



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 06:06 AM BST

PDB ID : 6ICX  
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](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.

---

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	:	2.13.1
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)	:	2.13.1

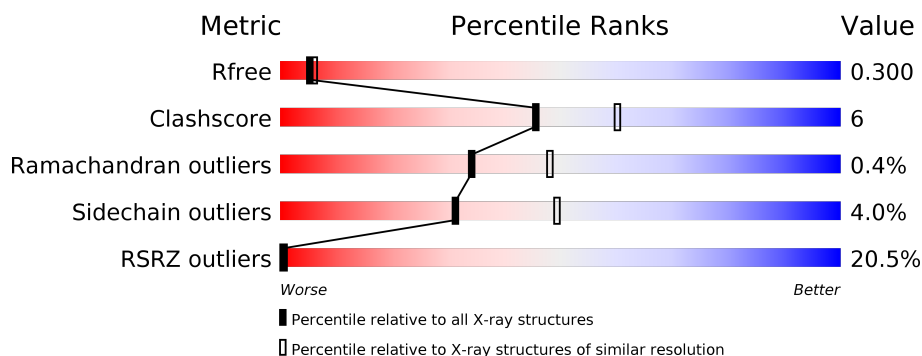
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	321	<div> <div>15%</div> <div>81%</div> <div>16%</div> <div>..</div> </div>
2	B	177	<div> <div>28%</div> <div>76%</div> <div>15%</div> <div>8%</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
3	NAG	A	601	-	-	-	X

## 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

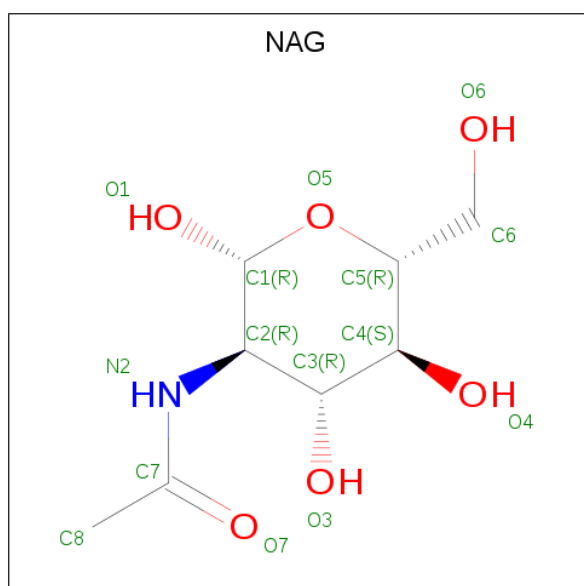
There is a discrepancy between the modelled and reference sequences:

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 (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by author).



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		

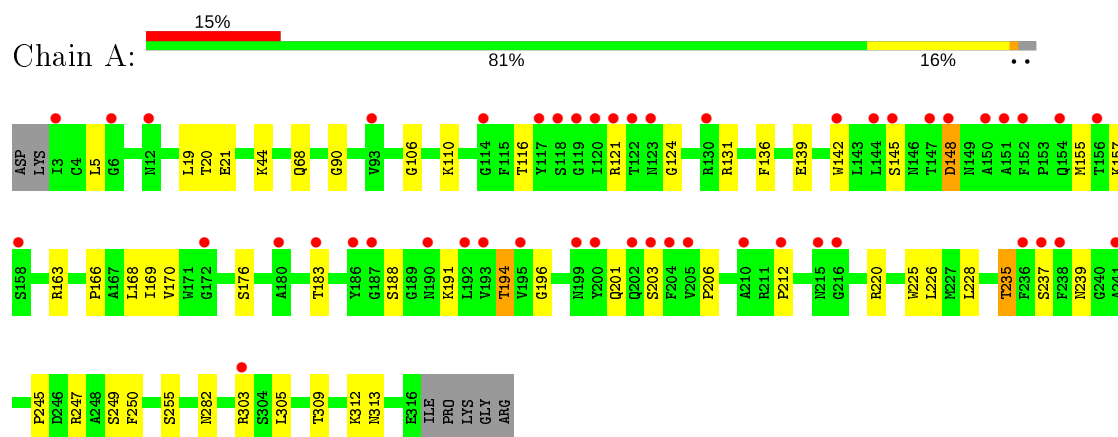
- Molecule 4 is water.

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

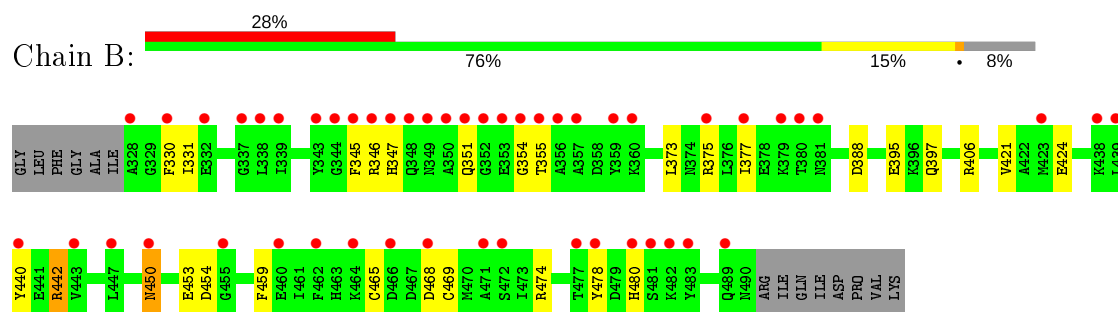
### 3 Residue-property plots

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, $\alpha$ , $\beta$ , $\gamma$	115.32Å 115.32Å 293.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.10 – 2.40 36.56 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (32.10-2.40) 99.1 (36.56-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.266 , 0.300 0.266 , 0.300	Depositor DCC
$R_{free}$ test set	1458 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.7	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 59.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<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

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	0.25	0/2430	0.45	0/3286
2	B	0.24	0/1351	0.41	0/1821
All	All	0.25	0/3781	0.43	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: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:170:VAL:O	1:A:245:PRO:HB3	2.13	0.48
1:A:90:GLY:N	4:A:710:HOH:O	2.44	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:HB3	2:B:442:ARG:HH11	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:44:LYS:NZ	4:A:704:HOH:O	2.39	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:HA	1:A:228:LEU:HD23	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

*Continued on next page...*

Continued from previous page...

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%)	25	36
2	B	161/177 (91%)	151 (94%)	10 (6%)	0	100	100
All	All	473/498 (95%)	446 (94%)	25 (5%)	2 (0%)	34	48

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%)	253 (97%)	7 (3%)	44	65
2	B	141/152 (93%)	132 (94%)	9 (6%)	17	28
All	All	401/420 (96%)	385 (96%)	16 (4%)	31	49

All (16) 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
2	B	330	PHE
2	B	331	ILE
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

Some 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 monosaccharides 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	0.27	0	17,19,21	0.46	0
3	NAG	A	602	1	14,14,15	0.38	0	17,19,21	0.48	0
3	NAG	B	501	2	14,14,15	0.28	0	17,19,21	0.42	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.

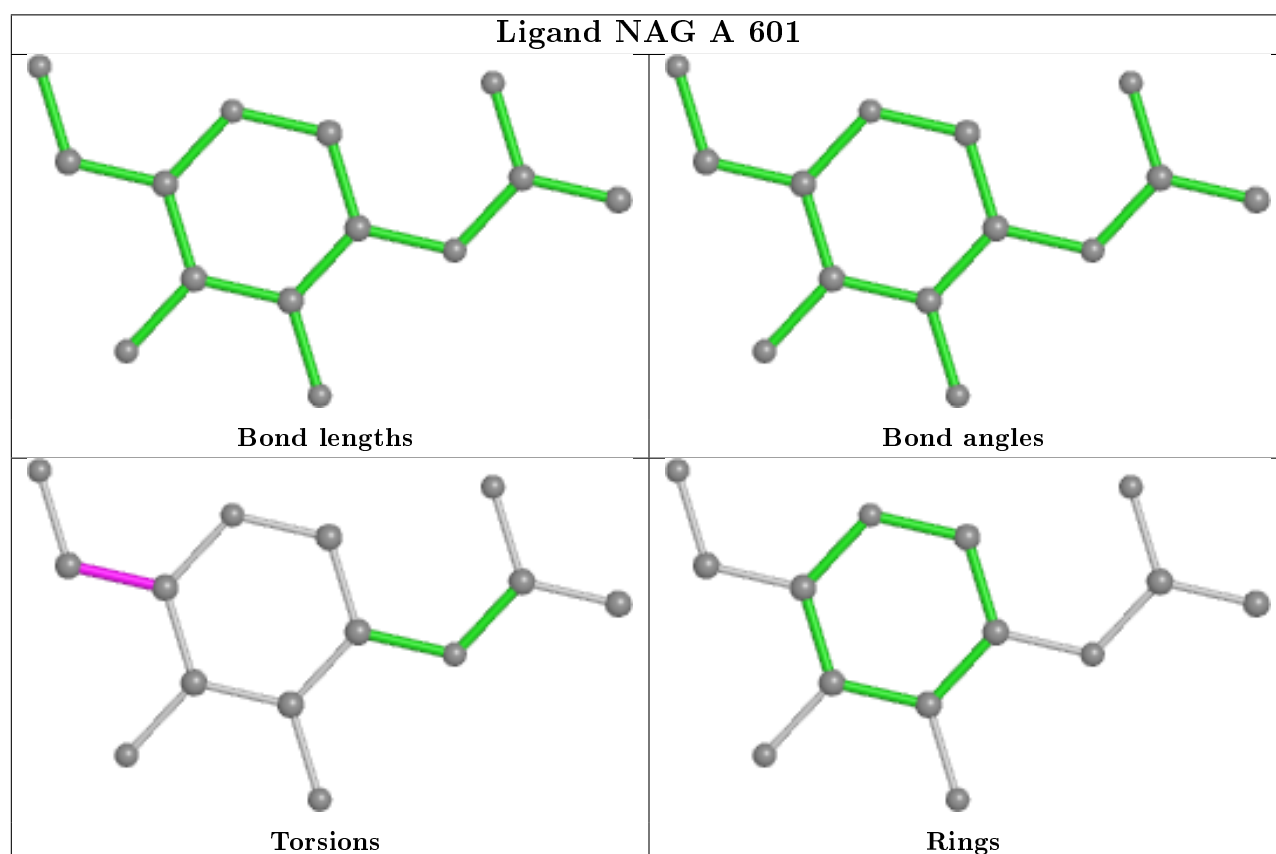
All (3) torsion outliers are listed below:

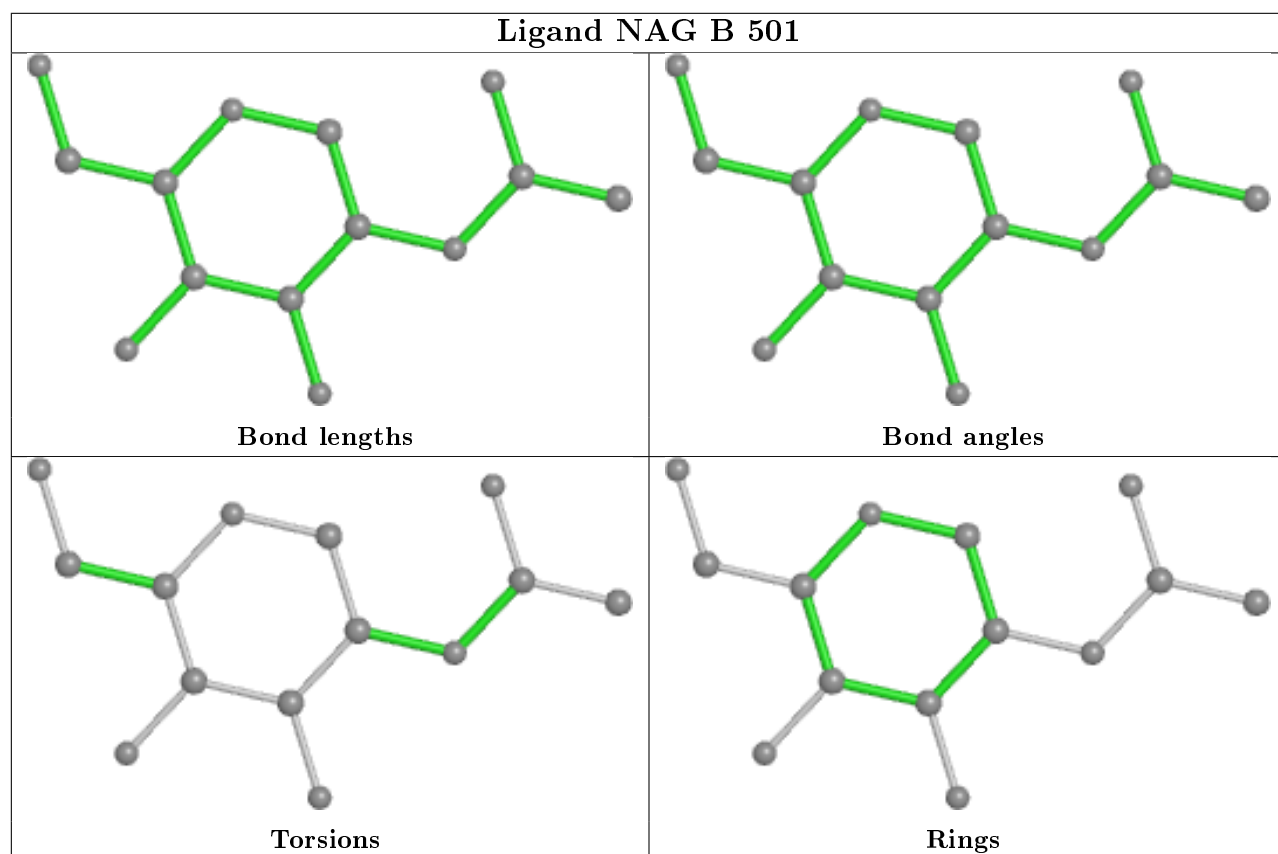
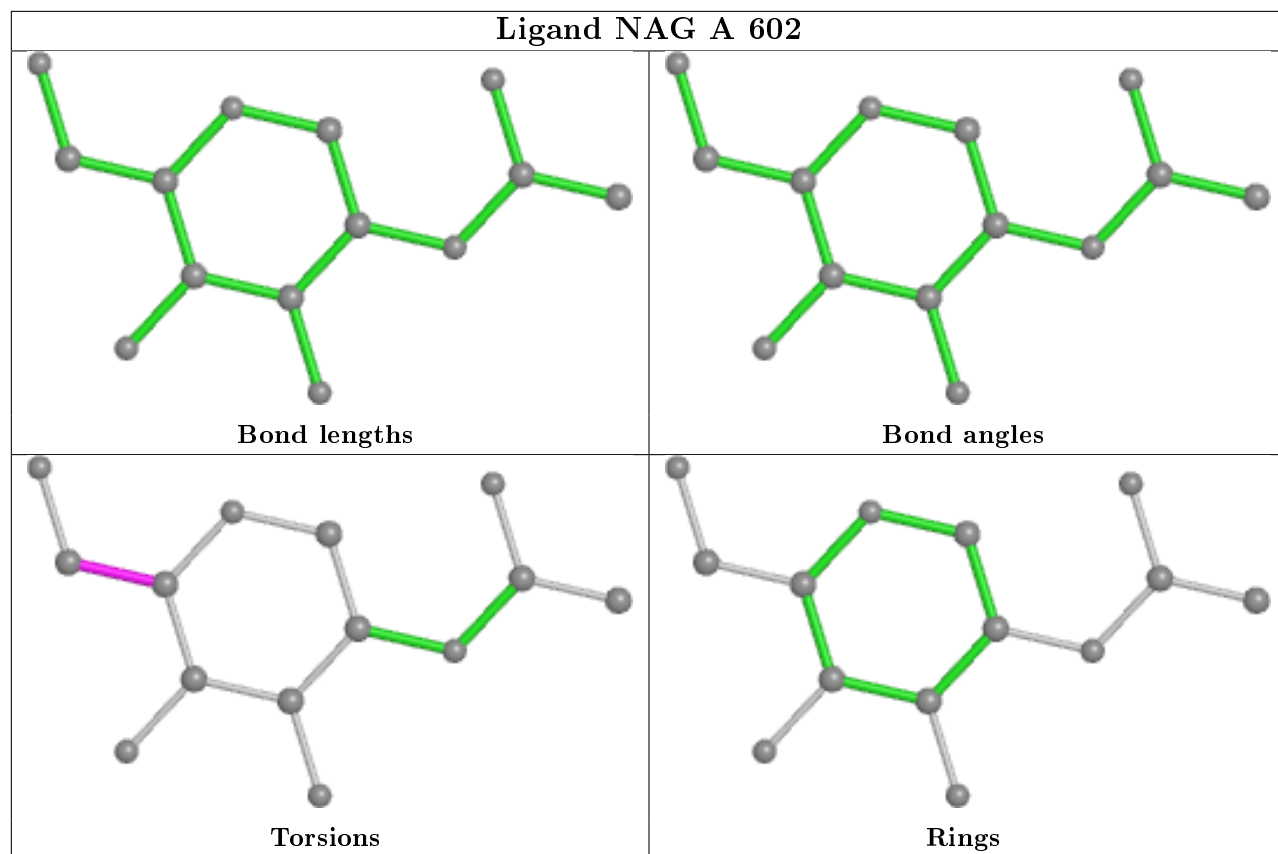
Mol	Chain	Res	Type	Atoms
3	A	601	NAG	O5-C5-C6-O6
3	A	602	NAG	O5-C5-C6-O6
3	A	602	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	314/321 (97%)	0.85	48 (15%)	2 1	40, 74, 127, 224	0
2	B	163/177 (92%)	1.67	50 (30%)	0 0	39, 105, 168, 202	0
All	All	477/498 (95%)	1.13	98 (20%)	1 0	39, 80, 154, 224	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	118	SER	6.7
1	A	6	GLY	6.7
2	B	480	HIS	6.6
2	B	348	GLN	6.3
1	A	148	ASP	6.3
1	A	186	TYR	6.3
2	B	379	LYS	6.2
2	B	351	GLN	6.2
2	B	471	ALA	5.9
2	B	462	PHE	5.9
2	B	464	LYS	5.8
2	B	353	GLU	5.6
1	A	156	THR	5.5
1	A	117	TYR	5.5
2	B	347	HIS	5.5
1	A	147	THR	5.4
2	B	468	ASP	5.2
2	B	472	SER	5.0
2	B	483	TYR	5.0
2	B	352	GLY	4.9
2	B	354	GLY	4.5
1	A	204	PHE	4.4
2	B	460	GLU	4.4
2	B	482	LYS	4.4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	144	LEU	4.4
2	B	381	ASN	4.3
1	A	3	ILE	4.2
2	B	350	ALA	4.2
1	A	12	ASN	4.0
2	B	359	TYR	4.0
1	A	190	ASN	4.0
2	B	332	GLU	3.9
1	A	203	SER	3.9
2	B	343	TYR	3.8
1	A	200	TYR	3.8
2	B	481	SER	3.8
2	B	447	LEU	3.8
1	A	145	SER	3.7
1	A	236	PHE	3.6
1	A	172	GLY	3.6
1	A	180	ALA	3.6
2	B	345	PHE	3.6
2	B	439	LEU	3.5
2	B	440	TYR	3.5
1	A	210	ALA	3.4
1	A	195	VAL	3.3
1	A	114	GLY	3.3
2	B	349	ASN	3.3
2	B	356	ALA	3.3
1	A	151	ALA	3.1
2	B	438	LYS	3.1
1	A	205	VAL	3.0
1	A	183	THR	3.0
1	A	199	ASN	3.0
1	A	193	VAL	3.0
1	A	241	ALA	3.0
1	A	152	PHE	3.0
2	B	478	TYR	2.9
1	A	122	THR	2.9
2	B	360	LYS	2.9
1	A	192	LEU	2.9
1	A	150	ALA	2.9
1	A	123	ASN	2.8
1	A	212	PRO	2.8
2	B	377	ILE	2.8
2	B	477	THR	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	215	ASN	2.7
2	B	328	ALA	2.7
2	B	489	GLN	2.7
2	B	338	LEU	2.6
1	A	202	GLN	2.6
2	B	346	ARG	2.6
1	A	121	ARG	2.5
2	B	344	GLY	2.5
1	A	154	GLN	2.4
2	B	330	PHE	2.4
2	B	443	VAL	2.4
1	A	158	SER	2.4
2	B	380	THR	2.4
1	A	93	VAL	2.3
2	B	450	ASN	2.3
1	A	216	GLY	2.3
2	B	355	THR	2.3
1	A	142	TRP	2.3
2	B	339	ILE	2.3
1	A	187	GLY	2.2
2	B	337	GLY	2.2
2	B	357	ALA	2.2
1	A	130	ARG	2.2
2	B	375	ARG	2.2
2	B	466	ASP	2.1
2	B	455	GLY	2.1
1	A	237	SER	2.1
1	A	120	ILE	2.1
2	B	423	MET	2.1
1	A	238	PHE	2.0
1	A	119	GLY	2.0
1	A	303	ARG	2.0

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

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

## 6.3 Carbohydrates ⓘ

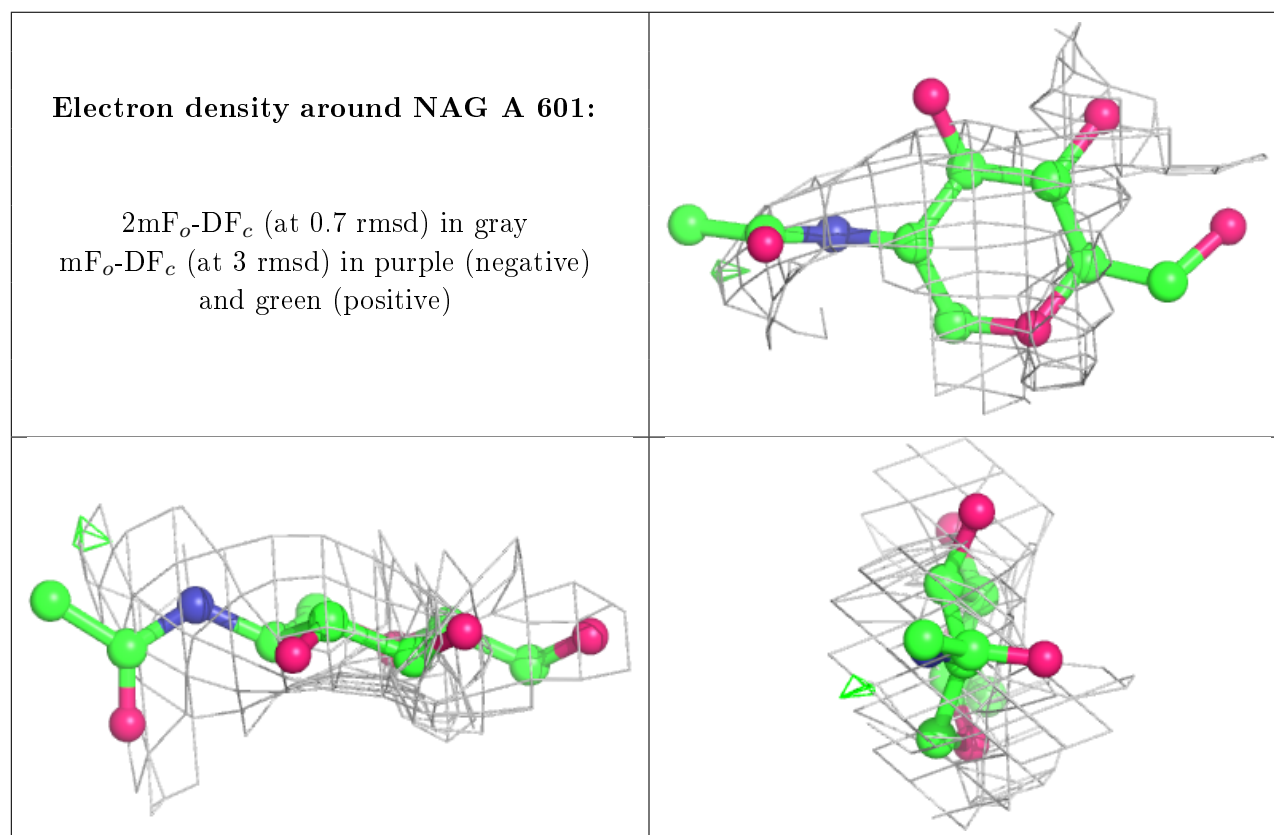
There are no monosaccharides in this entry.

## 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.

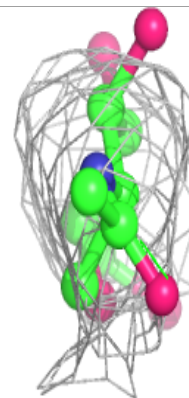
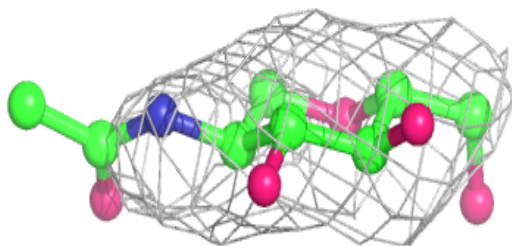
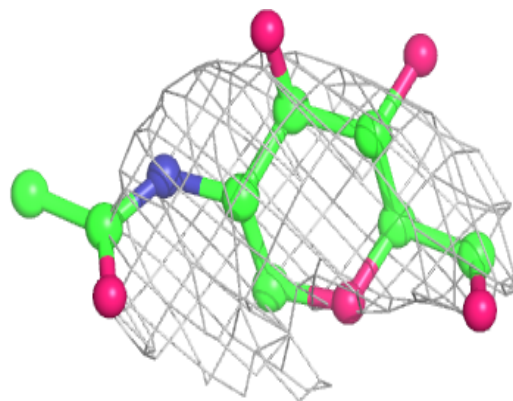
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	601	14/15	0.77	0.40	157,169,172,173	0
3	NAG	A	602	14/15	0.84	0.54	147,159,166,168	0
3	NAG	B	501	14/15	0.92	0.14	74,83,93,98	0

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.

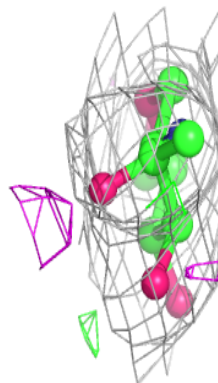
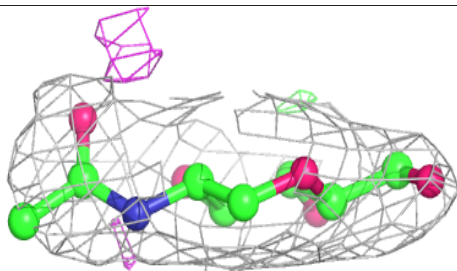
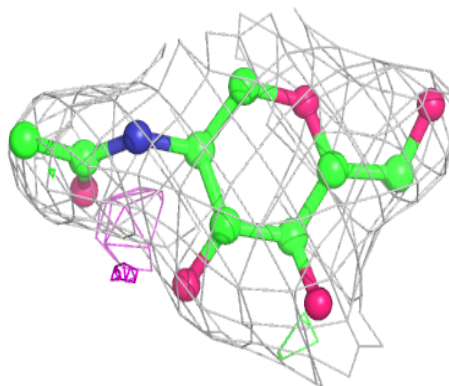


**Electron density around NAG A 602:**

$2mF_o-DF_c$  (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

There are no such residues in this entry.