



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2026 – 04:20 am BST

PDB ID : 30BC / pdb_000030bc
Title : Structure of the Hepatitis C Virus E2 Core from Genotype 6a in Complex with Germline Reverted Variants of the Broadly Neutralizing Antibody AR3A
Authors : Yechezkel, I.; Tzarum, N.
Deposited on : 2026-04-19
Resolution : 2.04 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

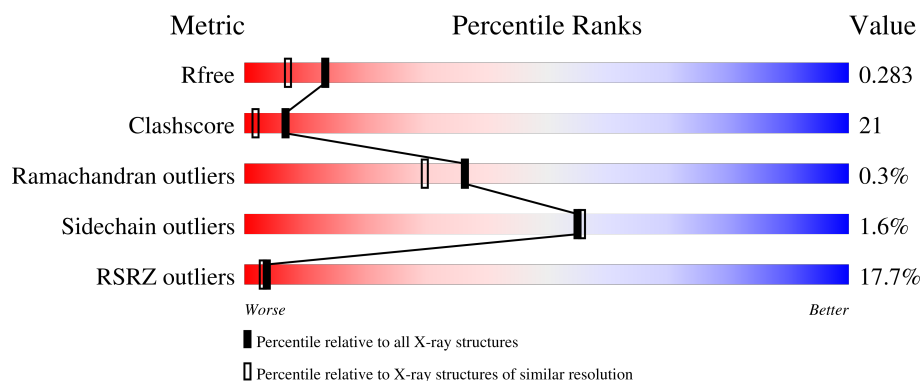
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	16% 73% 24% ..
2	E	189	30% 53% 32% .. 13%
3	L	233	6% 72% 19% 8%
4	A	2	50% 50%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4893 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 Fab AR3A 1-69 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	228	Total	C	N	O	S	0	0	0
			1689	1065	280	336	8			

- Molecule 2 is a protein called HCV E2 envelope protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	164	Total	C	N	O	S	0	0	0
			1260	801	215	231	13			

- Molecule 3 is a protein called Fab AR3A 1-69 light chain.

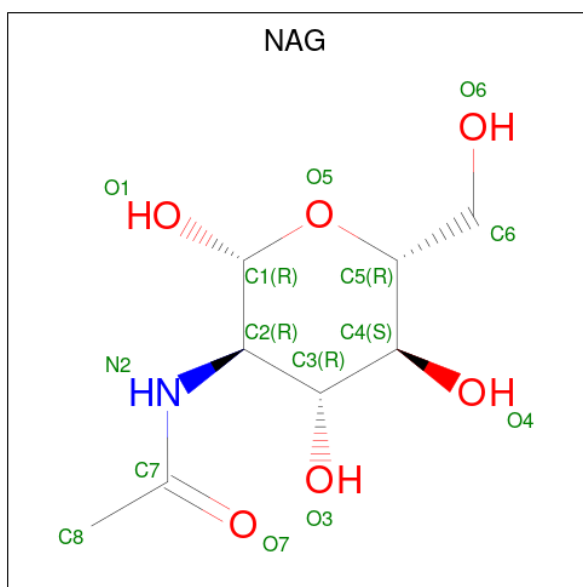
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	4	0
			1678	1042	292	339	5			

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

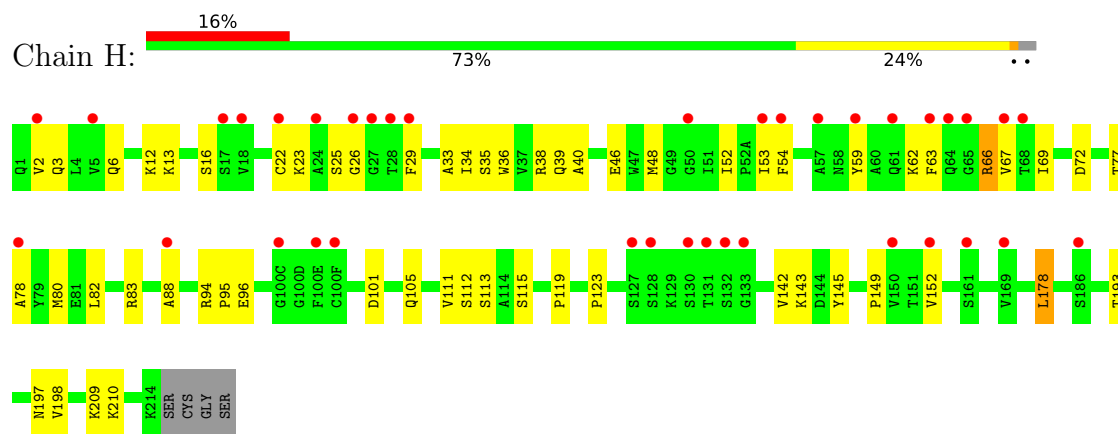
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	73	Total	O	0	0
			73	73		
6	E	15	Total	O	0	0
			15	15		
6	L	108	Total	O	0	0
			108	108		

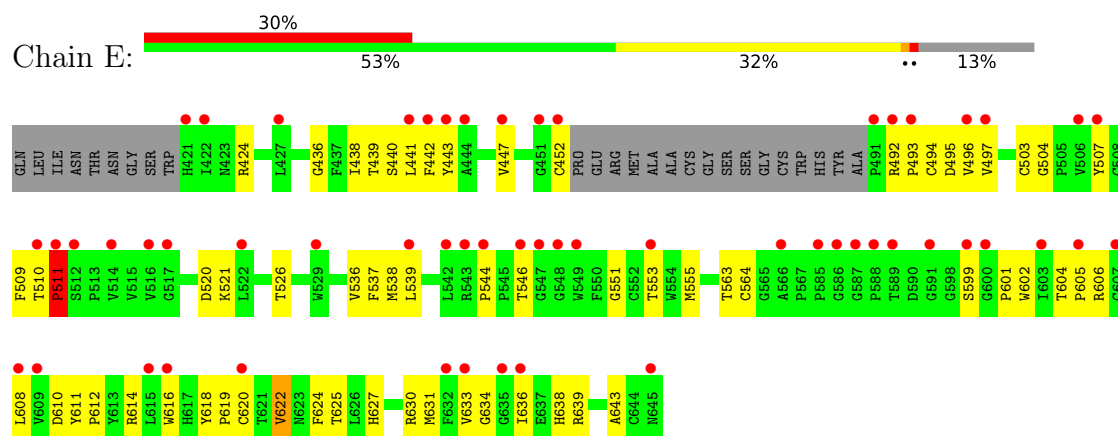
3 Residue-property plots

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.

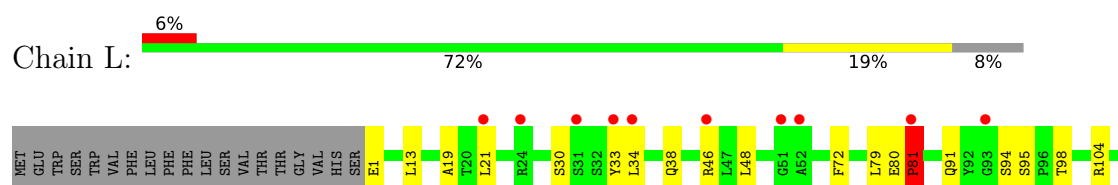
• Molecule 1: Fab AR3A 1-69 heavy chain



• Molecule 2: HCV E2 envelope protein



• Molecule 3: Fab AR3A 1-69 light chain





● 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	61.43Å 66.95Å 218.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.98 – 2.04 46.98 – 2.04	Depositor EDS
% Data completeness (in resolution range)	95.9 (46.98-2.04) 95.9 (46.98-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.235 , 0.281 0.238 , 0.283	Depositor DCC
R_{free} test set	2733 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4893	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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: 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	0.65	0/1730	0.86	0/2356
2	E	0.56	0/1302	0.84	2/1781 (0.1%)
3	L	0.83	4/1713 (0.2%)	0.97	6/2323 (0.3%)
All	All	0.70	4/4745 (0.1%)	0.90	8/6460 (0.1%)

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
3	L	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	81	PRO	N-CA	17.14	1.70	1.47
3	L	142	PRO	N-CA	13.34	1.70	1.47
3	L	80	GLU	C-N	7.77	1.45	1.33
3	L	141	TYR	C-N	5.85	1.45	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	80	GLU	CA-C-N	14.87	136.72	119.47
3	L	80	GLU	C-N-CA	14.87	136.72	119.47
2	E	511	PRO	CB-CA-C	9.57	127.35	111.56
3	L	142	PRO	CA-N-CD	-7.51	100.99	111.50
2	E	511	PRO	CA-N-CD	-7.14	102.01	112.00
3	L	81	PRO	CA-N-CD	-7.06	102.12	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	141	TYR	CA-C-N	5.19	139.45	127.00
3	L	141	TYR	C-N-CA	5.19	139.45	127.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	46	ARG	Sidechain
3	L	81	PRO	Mainchain

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	1689	0	1652	71	0
2	E	1260	0	1180	83	0
3	L	1678	0	1626	43	0
4	A	28	0	25	0	0
5	E	42	0	39	0	0
6	E	15	0	0	6	0
6	H	73	0	0	5	0
6	L	108	0	0	7	0
All	All	4893	0	4522	197	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 21.

All (197) 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)
3:L:81:PRO:N	3:L:81:PRO:CA	1.70	1.44
3:L:142:PRO:N	3:L:142:PRO:CA	1.69	1.39
2:E:452:CYS:SG	2:E:620:CYS:CB	2.14	1.35
2:E:452:CYS:SG	2:E:620:CYS:SG	1.28	1.27
1:H:67:VAL:HG22	1:H:82:LEU:HD13	1.23	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:23:LYS:HG2	1:H:77:THR:HG22	1.10	1.09
1:H:67:VAL:HG22	1:H:82:LEU:CD1	1.83	1.08
2:E:553:THR:HG22	2:E:563:THR:HG22	1.35	1.04
2:E:619:PRO:O	2:E:622:VAL:CG2	2.10	0.99
2:E:510:THR:O	2:E:510:THR:HG23	1.65	0.96
1:H:22:CYS:HB3	1:H:78:ALA:HB3	1.49	0.93
1:H:23:LYS:CG	1:H:77:THR:HG22	1.99	0.91
2:E:619:PRO:O	2:E:622:VAL:HG23	1.71	0.89
3:L:34:LEU:HD13	3:L:72:PHE:CG	2.10	0.86
1:H:178:LEU:O	1:H:178:LEU:HD23	1.77	0.84
2:E:510:THR:OG1	2:E:544:PRO:HG3	1.77	0.84
1:H:2:VAL:HG21	1:H:29:PHE:HD2	1.41	0.82
2:E:546:THR:HG21	2:E:634:GLY:CA	2.09	0.82
1:H:67:VAL:CG2	1:H:82:LEU:CD1	2.60	0.80
1:H:23:LYS:HG2	1:H:77:THR:CG2	2.03	0.80
2:E:627:HIS:CD2	6:E:813:HOH:O	2.36	0.78
2:E:510:THR:O	2:E:510:THR:CG2	2.30	0.77
1:H:34:ILE:HD13	1:H:94:ARG:CD	2.14	0.77
1:H:63:PHE:HB3	1:H:67:VAL:CG2	2.13	0.77
1:H:67:VAL:CG2	1:H:82:LEU:HD13	2.12	0.76
2:E:440:SER:HG	2:E:616:TRP:CD1	2.04	0.76
2:E:521:LYS:O	2:E:538:MET:HE1	1.86	0.75
2:E:619:PRO:O	2:E:622:VAL:HG22	1.84	0.75
1:H:34:ILE:HD11	1:H:94:ARG:CZ	2.16	0.74
1:H:66:ARG:HH11	1:H:66:ARG:HG3	1.51	0.73
1:H:34:ILE:HD13	1:H:94:ARG:HD3	1.69	0.73
2:E:452:CYS:SG	2:E:620:CYS:HB3	2.23	0.73
1:H:12:LYS:NZ	6:H:302:HOH:O	2.16	0.72
3:L:1:GLU:O	3:L:1:GLU:HG3	1.87	0.72
2:E:553:THR:HG21	2:E:601:PRO:HD3	1.71	0.71
1:H:66:ARG:HG3	1:H:66:ARG:NH1	2.04	0.71
1:H:178:LEU:HD23	1:H:178:LEU:C	2.14	0.71
3:L:38:GLN:HB2	3:L:48:LEU:HD11	1.72	0.71
2:E:546:THR:HG21	2:E:634:GLY:HA3	1.71	0.71
2:E:608:LEU:CD2	2:E:614:ARG:HD2	2.19	0.70
2:E:424:ARG:HD2	2:E:526:THR:O	1.91	0.70
3:L:123:ASP:O	3:L:127:LYS:HE2	1.92	0.70
1:H:36:TRP:CE2	1:H:80:MET:HB2	2.26	0.69
1:H:53:ILE:HG22	1:H:54:PHE:CD1	2.27	0.69
2:E:441:LEU:HD23	2:E:441:LEU:O	1.92	0.68
2:E:553:THR:HG21	2:E:618:TYR:OH	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:630:ARG:HD2	2:E:639:ARG:HE	1.57	0.68
2:E:546:THR:HG21	2:E:634:GLY:HA2	1.74	0.68
1:H:63:PHE:HB3	1:H:67:VAL:HG21	1.76	0.67
2:E:627:HIS:HD2	6:E:813:HOH:O	1.73	0.67
1:H:2:VAL:CG2	1:H:29:PHE:HD2	2.07	0.67
1:H:95:PRO:HA	1:H:101:ASP:OD1	1.95	0.67
1:H:33:ALA:HB2	1:H:52:ILE:HD13	1.75	0.66
2:E:495:ASP:CG	2:E:496:VAL:H	2.03	0.66
3:L:184:LYS:O	3:L:188:GLU:HG2	1.95	0.66
2:E:625:THR:O	2:E:643:ALA:HA	1.94	0.66
1:H:34:ILE:CD1	1:H:94:ARG:CZ	2.73	0.66
2:E:509:PHE:N	2:E:551:GLY:O	2.28	0.66
1:H:142:VAL:HB	1:H:178:LEU:CD2	2.25	0.65
1:H:72:ASP:HB2	1:H:77:THR:OG1	1.97	0.65
2:E:553:THR:CG2	2:E:601:PRO:HD3	2.26	0.65
1:H:143:LYS:HE2	6:L:346:HOH:O	1.96	0.65
1:H:2:VAL:HG12	1:H:26:GLY:HA3	1.78	0.65
2:E:630:ARG:HG2	2:E:639:ARG:HG2	1.79	0.65
1:H:63:PHE:HB3	1:H:67:VAL:HG23	1.77	0.64
1:H:6:GLN:N	6:H:301:HOH:O	2.25	0.64
2:E:631:MET:HE3	2:E:633:VAL:HG21	1.80	0.64
1:H:6:GLN:O	6:H:301:HOH:O	2.15	0.64
1:H:2:VAL:CG1	1:H:26:GLY:HA3	2.28	0.64
2:E:447:VAL:HG11	2:E:622:VAL:HG21	1.80	0.63
2:E:521:LYS:NZ	2:E:538:MET:HE1	2.14	0.63
2:E:452:CYS:SG	2:E:620:CYS:CA	2.85	0.62
3:L:121:PRO:HD3	3:L:133:VAL:HG22	1.81	0.62
2:E:511:PRO:HB2	2:E:638:HIS:CE1	2.34	0.62
3:L:125:GLN:NE2	6:L:306:HOH:O	2.32	0.62
2:E:539:LEU:HD23	2:E:564:CYS:SG	2.40	0.62
2:E:504:GLY:O	6:E:801:HOH:O	2.15	0.62
3:L:143[A]:ARG:HG3	3:L:174:TYR:CG	2.35	0.61
3:L:143[A]:ARG:HG3	3:L:174:TYR:CD2	2.36	0.61
2:E:611:TYR:HB2	2:E:612:PRO:CD	2.29	0.61
3:L:187:TYR:CZ	3:L:212:ARG:HG3	2.35	0.61
1:H:39:GLN:O	1:H:88:ALA:HB1	2.01	0.61
3:L:34:LEU:HD13	3:L:72:PHE:CD1	2.36	0.61
3:L:30:SER:HB3	3:L:33:TYR:CD2	2.36	0.60
2:E:447:VAL:HG11	2:E:622:VAL:CG2	2.31	0.60
2:E:630:ARG:HD2	2:E:639:ARG:NE	2.17	0.59
1:H:40:ALA:HA	1:H:88:ALA:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:211:ASN:HB2	3:L:214:GLU:HG3	1.85	0.58
1:H:96:GLU:HB2	1:H:101:ASP:OD2	2.04	0.58
1:H:59:TYR:HE1	1:H:69:ILE:HD12	1.69	0.57
2:E:509:PHE:CZ	2:E:601:PRO:HB3	2.39	0.57
3:L:34:LEU:CD1	3:L:72:PHE:CG	2.86	0.57
1:H:2:VAL:CG2	1:H:29:PHE:CD2	2.87	0.57
2:E:436:GLY:O	2:E:439:THR:HG23	2.04	0.57
2:E:630:ARG:CZ	2:E:630:ARG:HB3	2.35	0.56
2:E:604:THR:HG23	2:E:605:PRO:HD2	1.88	0.56
1:H:193:THR:HG23	1:H:210:LYS:HE3	1.87	0.55
2:E:631:MET:HE3	2:E:633:VAL:CG2	2.36	0.55
3:L:192:VAL:HG22	3:L:211:ASN:ND2	2.20	0.55
1:H:2:VAL:HG21	1:H:29:PHE:CD2	2.32	0.55
3:L:34:LEU:HD13	3:L:72:PHE:CD2	2.41	0.55
1:H:83:ARG:C	1:H:111:VAL:HG11	2.32	0.54
2:E:494:CYS:HB3	2:E:539:LEU:HB3	1.90	0.54
3:L:81:PRO:N	3:L:81:PRO:C	2.61	0.54
2:E:604:THR:HG22	2:E:606:ARG:H	1.73	0.54
3:L:34:LEU:CD1	3:L:72:PHE:CD2	2.91	0.54
2:E:610:ASP:OD1	2:E:614:ARG:NE	2.35	0.54
1:H:142:VAL:HB	1:H:178:LEU:HD22	1.89	0.53
2:E:563:THR:HB	2:E:599:SER:O	2.09	0.53
3:L:127:LYS:N	3:L:127:LYS:HD3	2.23	0.53
1:H:40:ALA:HA	1:H:88:ALA:CB	2.40	0.52
2:E:495:ASP:CG	2:E:496:VAL:N	2.67	0.52
1:H:39:GLN:C	1:H:88:ALA:HB1	2.34	0.52
1:H:3:GLN:O	1:H:25:SER:HB2	2.10	0.52
1:H:34:ILE:HD12	1:H:78:ALA:HB2	1.92	0.52
1:H:13:LYS:CD	1:H:113:SER:HA	2.40	0.51
2:E:507:TYR:OH	2:E:612:PRO:HG2	2.10	0.51
1:H:13:LYS:HD3	1:H:112:SER:O	2.11	0.51
2:E:520:ASP:O	2:E:538:MET:HE2	2.11	0.51
2:E:608:LEU:HD21	2:E:614:ARG:HD2	1.92	0.51
2:E:521:LYS:HZ2	2:E:538:MET:HE1	1.75	0.50
3:L:125:GLN:O	3:L:128:SER:OG	2.27	0.50
2:E:611:TYR:HB2	2:E:612:PRO:HD2	1.94	0.49
2:E:495:ASP:OD1	2:E:496:VAL:N	2.45	0.49
1:H:123:PRO:HD3	1:H:209:LYS:HE2	1.94	0.49
2:E:436:GLY:HA2	6:E:808:HOH:O	2.12	0.49
1:H:66:ARG:HH11	1:H:66:ARG:CG	2.20	0.49
2:E:610:ASP:HA	2:E:614:ARG:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:521:LYS:O	2:E:521:LYS:NZ	2.36	0.49
2:E:604:THR:CG2	2:E:605:PRO:HD2	2.42	0.49
1:H:36:TRP:HB3	1:H:48:MET:CE	2.43	0.48
1:H:34:ILE:HD11	1:H:94:ARG:NH1	2.28	0.48
1:H:59:TYR:CE1	1:H:69:ILE:HD12	2.46	0.48
3:L:21:LEU:HB3	6:L:345:HOH:O	2.12	0.48
2:E:496:VAL:HG23	2:E:536:VAL:HB	1.94	0.48
2:E:509:PHE:CE2	2:E:601:PRO:HB3	2.48	0.48
1:H:3:GLN:O	1:H:25:SER:CB	2.62	0.47
3:L:13:LEU:CD1	3:L:19:ALA:HB2	2.44	0.47
1:H:66:ARG:O	1:H:82:LEU:HD12	2.15	0.47
3:L:98:THR:HG22	6:L:367:HOH:O	2.14	0.47
3:L:137:LEU:CD2	3:L:197:VAL:HG21	2.45	0.47
1:H:101:ASP:OD1	1:H:101:ASP:N	2.43	0.47
3:L:126:LEU:O	3:L:184:LYS:HD2	2.15	0.47
3:L:184:LYS:O	3:L:188:GLU:CG	2.62	0.46
1:H:34:ILE:CD1	1:H:94:ARG:NE	2.78	0.46
2:E:439:THR:O	2:E:442:PHE:N	2.36	0.46
1:H:119:PRO:HB3	1:H:145:TYR:HB3	1.98	0.46
2:E:436:GLY:C	6:E:808:HOH:O	2.58	0.46
3:L:98:THR:CG2	6:L:367:HOH:O	2.63	0.46
1:H:13:LYS:CE	6:H:332:HOH:O	2.63	0.46
3:L:195:CYS:O	3:L:207:THR:HA	2.15	0.46
1:H:46:GLU:OE2	1:H:62:LYS:NZ	2.48	0.46
1:H:152:VAL:HG12	1:H:198:VAL:HG22	1.98	0.46
1:H:22:CYS:O	1:H:78:ALA:N	2.40	0.45
1:H:36:TRP:CD2	1:H:80:MET:HB2	2.50	0.45
2:E:440:SER:OG	2:E:616:TRP:CD1	2.67	0.45
3:L:150:LYS:HA	3:L:154:ALA:O	2.17	0.45
3:L:143[A]:ARG:HG3	3:L:174:TYR:CD1	2.52	0.45
3:L:104[B]:ARG:NH2	6:L:314:HOH:O	2.49	0.45
2:E:436:GLY:CA	6:E:808:HOH:O	2.65	0.44
2:E:636:ILE:H	2:E:636:ILE:HD12	1.83	0.44
1:H:53:ILE:HG22	1:H:54:PHE:HD1	1.79	0.44
3:L:94:SER:O	3:L:95:SER:C	2.59	0.44
2:E:496:VAL:CG2	2:E:536:VAL:HB	2.48	0.44
1:H:105:GLN:NE2	6:H:301:HOH:O	1.92	0.44
2:E:608:LEU:HD21	2:E:614:ARG:CD	2.48	0.44
2:E:521:LYS:HZ3	2:E:538:MET:HE1	1.81	0.44
1:H:152:VAL:HA	1:H:197:ASN:O	2.18	0.43
1:H:34:ILE:HD13	1:H:94:ARG:NE	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:29:PHE:HE1	1:H:94:ARG:HB3	1.84	0.43
3:L:19:ALA:HB2	3:L:79:LEU:HD11	2.01	0.43
3:L:91:GLN:NE2	3:L:94:SER:OG	2.51	0.43
2:E:553:THR:CG2	2:E:618:TYR:OH	2.64	0.43
3:L:137:LEU:HD21	3:L:197:VAL:HG21	2.01	0.43
2:E:608:LEU:HD22	2:E:614:ARG:HD2	1.99	0.43
2:E:636:ILE:HD12	2:E:636:ILE:N	2.33	0.43
2:E:492:ARG:HG3	2:E:493:PRO:HD2	2.01	0.42
1:H:13:LYS:HD2	1:H:113:SER:HA	2.01	0.42
3:L:172:SER:OG	6:L:303:HOH:O	2.22	0.42
2:E:608:LEU:CD2	2:E:614:ARG:CD	2.96	0.42
1:H:142:VAL:HB	1:H:178:LEU:HD23	2.00	0.41
2:E:503:CYS:O	2:E:555:MET:HB3	2.20	0.41
3:L:142:PRO:N	3:L:142:PRO:C	2.67	0.41
2:E:495:ASP:O	2:E:539:LEU:HB2	2.20	0.41
2:E:624:PHE:HB3	2:E:643:ALA:HB1	2.02	0.41
2:E:492:ARG:CG	2:E:493:PRO:HD2	2.51	0.41
2:E:497:VAL:CG2	2:E:537:PHE:HB2	2.51	0.41
2:E:438:ILE:O	2:E:438:ILE:HG22	2.19	0.41
2:E:452:CYS:SG	2:E:620:CYS:HA	2.60	0.41
1:H:13:LYS:O	1:H:16:SER:OG	2.38	0.41
2:E:497:VAL:HG22	2:E:537:PHE:HB2	2.03	0.41
2:E:602:TRP:CZ2	2:E:608:LEU:HD12	2.56	0.41
3:L:187:TYR:OH	3:L:212:ARG:HG3	2.21	0.41
3:L:122:SER:OG	3:L:124:GLU:HG2	2.22	0.40
3:L:143[A]:ARG:HG3	3:L:174:TYR:CE2	2.55	0.40
3:L:187:TYR:CE2	3:L:212:ARG:HG3	2.56	0.40
2:E:511:PRO:HB2	2:E:638:HIS:ND1	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	226/232 (97%)	219 (97%)	6 (3%)	1 (0%)	30	22
2	E	160/189 (85%)	151 (94%)	8 (5%)	1 (1%)	21	13
3	L	216/233 (93%)	213 (99%)	3 (1%)	0	100	100
All	All	602/654 (92%)	583 (97%)	17 (3%)	2 (0%)	36	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	511	PRO
1	H	149	PRO

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	190/193 (98%)	185 (97%)	5 (3%)	40	37
2	E	140/159 (88%)	137 (98%)	3 (2%)	47	46
3	L	189/203 (93%)	189 (100%)	0	100	100
All	All	519/555 (94%)	511 (98%)	8 (2%)	55	58

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	35	SER
1	H	38	ARG
1	H	66	ARG
1	H	115	SER
1	H	178	LEU
2	E	443	TYR
2	E	511	PRO
2	E	622	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	58	ASN
1	H	102	ASN
2	E	428	ASN
2	E	434	GLN
2	E	532	ASN
2	E	638	HIS
3	L	91	GLN
3	L	148	GLN
3	L	211	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	A	1	2,4	14,14,15	0.17	0	17,19,21	0.70	1 (5%)
4	NAG	A	2	4	14,14,15	0.28	0	17,19,21	0.51	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	2,4	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	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	A	1	NAG	C1-O5-C5	2.39	115.43	112.19

There are no chirality outliers.

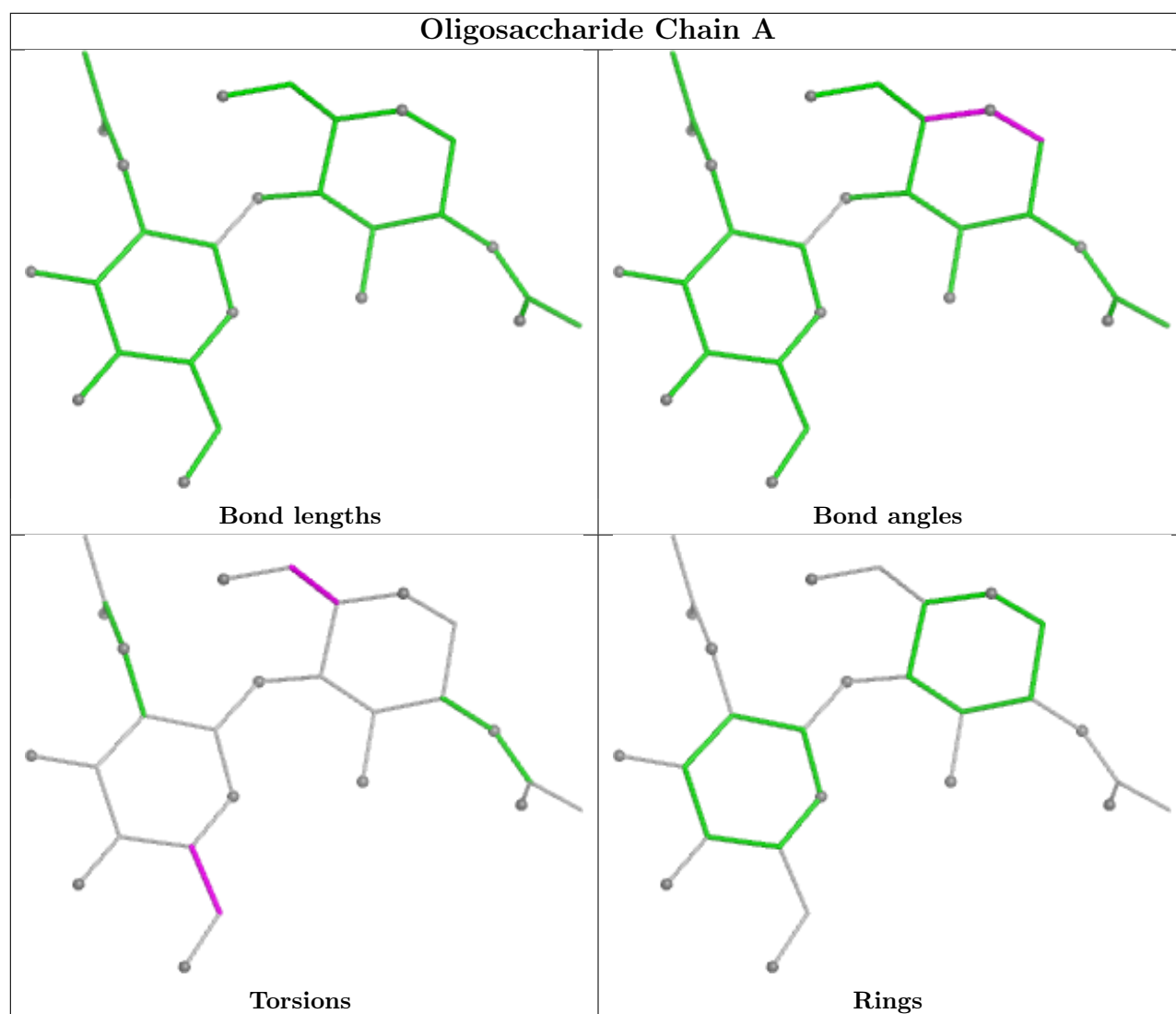
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2	NAG	O5-C5-C6-O6
4	A	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](#)

3 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	NAG	E	702	2	14,14,15	0.17	0	17,19,21	0.35	0
5	NAG	E	701	2	14,14,15	0.25	0	17,19,21	0.59	0
5	NAG	E	703	2	14,14,15	0.24	0	17,19,21	0.37	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	NAG	E	702	2	-	3/6/23/26	0/1/1/1
5	NAG	E	701	2	-	2/6/23/26	0/1/1/1
5	NAG	E	703	2	-	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.

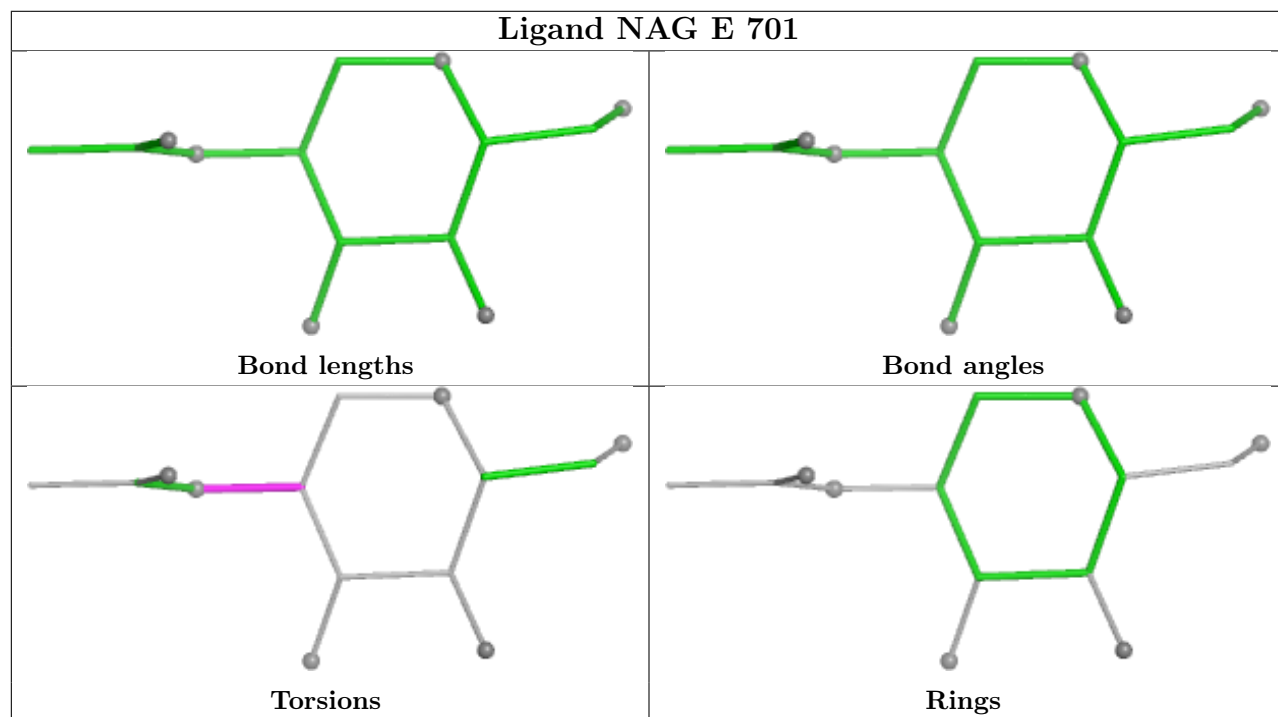
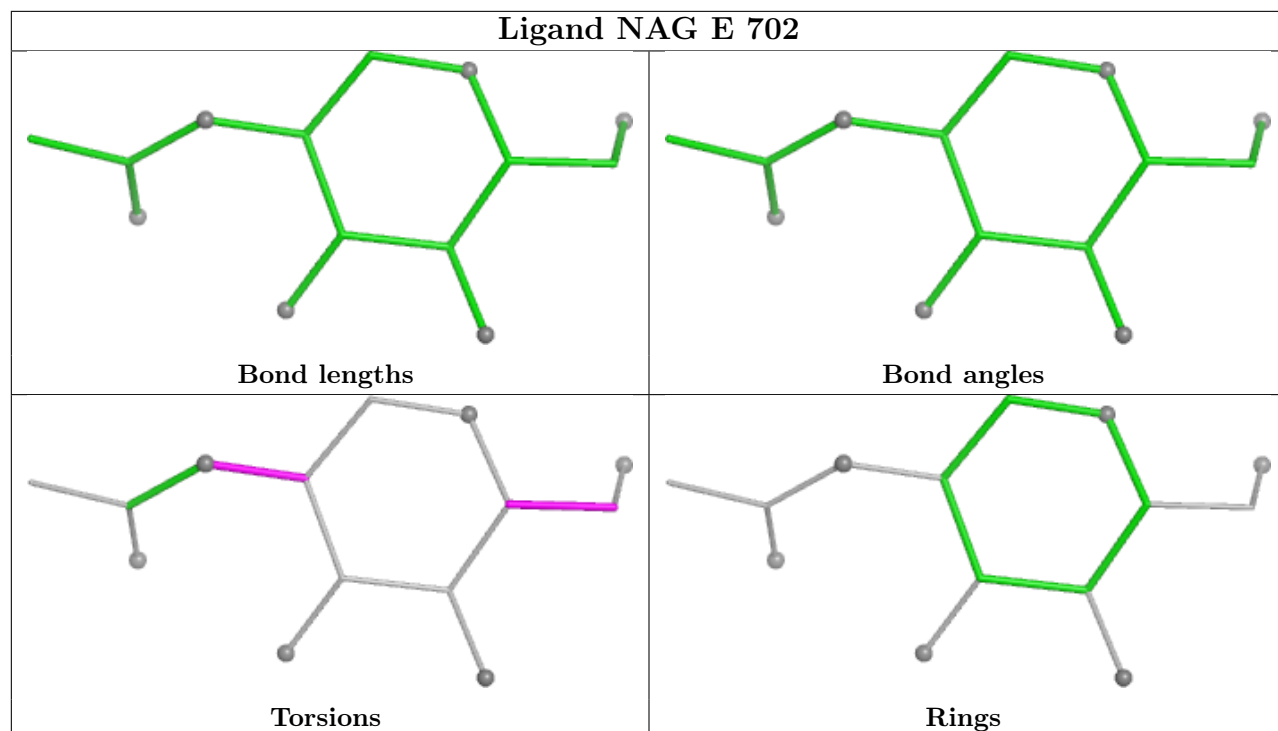
All (5) torsion outliers are listed below:

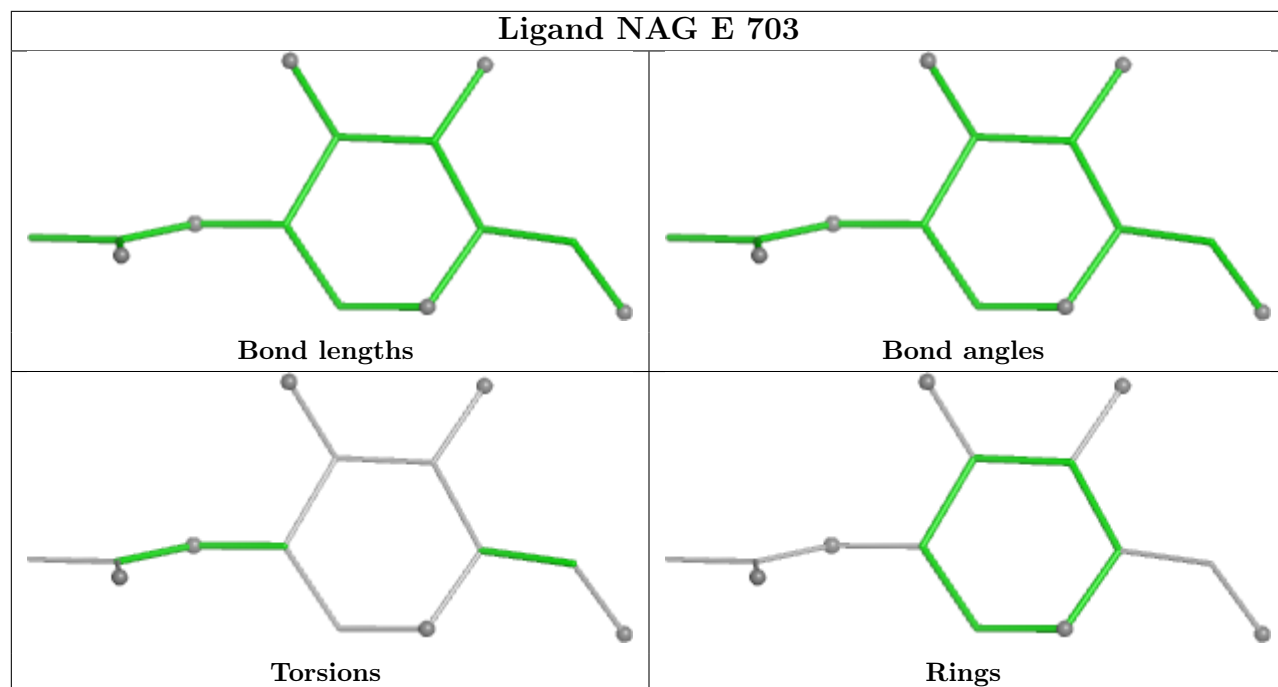
Mol	Chain	Res	Type	Atoms
5	E	702	NAG	O5-C5-C6-O6
5	E	702	NAG	C4-C5-C6-O6
5	E	701	NAG	C3-C2-N2-C7
5	E	701	NAG	C1-C2-N2-C7
5	E	702	NAG	C1-C2-N2-C7

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 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	228/232 (98%)	1.07	37 (16%) 4 4	40, 61, 107, 129	0
2	E	164/189 (86%)	1.78	56 (34%) 1 0	62, 85, 110, 129	0
3	L	214/233 (91%)	0.71	14 (6%) 25 24	24, 53, 72, 102	4 (1%)
All	All	606/654 (92%)	1.13	107 (17%) 4 3	24, 63, 104, 129	4 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	585	PRO	4.9
1	H	54	PHE	4.6
1	H	131	THR	4.5
2	E	600	GLY	4.4
2	E	510	THR	4.3
2	E	491	PRO	4.2
2	E	447	VAL	4.1
1	H	26	GLY	4.1
1	H	2	VAL	4.1
2	E	511	PRO	4.1
2	E	566	ALA	4.0
2	E	542	LEU	4.0
3	L	34	LEU	4.0
3	L	51	GLY	4.0
1	H	29	PHE	3.9
1	H	65	GLY	3.9
2	E	452	CYS	3.6
2	E	514	VAL	3.5
1	H	133	GLY	3.4
2	E	548	GLY	3.4
2	E	522	LEU	3.4
2	E	443	TYR	3.4
3	L	81	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
2	E	589	THR	3.3
2	E	497	VAL	3.3
2	E	512	SER	3.2
2	E	620	CYS	3.2
1	H	169	VAL	3.2
2	E	496	VAL	3.1
2	E	422	ILE	3.1
2	E	441	LEU	3.1
2	E	549	TRP	3.1
2	E	588	PRO	3.0
1	H	50	GLY	3.0
1	H	27	GLY	3.0
3	L	93	GLY	2.9
1	H	78	ALA	2.9
1	H	53	ILE	2.9
2	E	442	PHE	2.9
1	H	18	VAL	2.8
1	H	67	VAL	2.8
3	L	24[A]	ARG	2.8
2	E	421	HIS	2.8
3	L	46	ARG	2.8
2	E	603	ILE	2.8
2	E	607	CYS	2.7
1	H	128	SER	2.7
2	E	608	LEU	2.7
1	H	63	PHE	2.7
2	E	539	LEU	2.7
2	E	493	PRO	2.7
1	H	132	SER	2.7
2	E	599	SER	2.6
1	H	152	VAL	2.6
2	E	492	ARG	2.6
1	H	17	SER	2.6
3	L	215	CYS	2.6
3	L	21	LEU	2.6
2	E	553	THR	2.6
2	E	516	VAL	2.5
1	H	186	SER	2.5
3	L	127	LYS	2.5
1	H	22	CYS	2.5
3	L	33	TYR	2.5
1	H	88	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	506	VAL	2.4
2	E	507	TYR	2.4
1	H	100(C)	GLY	2.4
1	H	24	ALA	2.3
2	E	586	GLY	2.3
1	H	100(E)	PHE	2.3
1	H	127	SER	2.3
2	E	636	ILE	2.3
1	H	57	ALA	2.3
1	H	68	THR	2.3
2	E	615	LEU	2.3
1	H	150	VAL	2.2
2	E	546	THR	2.2
2	E	609	VAL	2.2
2	E	427	LEU	2.2
2	E	529	TRP	2.2
2	E	632	PHE	2.2
3	L	192	VAL	2.2
2	E	591	GLY	2.2
2	E	444	ALA	2.2
2	E	616	TRP	2.2
1	H	130	SER	2.2
2	E	633	VAL	2.1
1	H	64	GLN	2.1
2	E	517	GLY	2.1
2	E	547	GLY	2.1
3	L	31	SER	2.1
1	H	28	THR	2.1
1	H	5	VAL	2.1
2	E	587	GLY	2.1
2	E	544	PRO	2.1
1	H	100(F)	CYS	2.1
3	L	124	GLU	2.1
1	H	61	GLN	2.1
2	E	543	ARG	2.1
2	E	451	GLY	2.1
2	E	635	GLY	2.1
1	H	161	SER	2.1
2	E	645	ASN	2.0
2	E	605	PRO	2.0
1	H	59	TYR	2.0
3	L	52	ALA	2.0

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

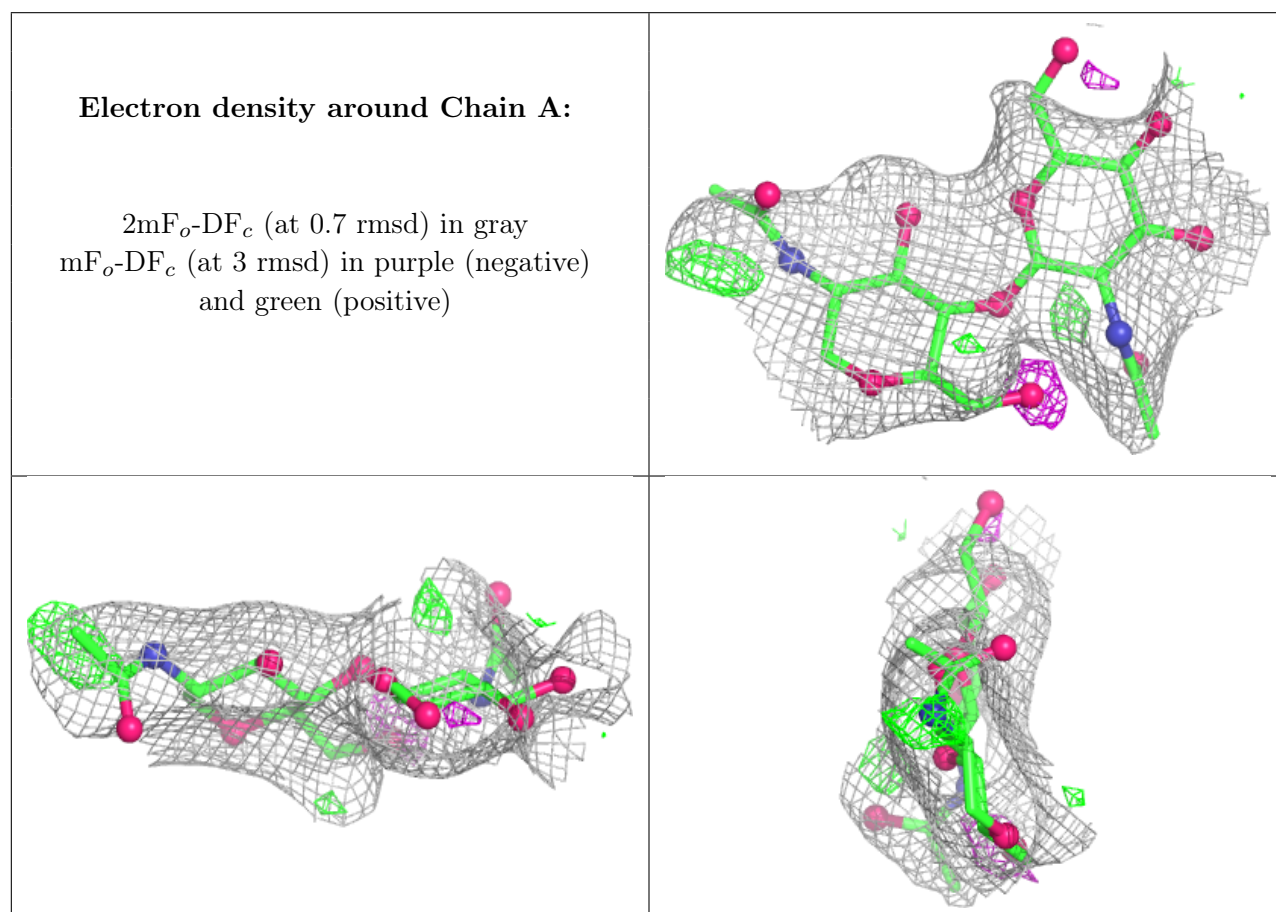
There are no non-standard protein/DNA/RNA residues in this entry.

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	A	1	14/15	-	-	79,87,107,107	0
4	NAG	A	2	14/15	-	-	93,104,109,115	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.

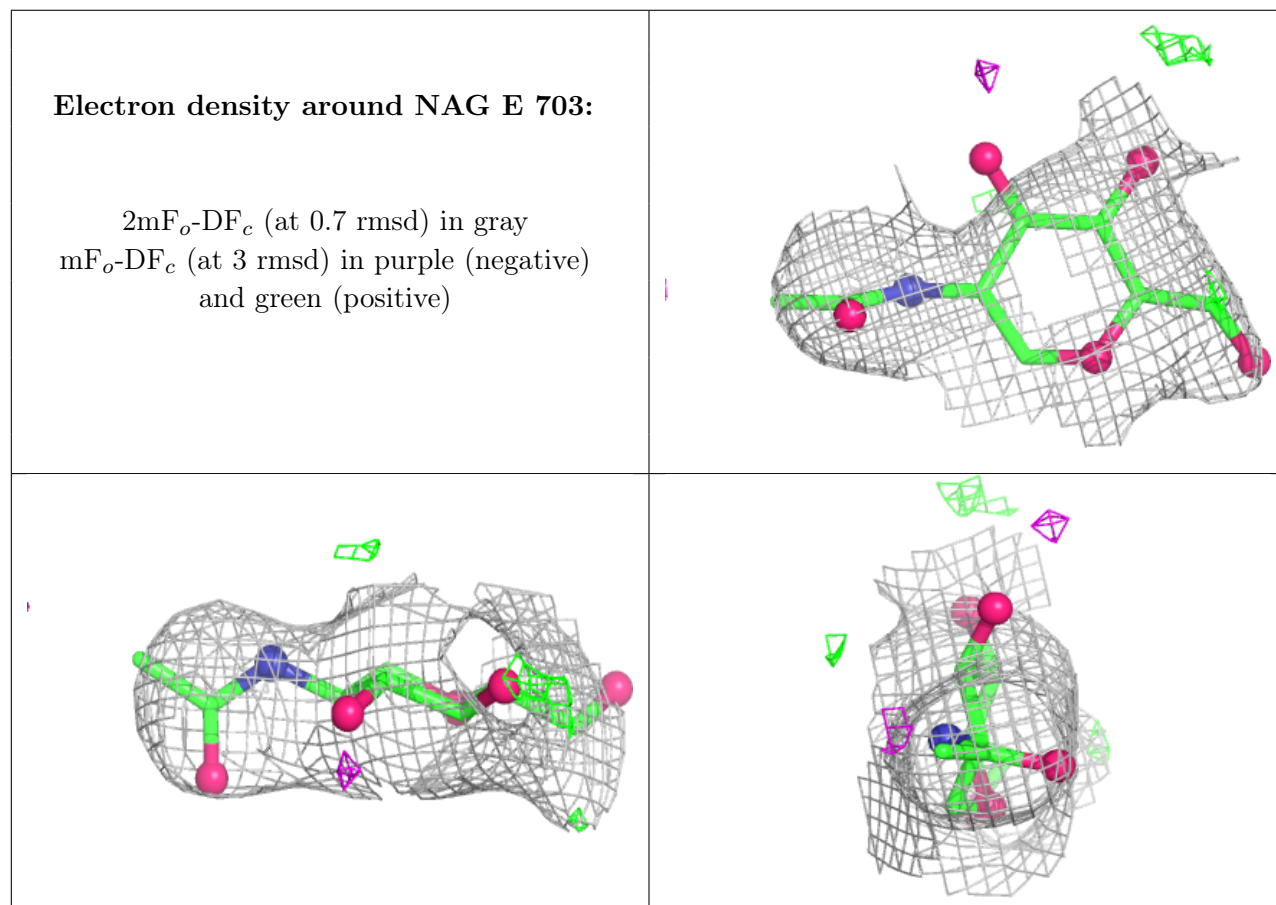


6.4 Ligands ⓘ

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, 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.

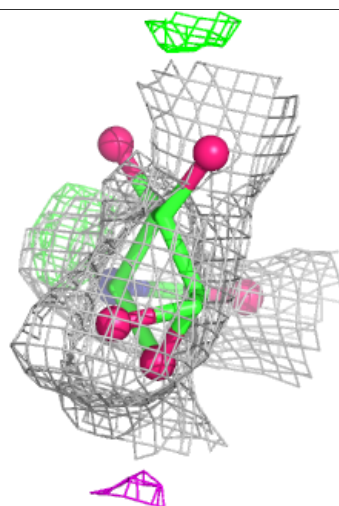
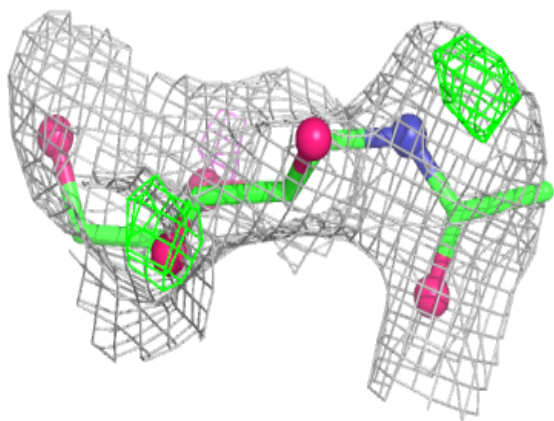
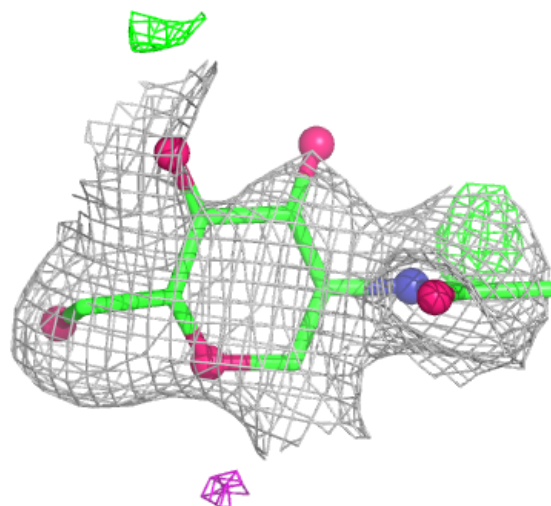
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	E	703	14/15	0.57	0.16	100,111,117,120	0
5	NAG	E	701	14/15	0.71	0.19	92,99,101,107	0
5	NAG	E	702	14/15	0.77	0.15	86,95,101,103	0

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.



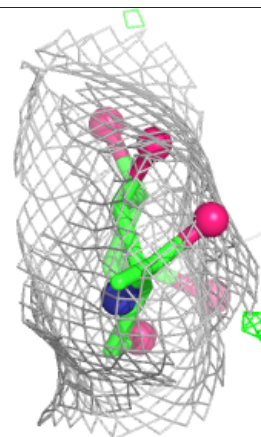
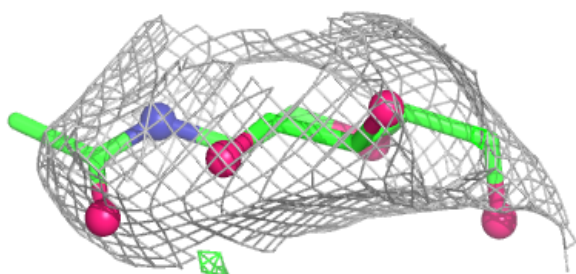
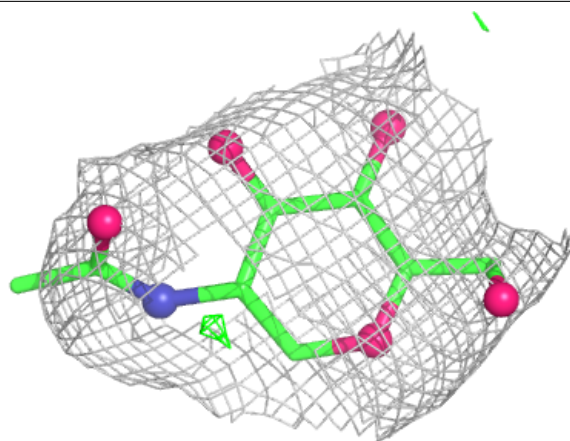
Electron density around NAG E 701:

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



Electron density around NAG 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.