



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:08 AM UTC

PDB ID : 6ICX / pdb_00006icx
Title : Crystal structure of H7 hemagglutinin mutant AH-AGPL (V186G) from the influenza virus A/Anhui/1/2013 (H7N9)
Authors : Gao, G.F.; Xu, Y.; Qi, J.X.
Deposited on : 2018-09-07
Resolution : 2.40 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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

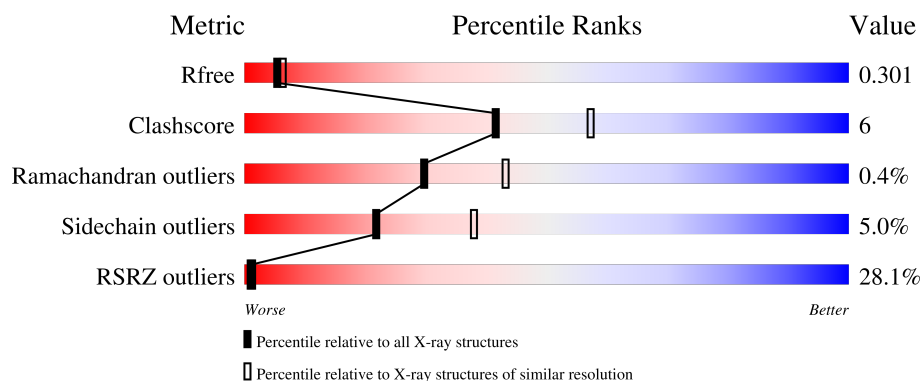
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	A	321	24% 81% 15% ..
2	B	177	32% 74% 17% 8%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3829 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	314	2384	1480	432	457	15	0	0	0

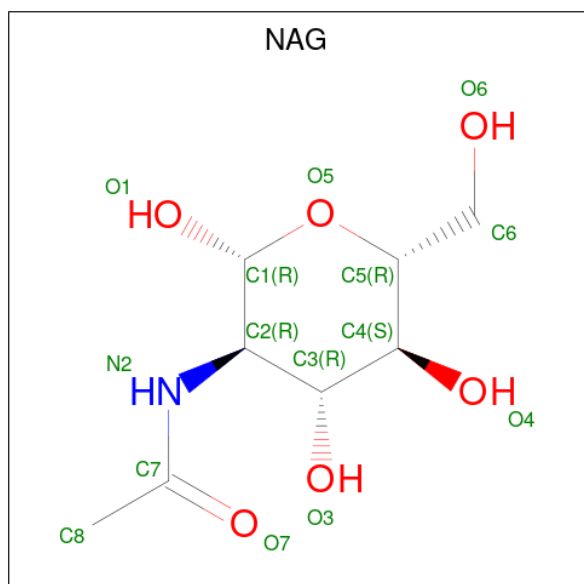
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	177	GLY	VAL	engineered mutation	UNP R4NN21

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	163	1328	817	231	273	7	0	0	0

- Molecule 3 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
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

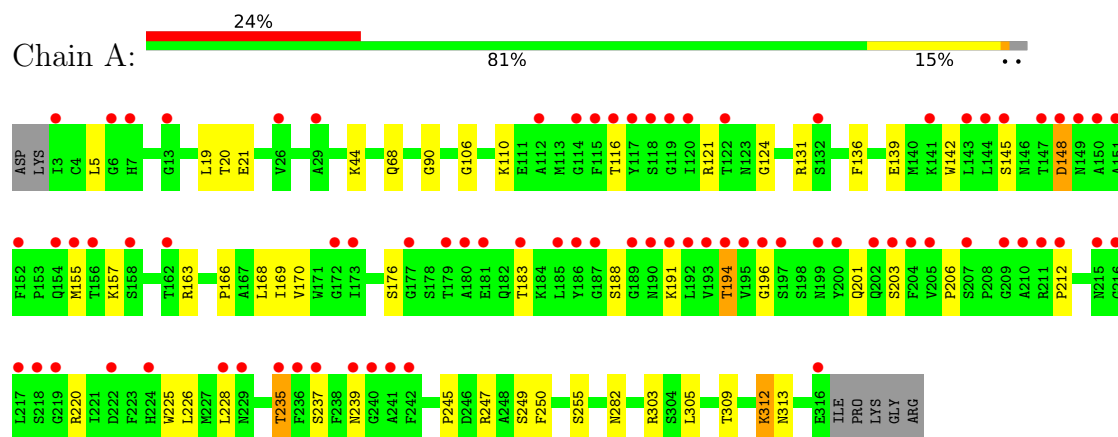
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total	O	0	0
			55	55		
4	B	20	Total	O	0	0
			20	20		

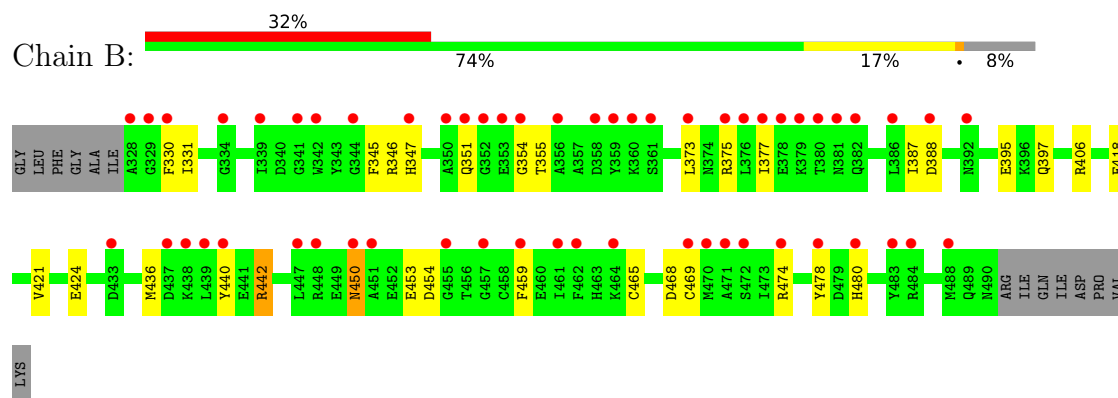
3 Residue-property plots [i](#)

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: Hemagglutinin HA1 chain



• Molecule 2: Hemagglutinin HA2 chain



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	115.32Å 115.32Å 293.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.10 – 2.40 32.10 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (32.10-2.40) 99.0 (32.10-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.266 , 0.300 0.267 , 0.301	Depositor DCC
R_{free} test set	1459 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	57.7	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for $-1/3^*h+1/3^*k+1/3^*l,-k,8/3^*h+4/3^*k+1/3^*l$ 0.023 for $-2/3^*h-1/3^*k-1/3^*l,-1/3^*h-2/3^*k+1/3^*l,-4/3^*h+4/3^*k+1/3^*l$ 0.015 for $-h,1/3^*h-1/3^*k-1/3^*l,-4/3^*h-8/3^*k+1/3^*l$	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3829	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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	A	0.12	0/2430	0.34	0/3286
2	B	0.10	0/1351	0.28	0/1821
All	All	0.11	0/3781	0.32	0/5107

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2384	0	2331	34	1
2	B	1328	0	1222	18	0
3	A	28	0	26	0	0
3	B	14	0	13	0	0
4	A	55	0	0	7	0
4	B	20	0	0	0	0
All	All	3829	0	3592	47	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 6.

All (47) 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:235:THR:O	4:A:701:HOH:O	2.02	0.77
2:B:345:PHE:O	2:B:355:THR:HA	1.94	0.67
1:A:20:THR:HG22	1:A:21:GLU:HG3	1.76	0.66
1:A:116:THR:O	1:A:157:LYS:NZ	2.31	0.64
2:B:375:ARG:NH2	2:B:424:GLU:OE2	2.31	0.64
1:A:121:ARG:NH1	1:A:145:SER:O	2.33	0.60
2:B:346:ARG:HA	2:B:354:GLY:O	2.02	0.59
1:A:5:LEU:HD11	2:B:440:TYR:HA	1.85	0.59
2:B:388:ASP:OD2	2:B:406:ARG:NH2	2.32	0.59
1:A:196:GLY:O	4:A:701:HOH:O	2.17	0.56
1:A:170:VAL:HG22	1:A:225:TRP:HB3	1.88	0.55
1:A:282:ASN:HB3	2:B:377:ILE:HG23	1.87	0.55
2:B:450:ASN:N	2:B:450:ASN:OD1	2.39	0.55
1:A:191:LYS:HB2	1:A:206:PRO:HG3	1.87	0.55
1:A:44:LYS:NZ	4:A:704:HOH:O	2.39	0.54
1:A:106:GLY:HA2	1:A:255:SER:HB3	1.91	0.52
1:A:139:GLU:OE1	1:A:247:ARG:HD3	2.12	0.49
1:A:196:GLY:N	4:A:701:HOH:O	2.24	0.49
1:A:312:LYS:HD3	1:A:313:ASN:N	2.28	0.49
1:A:169:ILE:O	1:A:225:TRP:HA	2.13	0.49
1:A:90:GLY:N	4:A:710:HOH:O	2.44	0.48
1:A:170:VAL:O	1:A:245:PRO:HB3	2.13	0.48
1:A:5:LEU:HD21	2:B:440:TYR:HD1	1.80	0.46
2:B:347:HIS:HD2	2:B:474:ARG:HH12	1.62	0.46
2:B:450:ASN:ND2	2:B:478:TYR:OH	2.48	0.46
1:A:212:PRO:O	1:A:220:ARG:NH2	2.35	0.46
1:A:131:ARG:NH1	1:A:136:PHE:O	2.43	0.46
1:A:194:THR:OG1	1:A:203:SER:HB3	2.16	0.46
2:B:442:ARG:HH11	2:B:442:ARG:HB3	1.81	0.45
2:B:395:GLU:OE2	2:B:397:GLN:HB3	2.16	0.45
1:A:305:LEU:HB3	2:B:421:VAL:HG21	1.98	0.45
1:A:191:LYS:HA	1:A:239:ASN:HD21	1.82	0.45
1:A:110:LYS:NZ	1:A:139:GLU:OE2	2.36	0.44
1:A:183:THR:HG22	1:A:188:SER:HA	1.99	0.44
1:A:169:ILE:HB	1:A:226:LEU:HD23	2.00	0.44
2:B:453:GLU:HG2	2:B:459:PHE:HE2	1.82	0.44
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.92	0.43
1:A:235:THR:N	4:A:701:HOH:O	2.38	0.43
2:B:351:GLN:HE21	2:B:351:GLN:HB3	1.62	0.43
1:A:309:THR:HG22	2:B:373:LEU:HD11	2.01	0.42
1:A:124:GLY:HA3	1:A:142:TRP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LEU:HB3	1:A:249:SER:HB2	2.01	0.41
1:A:237:SER:N	4:A:703:HOH:O	2.53	0.41
2:B:346:ARG:HH21	2:B:355:THR:HG21	1.84	0.41
2:B:347:HIS:NE2	2:B:354:GLY:HA3	2.36	0.41
1:A:163:ARG:HD3	1:A:250:PHE:CZ	2.55	0.41
1:A:166:PRO:HA	1:A:228:LEU:O	2.21	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:44:LYS:NZ	1:A:68:GLN:O[5_555]	2.18	0.02

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	312/321 (97%)	295 (95%)	15 (5%)	2 (1%)	21	32
2	B	161/177 (91%)	151 (94%)	10 (6%)	0	100	100
All	All	473/498 (95%)	446 (94%)	25 (5%)	2 (0%)	30	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ASP
1	A	201	GLN

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	260/268 (97%)	252 (97%)	8 (3%)	35	57
2	B	141/152 (93%)	129 (92%)	12 (8%)	10	16
All	All	401/420 (96%)	381 (95%)	20 (5%)	22	38

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

Mol	Chain	Res	Type
1	A	19	LEU
1	A	148	ASP
1	A	155	MET
1	A	176	SER
1	A	194	THR
1	A	235	THR
1	A	303	ARG
1	A	312	LYS
2	B	330	PHE
2	B	331	ILE
2	B	387	ILE
2	B	418	GLU
2	B	436	MET
2	B	442	ARG
2	B	450	ASN
2	B	454	ASP
2	B	465	CYS
2	B	468	ASP
2	B	469	CYS
2	B	480	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	351	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	NAG	A	601	1	14,14,15	0.29	0	17,19,21	0.47	0
3	NAG	A	602	1	14,14,15	0.41	0	17,19,21	0.50	0
3	NAG	B	501	2	14,14,15	0.29	0	17,19,21	0.44	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	A	601	1	-	1/6/23/26	0/1/1/1
3	NAG	A	602	1	-	2/6/23/26	0/1/1/1
3	NAG	B	501	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.

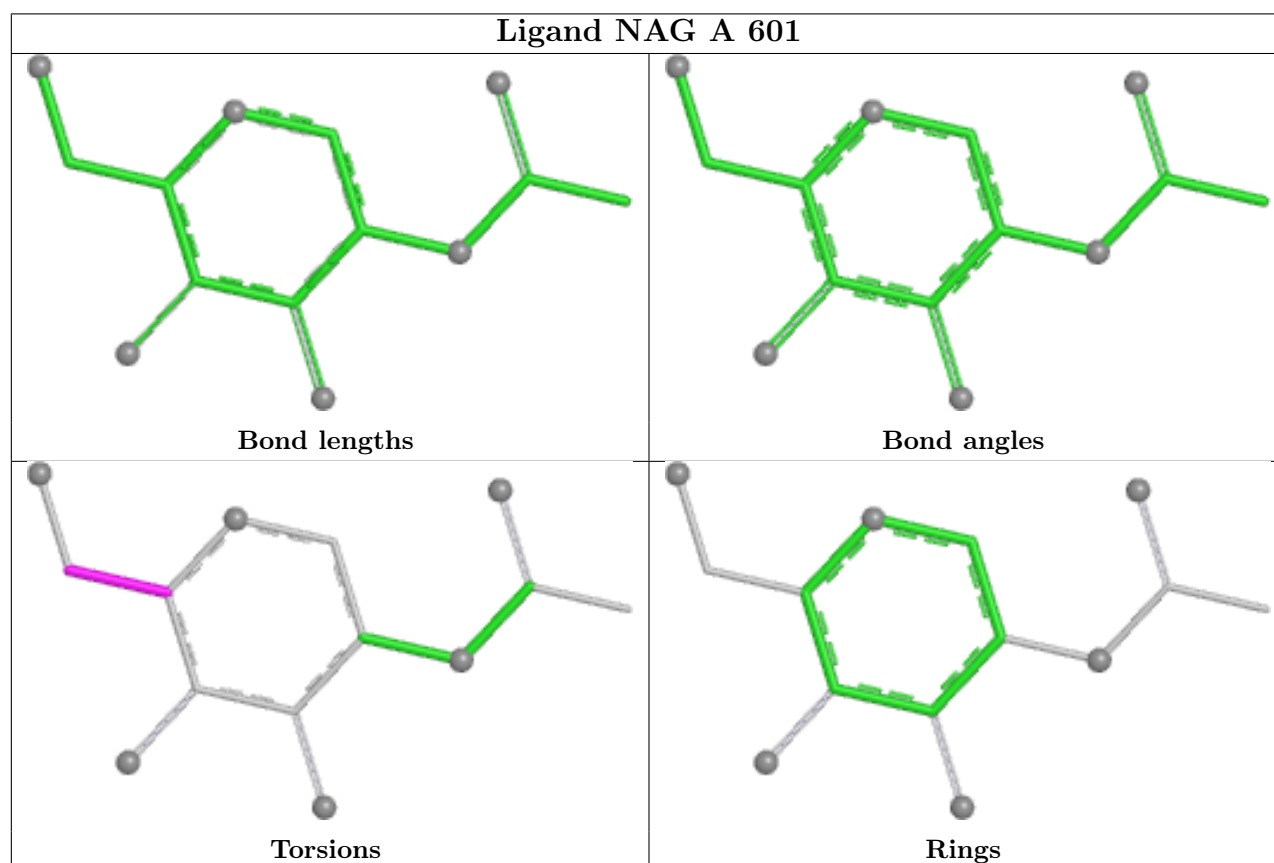
All (3) torsion outliers are listed below:

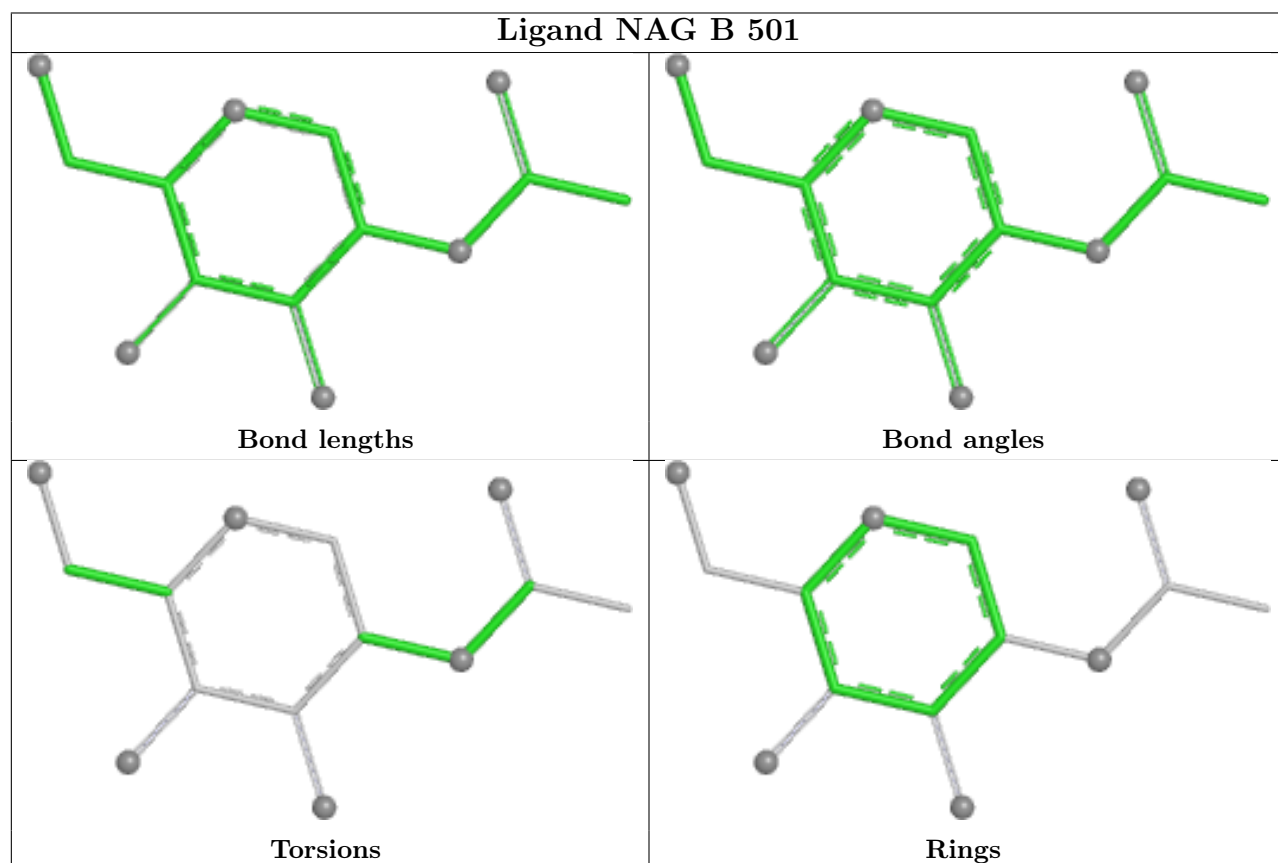
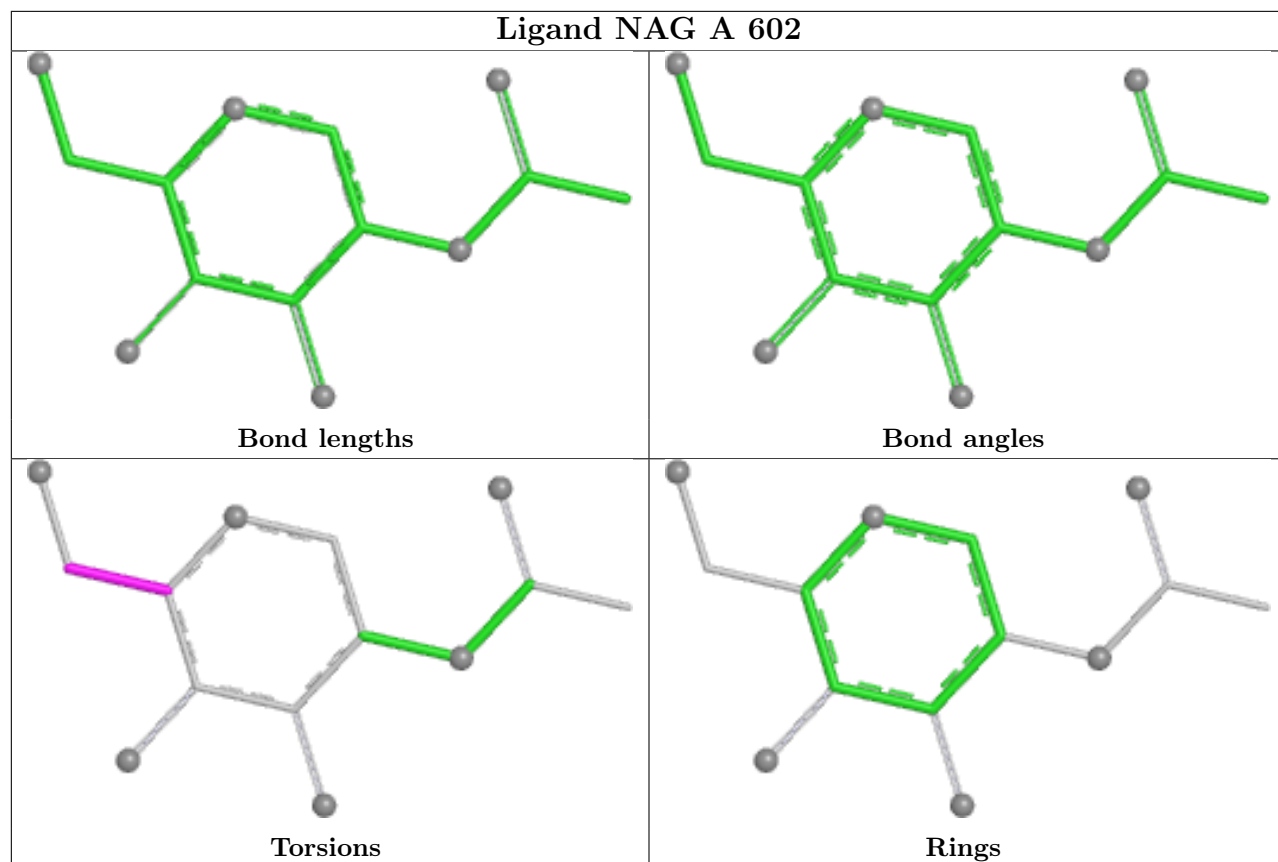
Mol	Chain	Res	Type	Atoms
3	A	601	NAG	O5-C5-C6-O6
3	A	602	NAG	C4-C5-C6-O6
3	A	602	NAG	O5-C5-C6-O6

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 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	A	314/321 (97%)	1.31	78 (24%) 2 1	40, 74, 127, 224	0
2	B	163/177 (92%)	1.68	56 (34%) 1 1	39, 105, 168, 202	0
All	All	477/498 (95%)	1.43	134 (28%) 1 1	39, 80, 154, 224	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	GLY	8.0
1	A	147	THR	7.5
2	B	483	TYR	5.9
1	A	212	PRO	5.7
2	B	461	ILE	5.5
1	A	172	GLY	5.5
1	A	186	TYR	5.4
1	A	158	SER	5.3
2	B	447	LEU	5.1
2	B	328	ALA	5.0
2	B	480	HIS	4.9
2	B	439	LEU	4.9
1	A	236	PHE	4.9
1	A	180	ALA	4.7
2	B	373	LEU	4.6
1	A	204	PHE	4.5
1	A	118	SER	4.5
1	A	156	THR	4.4
1	A	151	ALA	4.3
1	A	200	TYR	4.3
1	A	195	VAL	4.2
2	B	462	PHE	4.2
1	A	197	SER	4.2
1	A	203	SER	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	378	GLU	4.1
1	A	149	ASN	4.0
1	A	145	SER	4.0
2	B	375	ARG	3.9
2	B	380	THR	3.9
1	A	192	LEU	3.9
1	A	202	GLN	3.8
1	A	179	THR	3.8
1	A	193	VAL	3.7
1	A	199	ASN	3.7
2	B	451	ALA	3.7
1	A	148	ASP	3.7
1	A	3	ILE	3.7
1	A	189	GLY	3.7
1	A	183	THR	3.6
1	A	210	ALA	3.6
1	A	316	GLU	3.6
1	A	152	PHE	3.6
1	A	116	THR	3.6
2	B	330	PHE	3.6
2	B	358	ASP	3.6
2	B	360	LYS	3.6
1	A	162	THR	3.5
2	B	350	ALA	3.5
2	B	438	LYS	3.4
1	A	191	LYS	3.3
1	A	13	GLY	3.3
1	A	190	ASN	3.3
2	B	356	ALA	3.2
1	A	177	GLY	3.2
1	A	239	ASN	3.2
2	B	377	ILE	3.2
2	B	484	ARG	3.2
1	A	222	ASP	3.2
2	B	361	SER	3.1
2	B	472	SER	3.1
1	A	141	LYS	3.1
1	A	215	ASN	3.1
1	A	217	LEU	3.1
1	A	181	GLU	3.1
2	B	334	GLY	3.1
2	B	352	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	376	LEU	3.1
1	A	205	VAL	3.1
1	A	219	GLY	3.0
2	B	437	ASP	3.0
1	A	154	GLN	3.0
2	B	450	ASN	3.0
2	B	488	MET	3.0
1	A	211	ARG	3.0
1	A	196	GLY	2.9
2	B	329	GLY	2.9
2	B	344	GLY	2.9
2	B	469	CYS	2.9
1	A	185	LEU	2.8
1	A	242	PHE	2.8
2	B	353	GLU	2.8
2	B	464	LYS	2.8
1	A	207	SER	2.8
2	B	381	ASN	2.8
1	A	228	LEU	2.8
1	A	237	SER	2.7
2	B	455	GLY	2.7
1	A	119	GLY	2.7
1	A	120	ILE	2.7
1	A	235	THR	2.7
1	A	29	ALA	2.6
2	B	433	ASP	2.6
2	B	359	TYR	2.6
2	B	354	GLY	2.6
2	B	478	TYR	2.6
1	A	7	HIS	2.6
2	B	339	ILE	2.6
2	B	471	ALA	2.5
2	B	388	ASP	2.5
1	A	194	THR	2.5
2	B	470	MET	2.5
1	A	150	ALA	2.5
1	A	117	TYR	2.5
2	B	347	HIS	2.5
2	B	342	TRP	2.4
1	A	216	GLY	2.4
2	B	386	LEU	2.4
2	B	474	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	457	GLY	2.3
1	A	122	THR	2.3
1	A	144	LEU	2.3
1	A	240	GLY	2.3
1	A	241	ALA	2.3
1	A	209	GLY	2.3
1	A	218	SER	2.2
1	A	187	GLY	2.2
1	A	112	ALA	2.2
2	B	379	LYS	2.2
2	B	459	PHE	2.2
1	A	229	ASN	2.2
1	A	155	MET	2.2
1	A	224	HIS	2.2
1	A	115	PHE	2.2
1	A	143	LEU	2.1
2	B	392	ASN	2.1
2	B	341	GLY	2.1
1	A	132	SER	2.1
2	B	440	TYR	2.1
1	A	173	ILE	2.1
2	B	382	GLN	2.1
1	A	26	VAL	2.1
1	A	114	GLY	2.1
2	B	448	ARG	2.1
2	B	351	GLN	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](#)

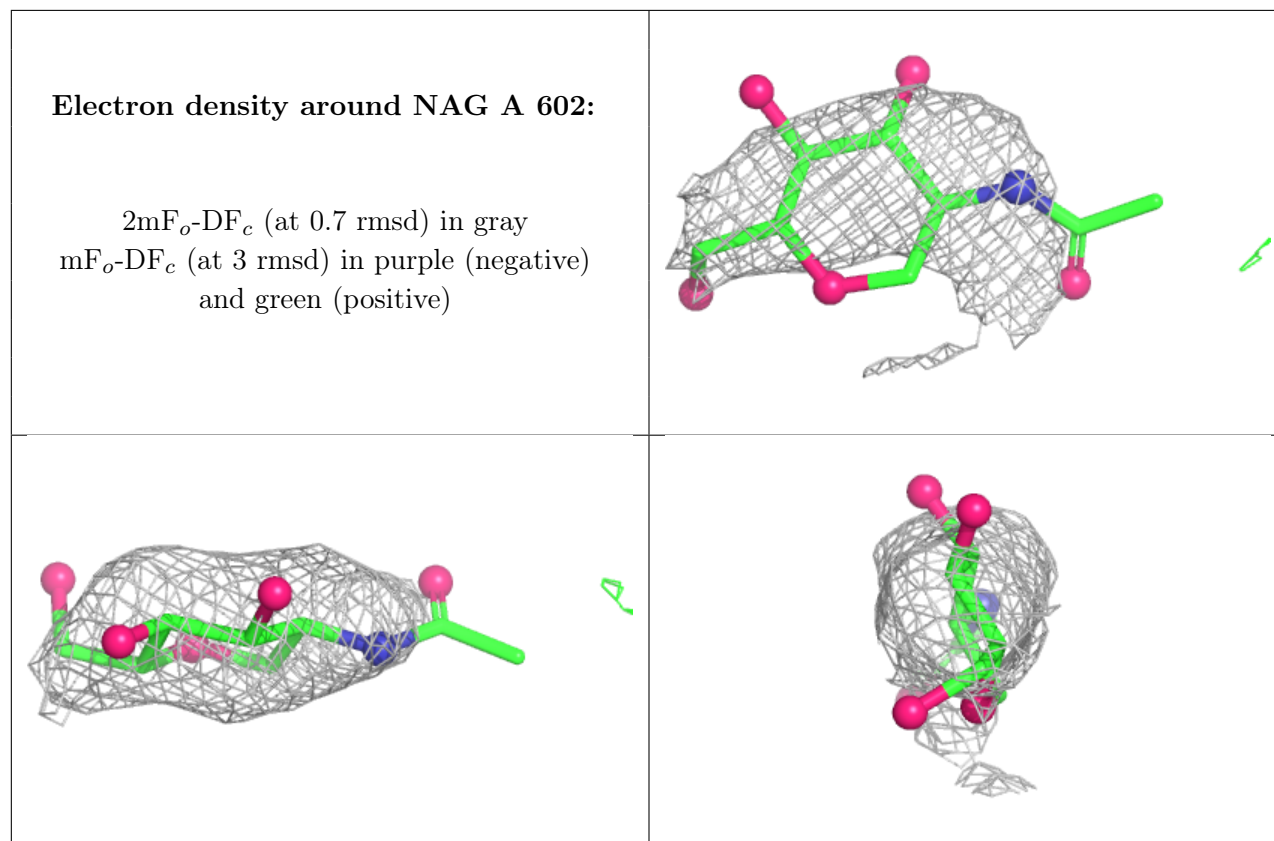
There are no oligosaccharides in this entry.

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.

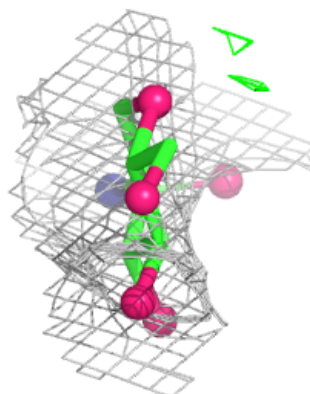
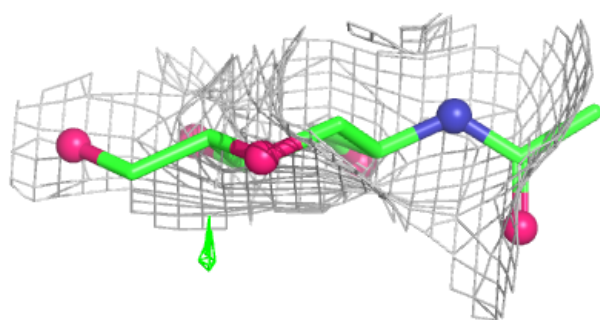
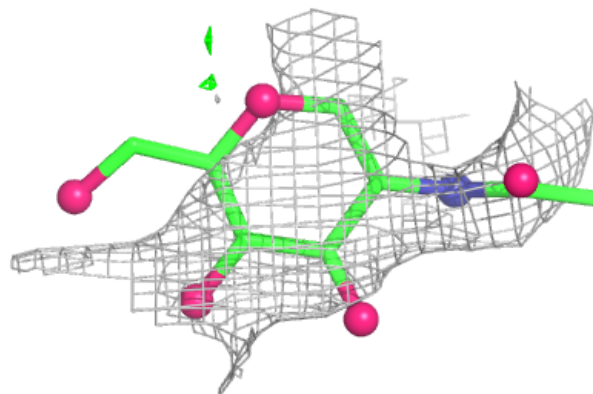
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	A	602	14/15	0.53	0.19	147,159,166,168	0
3	NAG	A	601	14/15	0.69	0.18	157,169,172,173	0
3	NAG	B	501	14/15	0.83	0.14	74,83,93,98	0

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.

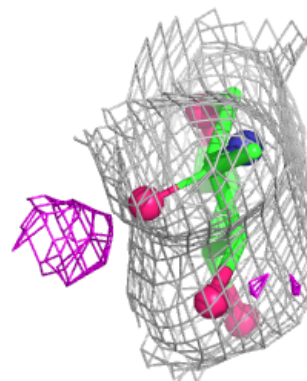
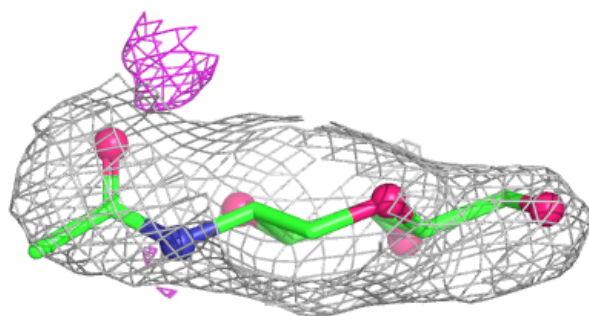
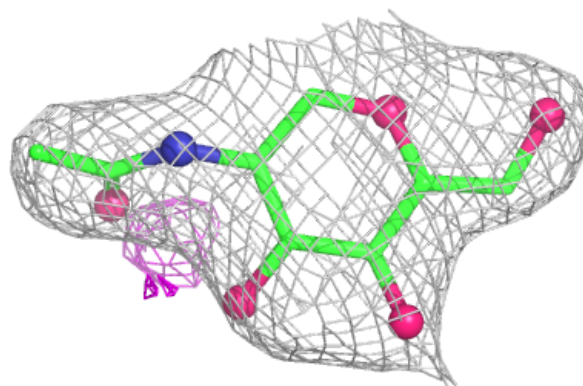


Electron density around NAG A 601:

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

**Electron density around NAG B 501:**

$2mF_o-DF_c$ (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.