOH:O	2.64	0.44
2:L:161:GLU:HA	2:L:176:SER:O	2.17	0.44
1:H:201:LYS:HD3	1:H:201:LYS:C	2.43	0.44
2:L:175:LEU:C	2:L:175:LEU:HD23	2.43	0.44
1:H:143:LYS:HG2	1:H:177[B]:SER:OG	2.18	0.43
1:H:143:LYS:NZ	7:H:405:HOH:O	2.52	0.43
1:H:206:LYS:HE3	1:H:206:LYS:HB2	1.75	0.43
2:L:163[B]:VAL:CG2	2:L:175:LEU:HD12	2.49	0.43
2:L:1:GLU:N	2:L:95:PRO:HG2	2.34	0.42
1:H:13:LYS:HE2	7:H:450:HOH:O	2.20	0.41
2:L:47:LEU:HD21	2:L:62:PHE:CD1	2.55	0.41
2:L:203:SER:OG	2:L:204:PRO:HD2	2.21	0.41
2:L:50:GLY:O	2:L:51:ALA:HB3	2.20	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)
7:D0A0:871:HOH:O	7:D0A0:881:HOH:O[4_465]	2.19	0.01

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	H	236/232 (102%)	232 (98%)	4 (2%)	0	100	100
2	L	214/233 (92%)	206 (96%)	8 (4%)	0	100	100
3	D0A0	170/189 (90%)	165 (97%)	4 (2%)	1 (1%)	21	11
All	All	620/654 (95%)	603 (97%)	16 (3%)	1 (0%)	43	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D0A0	510	THR

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	H	199/192 (104%)	196 (98%)	3 (2%)	57	49
2	L	186/202 (92%)	182 (98%)	4 (2%)	45	35
3	D0A0	149/159 (94%)	147 (99%)	2 (1%)	61	54
All	All	534/553 (97%)	525 (98%)	9 (2%)	51	44

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	2	VAL
1	H	150	VAL
1	H	201	LYS
2	L	33	LEU
2	L	74	THR
2	L	78	LEU
2	L	132	VAL
3	D0A0	449	SER

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Mol	Chain	Res	Type
3	D0A0	542	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	79	GLN
2	L	210	ASN

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	$\# Z > 2$
4	NAG	E	1	4,3	14,14,15	0.19	0	17,19,21	0.69	1 (5%)
4	NAG	E	2	4	14,14,15	0.29	0	17,19,21	0.50	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	E	1	4,3	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	2	4	-	1/6/23/26	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(°)
4	E	1	NAG	C1-O5-C5	2.35	115.37	112.19

There are no chirality outliers.

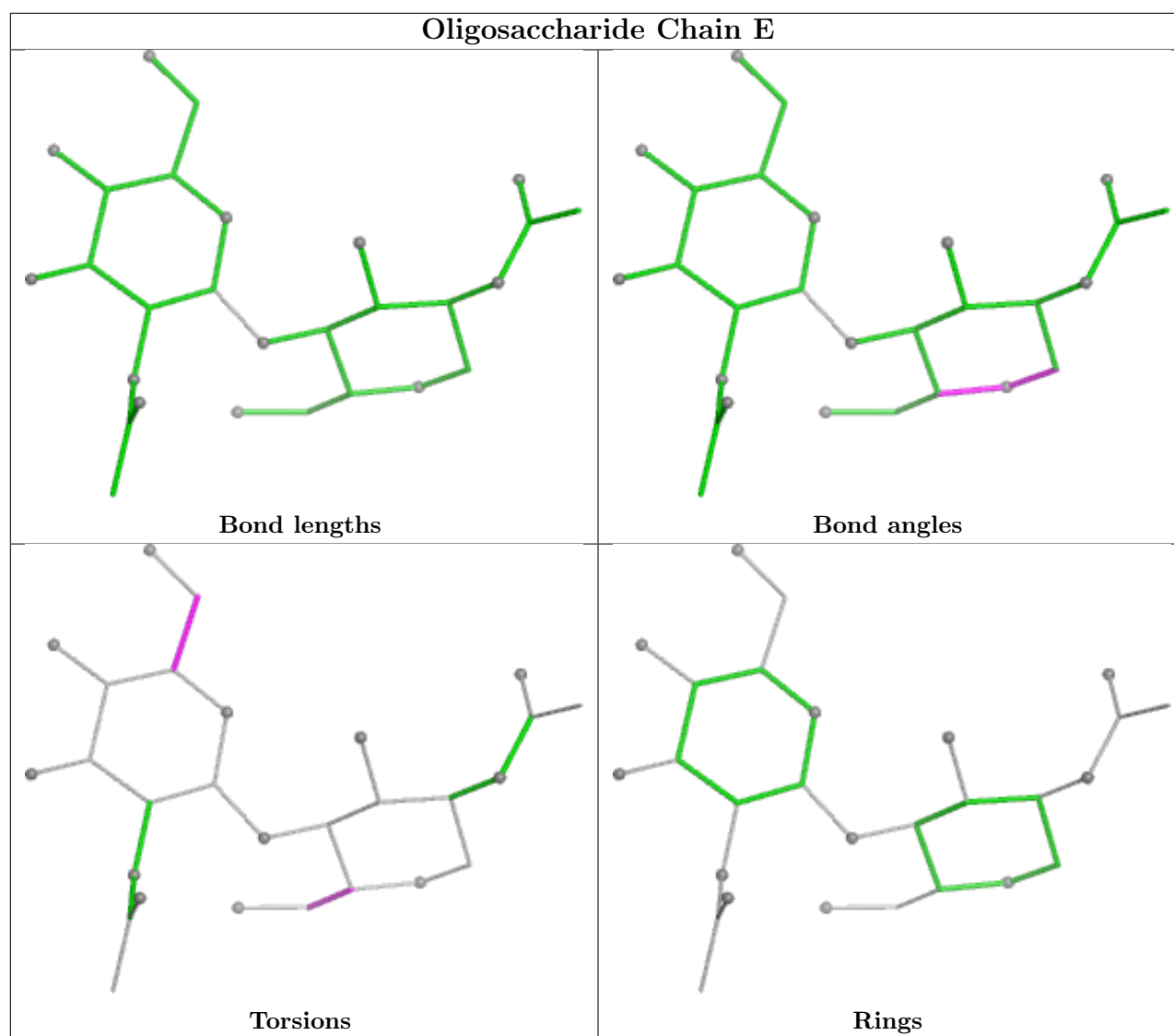
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	2	NAG	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
5	PEG	D0A0	704	-	6,6,6	0.11	0	5,5,5	0.09	0
5	PEG	H	301	-	6,6,6	0.10	0	5,5,5	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PEG	D0A0	705	-	6,6,6	0.14	0	5,5,5	0.13	0
5	PEG	H	305	-	6,6,6	0.11	0	5,5,5	0.08	0
5	PEG	H	302	-	6,6,6	0.15	0	5,5,5	0.10	0
6	NAG	D0A0	702	3	14,14,15	0.24	0	17,19,21	0.37	0
6	NAG	D0A0	701	3	14,14,15	0.25	0	17,19,21	0.60	0
5	PEG	D0A0	703	-	6,6,6	0.09	0	5,5,5	0.07	0
5	PEG	H	303	-	6,6,6	0.16	0	5,5,5	0.14	0
5	PEG	L	301	-	6,6,6	0.13	0	5,5,5	0.11	0
5	PEG	H	304	-	6,6,6	0.13	0	5,5,5	0.12	0
5	PEG	D0A0	706	-	6,6,6	0.12	0	5,5,5	0.10	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
5	PEG	D0A0	704	-	-	1/4/4/4	-
5	PEG	H	301	-	-	2/4/4/4	-
5	PEG	D0A0	705	-	-	1/4/4/4	-
5	PEG	H	305	-	-	2/4/4/4	-
5	PEG	H	302	-	-	2/4/4/4	-
6	NAG	D0A0	702	3	-	0/6/23/26	0/1/1/1
6	NAG	D0A0	701	3	-	2/6/23/26	0/1/1/1
5	PEG	D0A0	703	-	-	3/4/4/4	-
5	PEG	H	303	-	-	1/4/4/4	-
5	PEG	L	301	-	-	2/4/4/4	-
5	PEG	H	304	-	-	3/4/4/4	-
5	PEG	D0A0	706	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	304	PEG	O1-C1-C2-O2
5	H	304	PEG	O2-C3-C4-O4
5	H	301	PEG	O2-C3-C4-O4

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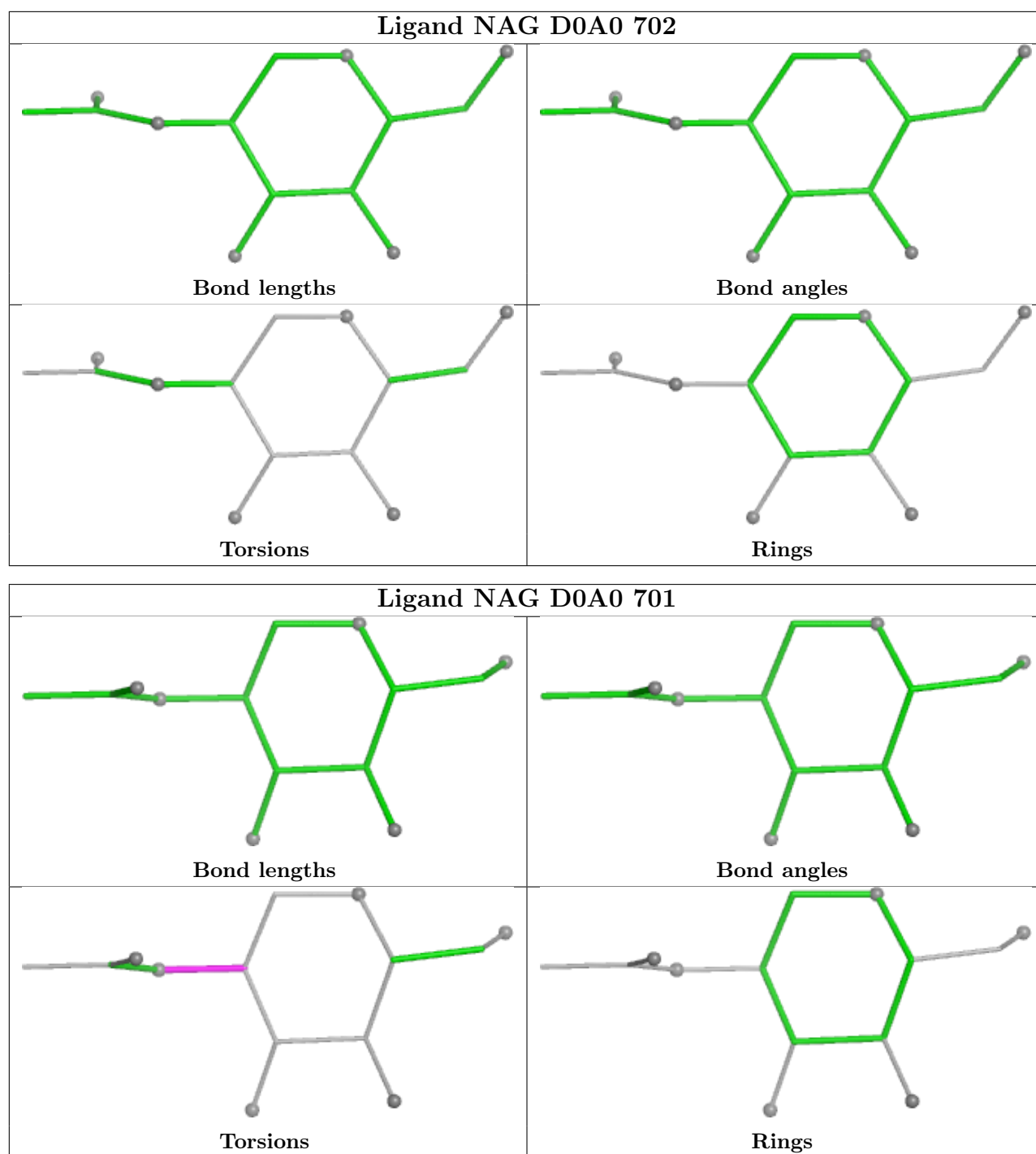
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Mol	Chain	Res	Type	Atoms
5	H	301	PEG	O1-C1-C2-O2
5	D0A0	704	PEG	O1-C1-C2-O2
5	D0A0	703	PEG	O1-C1-C2-O2
5	H	302	PEG	O1-C1-C2-O2
5	H	305	PEG	O1-C1-C2-O2
5	D0A0	705	PEG	O1-C1-C2-O2
5	H	302	PEG	C1-C2-O2-C3
5	D0A0	706	PEG	C4-C3-O2-C2
5	D0A0	703	PEG	O2-C3-C4-O4
5	D0A0	703	PEG	C1-C2-O2-C3
5	H	304	PEG	C4-C3-O2-C2
5	L	301	PEG	C4-C3-O2-C2
6	D0A0	701	NAG	C3-C2-N2-C7
6	D0A0	701	NAG	C1-C2-N2-C7
5	H	303	PEG	O1-C1-C2-O2
5	D0A0	706	PEG	O2-C3-C4-O4
5	H	305	PEG	C4-C3-O2-C2
5	L	301	PEG	O1-C1-C2-O2

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, 95th 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 ²)	Q<0.9
1	H	229/232 (98%)	0.28	7 (3%) 51 57	15, 40, 66, 82	4 (1%)
2	L	212/233 (90%)	0.39	11 (5%) 33 37	17, 40, 70, 91	2 (0%)
3	D0A0	167/189 (88%)	0.25	13 (7%) 19 21	15, 33, 75, 102	4 (2%)
All	All	608/654 (92%)	0.31	31 (5%) 33 38	15, 39, 70, 102	10 (1%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	94	SER	6.1
2	L	212	GLY	5.1
3	D0A0	587	GLY	5.0
2	L	95	PRO	4.5
3	D0A0	586	GLY	4.5
1	H	29	PHE	3.9
3	D0A0	633	VAL	3.9
1	H	203	SER	3.7
3	D0A0	585	PRO	3.7
2	L	211	ARG	3.4
2	L	210	ASN	3.3
3	D0A0	420	TRP	3.3
3	D0A0	566	ALA	3.2
2	L	8	PRO	3.2
3	D0A0	588	PRO	2.9
2	L	77	SER	2.8
3	D0A0	546	THR	2.6
2	L	76	SER	2.4
1	H	1	GLN	2.4
3	D0A0	451	GLY	2.3
2	L	157	GLY	2.3
1	H	146	PHE	2.3
2	L	169	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	147	PRO	2.3
3	D0A0	491	PRO	2.2
3	D0A0	547	GLY	2.2
1	H	202	PRO	2.1
2	L	7	SER	2.1
3	D0A0	639	ARG	2.1
1	H	42	GLY	2.0
3	D0A0	450	SER	2.0

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

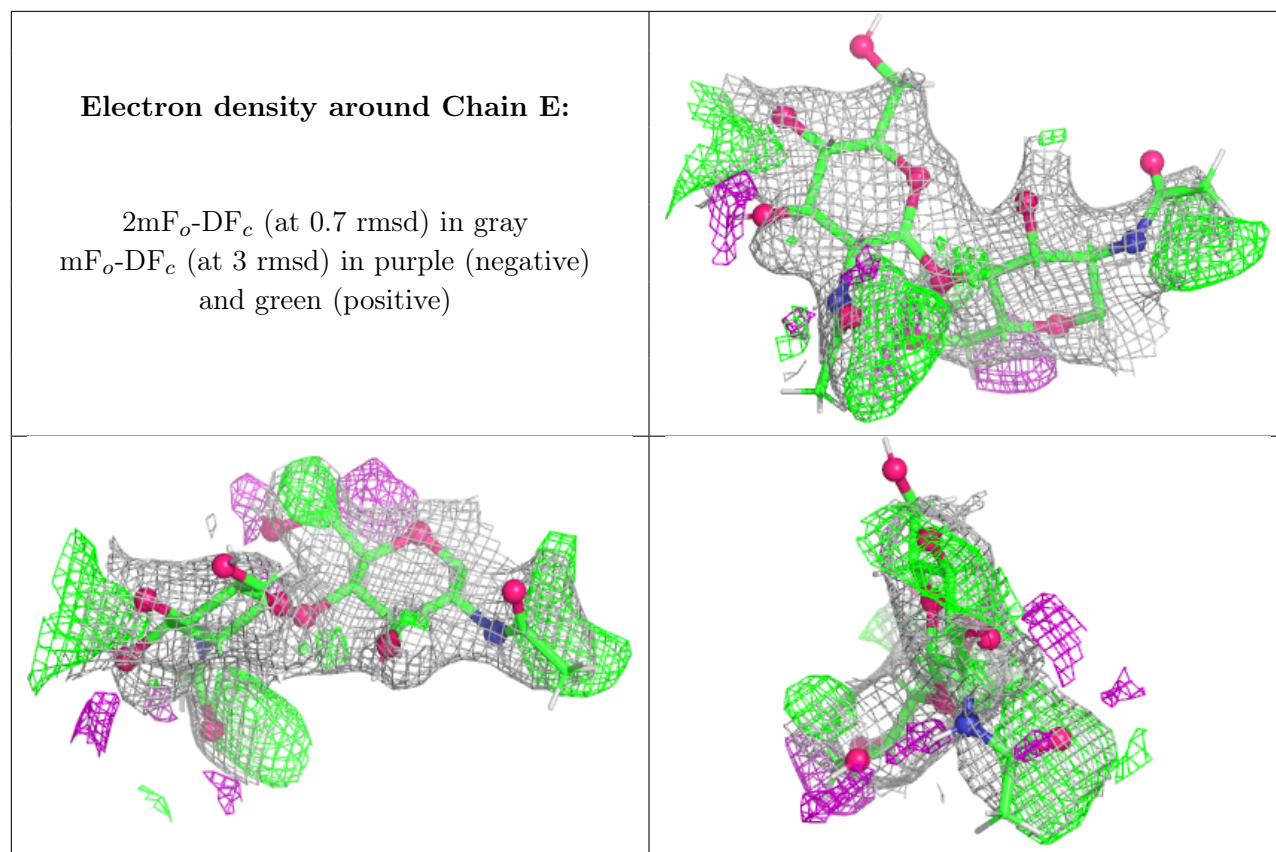
There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th 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	1	14/15	-	-	41,66,107,109	0
4	NAG	E	2	14/15	-	-	70,89,107,165	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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.

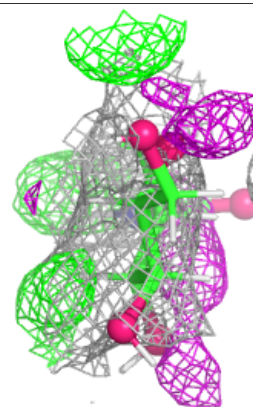
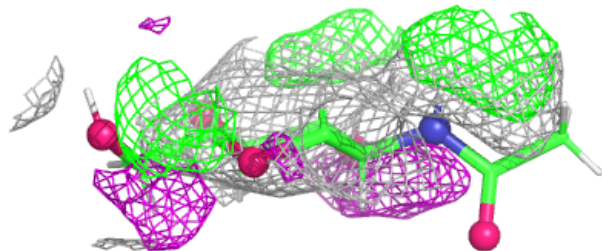
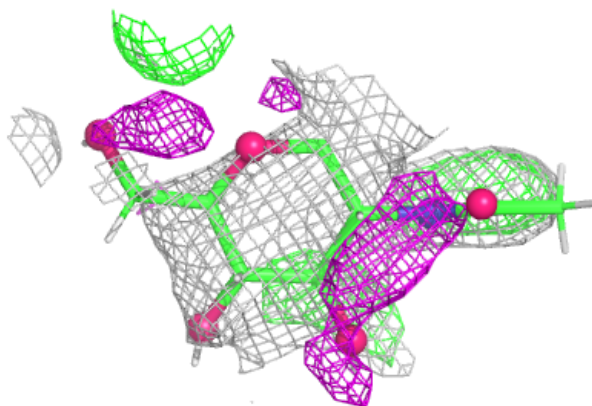
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	D0A0	702	14/15	0.54	0.24	65,97,124,145	0
6	NAG	D0A0	701	14/15	0.71	0.20	45,76,93,97	0
5	PEG	H	305	7/7	0.79	0.17	54,71,85,98	0
5	PEG	D0A0	706	7/7	0.80	0.17	55,66,79,79	0
5	PEG	H	301	7/7	0.82	0.16	47,57,79,89	0
5	PEG	D0A0	705	7/7	0.87	0.16	44,55,66,66	0
5	PEG	H	302	7/7	0.88	0.14	36,50,63,64	0
5	PEG	H	303	7/7	0.89	0.16	31,53,74,83	0
5	PEG	D0A0	703	7/7	0.89	0.15	61,78,94,94	0
5	PEG	L	301	7/7	0.91	0.10	42,53,66,66	0
5	PEG	H	304	7/7	0.91	0.11	49,66,73,73	0
5	PEG	D0A0	704	7/7	0.92	0.11	46,55,66,66	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.

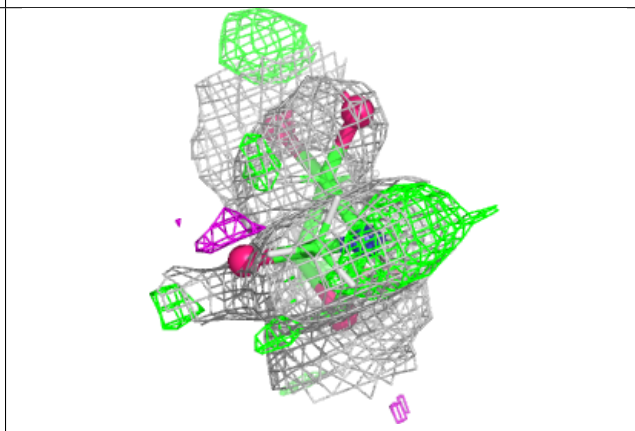
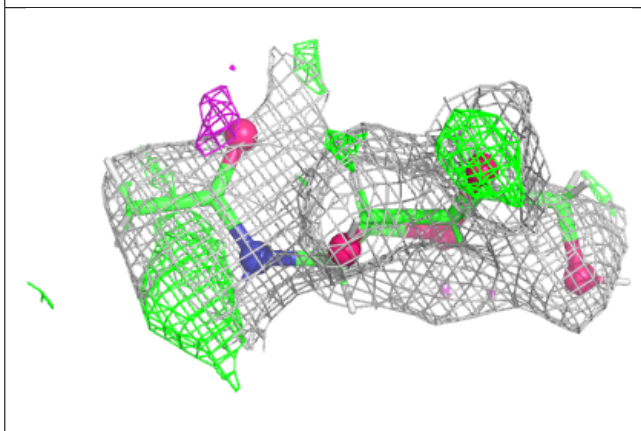
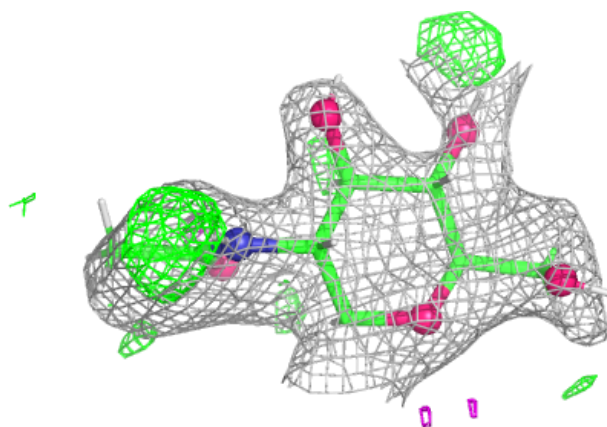
Electron density around NAG D0A0 702:

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



Electron density around NAG D0A0 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 [i](#)

There are no such residues in this entry.