



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2021 – 02:11 PM JST

PDB ID : 7EAN  
Title : immune complex of SARS-CoV-2 RBD and cross-neutralizing antibody 6D6  
Authors : Li, T.T.; Gu, Y.; Li, S.W.  
Deposited on : 2021-03-07  
Resolution : 1.91 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

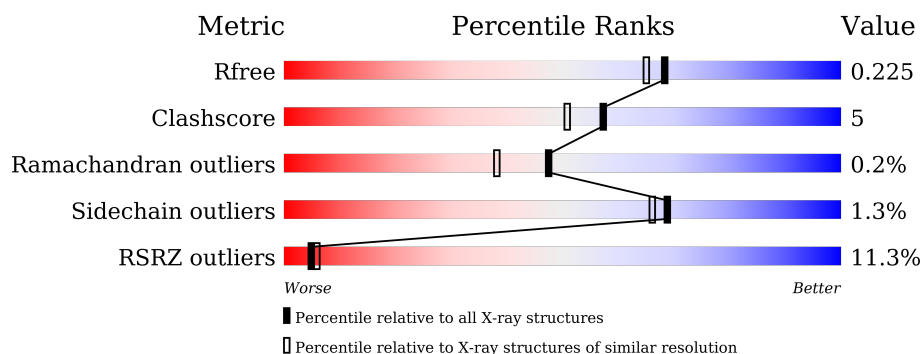
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.91 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	223	<div> <div>11%</div> <div> <div></div> <div>81%</div> <div>7%</div> <div>13%</div> </div> </div>
2	H	222	<div> <div>10%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>.</div> </div> </div>
3	L	210	<div> <div>11%</div> <div> <div></div> <div>85%</div> <div>14%</div> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9677 atoms, of which 4645 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 Spike protein S1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	195	3001	989	1458	257	289	8	0	0	0

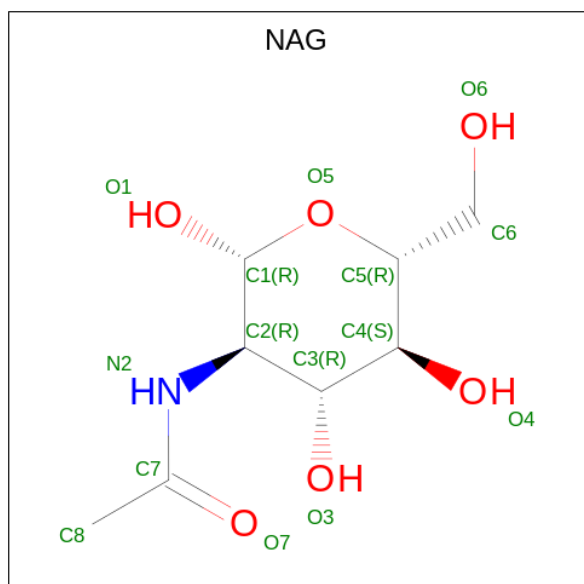
- Molecule 2 is a protein called Heavy chain of SARS-CoV-2 cross-neutralizing mAb 6D6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	H	222	3279	1056	1608	271	338	6	0	0	0

- Molecule 3 is a protein called Light chain of SARS-CoV-2 cross-neutralizing mAb 6D6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	L	210	3204	1023	1565	275	334	7	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



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

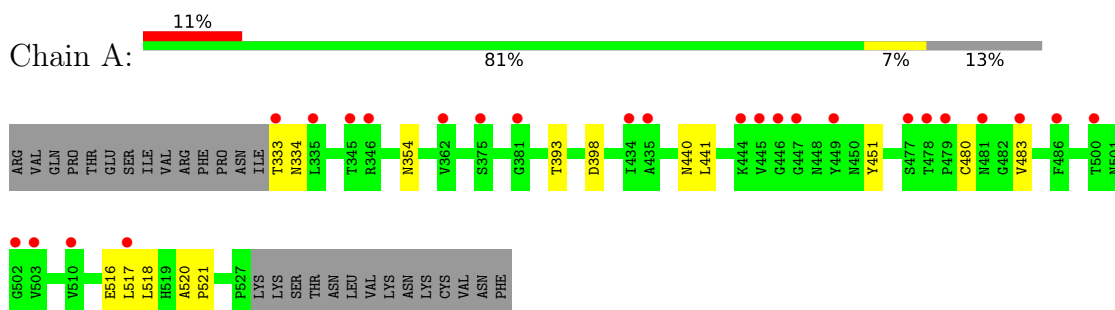
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	43	Total	O	0	0
			43	43		
5	H	75	Total	O	0	0
			75	75		
5	L	47	Total	O	0	0
			47	47		

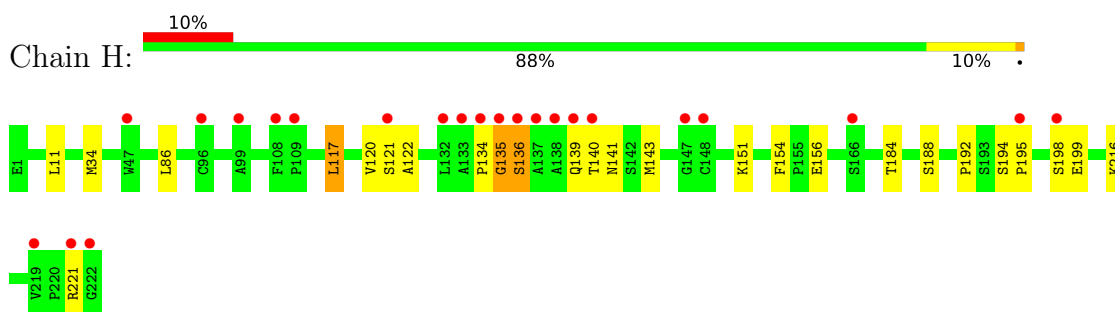
### 3 Residue-property plots [i](#)

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.

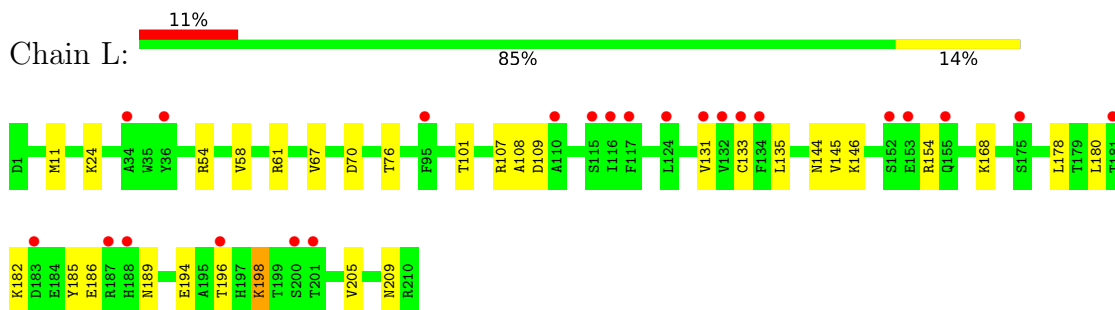
- Molecule 1: Spike protein S1



- Molecule 2: Heavy chain of SARS-CoV-2 cross-neutralizing mAb 6D6



- Molecule 3: Light chain of SARS-CoV-2 cross-neutralizing mAb 6D6



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.28Å 85.34Å 160.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.25 – 1.91 30.08 – 1.91	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.25-1.91) 89.0 (30.08-1.91)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.191 , 0.224 0.192 , 0.225	Depositor DCC
$R_{free}$ test set	2000 reflections (3.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 54.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9677	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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	0.59	0/1587	0.61	0/2161
2	H	0.71	2/1718 (0.1%)	0.74	2/2357 (0.1%)
3	L	0.63	1/1676 (0.1%)	0.65	0/2274
All	All	0.65	3/4981 (0.1%)	0.67	2/6792 (0.0%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	34	MET	SD-CE	-5.94	1.44	1.77
2	H	156	GLU	CD-OE1	5.62	1.31	1.25
3	L	133	CYS	CB-SG	-5.22	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	117	LEU	CB-CG-CD1	-9.05	95.61	111.00
2	H	34	MET	CG-SD-CE	7.53	112.24	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	136	SER	Peptide

## 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	1543	1458	1458	11	0
2	H	1671	1608	1608	18	0
3	L	1639	1565	1563	19	0
4	A	14	14	13	0	0
5	A	43	0	0	3	0
5	H	75	0	0	1	0
5	L	47	0	0	0	0
All	All	5032	4645	4642	47	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 5.

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)
2:H:11:LEU:HD11	2:H:120:VAL:CG1	1.97	0.95
2:H:216:LYS:NZ	5:H:301:HOH:O	2.03	0.90
2:H:11:LEU:HD11	2:H:120:VAL:HG12	1.54	0.89
2:H:120:VAL:HG22	2:H:122:ALA:H	1.52	0.75
1:A:333:THR:O	5:A:701:HOH:O	2.05	0.74
3:L:135:LEU:HD11	3:L:145:VAL:HG22	1.73	0.70
2:H:195:PRO:O	2:H:199:GLU:N	2.23	0.66
3:L:107:ARG:NH1	3:L:108:ALA:O	2.31	0.64
1:A:451:TYR:OH	5:A:702:HOH:O	2.15	0.64
2:H:11:LEU:CD1	2:H:120:VAL:HG12	2.28	0.63
1:A:518:LEU:HD22	3:L:67:VAL:HG21	1.81	0.62
2:H:139:GLN:HG2	2:H:140:THR:HA	1.83	0.60
3:L:189:ASN:OD1	3:L:209:ASN:OD1	2.20	0.59
1:A:517:LEU:HD23	1:A:517:LEU:H	1.67	0.59
3:L:180:LEU:HD11	3:L:185:TYR:HB2	1.87	0.56
2:H:192:PRO:HB2	2:H:195:PRO:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:24:LYS:HE2	3:L:70:ASP:OD1	2.09	0.53
3:L:146:LYS:HB3	3:L:146:LYS:NZ	2.23	0.52
2:H:139:GLN:CG	2:H:140:THR:HA	2.39	0.52
2:H:141:ASN:HB2	2:H:143:MET:O	2.10	0.52
3:L:182:LYS:O	3:L:186:GLU:HG3	2.10	0.51
2:H:194:SER:OG	2:H:195:PRO:HD3	2.10	0.51
2:H:120:VAL:HG11	2:H:154:PHE:CE2	2.45	0.51
3:L:109:ASP:OD2	3:L:198:LYS:HE3	2.11	0.51
2:H:192:PRO:O	2:H:195:PRO:HD2	2.12	0.50
2:H:86:LEU:CD2	2:H:117:LEU:HD21	2.42	0.49
2:H:120:VAL:HG11	2:H:154:PHE:HE2	1.81	0.44
1:A:354:ASN:O	1:A:398:ASP:HA	2.17	0.44
3:L:61:ARG:HB2	3:L:76:THR:O	2.17	0.44
1:A:440:ASN:OD1	1:A:441:LEU:HG	2.17	0.44
3:L:131:VAL:CG1	3:L:178:LEU:HB3	2.48	0.43
1:A:480:CYS:O	1:A:483:VAL:HG12	2.18	0.43
2:H:86:LEU:HD21	2:H:117:LEU:HD21	2.01	0.43
1:A:517:LEU:HG	1:A:517:LEU:O	2.18	0.43
1:A:393:THR:HG22	1:A:516:GLU:O	2.19	0.42
1:A:520:ALA:HB1	1:A:521:PRO:HD2	2.01	0.42
3:L:146:LYS:HB3	3:L:146:LYS:HZ1	1.83	0.42
3:L:194:GLU:HG2	3:L:205:VAL:HG22	2.01	0.42
3:L:11:MET:HG3	3:L:101:THR:CG2	2.50	0.42
2:H:134:PRO:HA	2:H:135:GLY:HA3	1.89	0.41
3:L:131:VAL:HG13	3:L:178:LEU:HB3	2.01	0.41
3:L:54:ARG:HG2	3:L:58:VAL:HB	2.03	0.41
3:L:180:LEU:CD1	3:L:185:TYR:HB2	2.50	0.41
2:H:151:LYS:HA	2:H:184:THR:HG23	2.03	0.41
3:L:168:LYS:HD2	3:L:168:LYS:HA	1.87	0.41
3:L:144:ASN:HB3	3:L:196:THR:OG1	2.21	0.40
1:A:334:ASN:ND2	5:A:701:HOH:O	2.32	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	193/223 (86%)	185 (96%)	8 (4%)	0	100	100
2	H	220/222 (99%)	217 (99%)	2 (1%)	1 (0%)	29	18
3	L	208/210 (99%)	205 (99%)	3 (1%)	0	100	100
All	All	621/655 (95%)	607 (98%)	13 (2%)	1 (0%)	47	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	135	GLY

### 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	168/196 (86%)	168 (100%)	0	100	100
2	H	191/191 (100%)	186 (97%)	5 (3%)	46	37
3	L	187/187 (100%)	185 (99%)	2 (1%)	73	72
All	All	546/574 (95%)	539 (99%)	7 (1%)	69	66

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	121	SER
2	H	136	SER
2	H	188	SER
2	H	198	SER
2	H	221	ARG
3	L	154	ARG
3	L	198	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	ASN
1	A	487	ASN
2	H	141	ASN
2	H	172	HIS
3	L	209	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](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	601	1	14,14,15	0.23	0	17,19,21	0.47	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	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

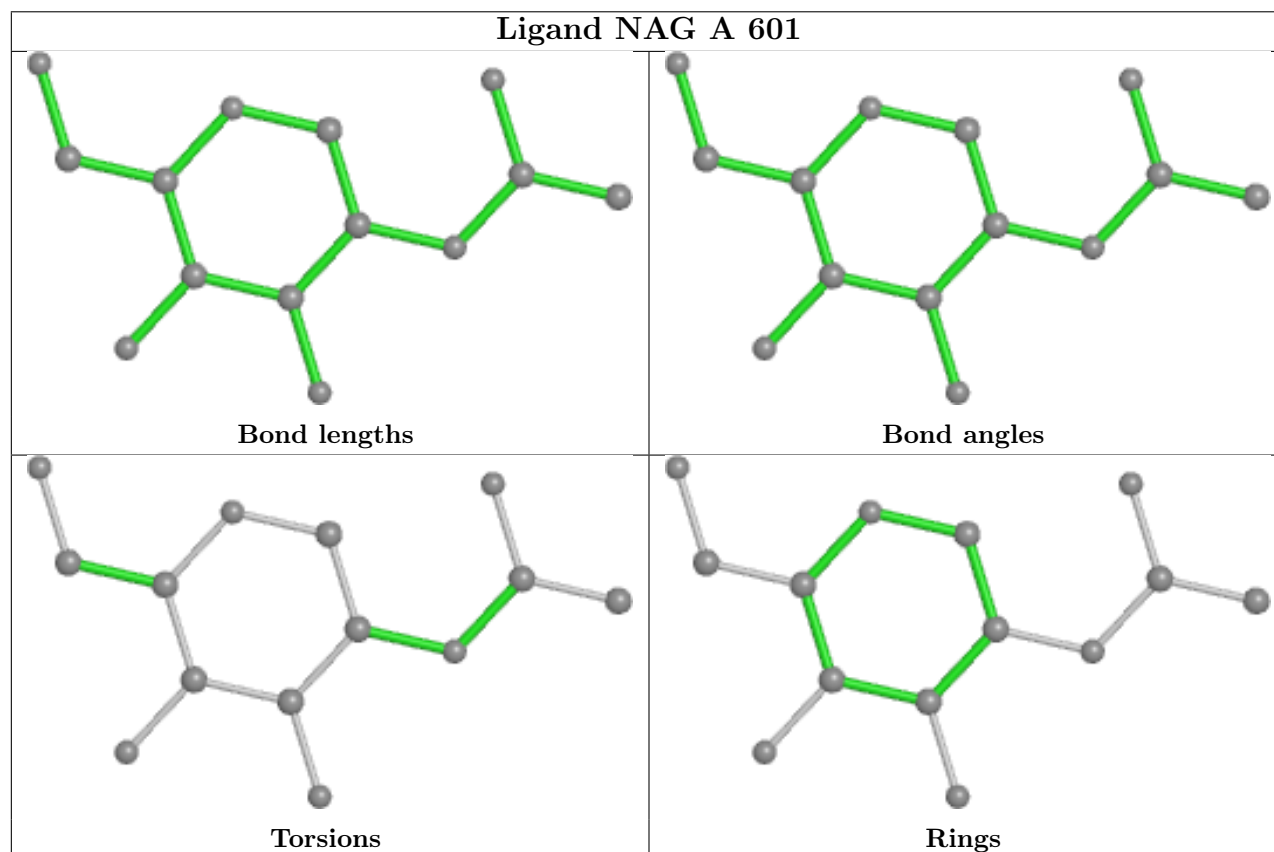
There are no chirality outliers.

There are no torsion outliers.

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, 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	195/223 (87%)	0.84	25 (12%) <b>3</b> <b>4</b>	39, 60, 88, 104	0
2	H	222/222 (100%)	0.65	23 (10%) <b>6</b> <b>7</b>	34, 46, 95, 136	0
3	L	210/210 (100%)	0.79	23 (10%) <b>5</b> <b>6</b>	38, 56, 88, 123	0
All	All	627/655 (95%)	0.76	71 (11%) <b>5</b> <b>6</b>	34, 54, 88, 136	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	137	ALA	14.3
1	A	445	VAL	7.2
2	H	135	GLY	5.9
2	H	140	THR	5.7
3	L	187	ARG	5.6
2	H	222	GLY	4.8
2	H	148	CYS	4.8
3	L	132	VAL	4.8
1	A	449	TYR	4.6
1	A	345	THR	4.5
2	H	139	GLN	4.4
3	L	134	PHE	4.3
3	L	117	PHE	4.1
2	H	138	ALA	4.0
3	L	183	ASP	4.0
2	H	136	SER	3.9
1	A	503	VAL	3.7
1	A	333	THR	3.5
1	A	447	GLY	3.4
2	H	108	PHE	3.4
2	H	221	ARG	3.3
1	A	362	VAL	3.2
1	A	478	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	346	ARG	3.1
3	L	155	GLN	3.1
3	L	133	CYS	3.1
3	L	188	HIS	3.0
3	L	115	SER	3.0
2	H	121	SER	2.9
1	A	444	LYS	2.9
2	H	198	SER	2.9
1	A	335	LEU	2.8
1	A	486	PHE	2.7
2	H	132	LEU	2.7
3	L	175	SER	2.7
2	H	99	ALA	2.6
2	H	47	TRP	2.6
3	L	116	ILE	2.6
1	A	479	PRO	2.6
3	L	201	THR	2.6
2	H	147	GLY	2.6
3	L	153	GLU	2.6
3	L	95	PHE	2.5
3	L	181	THR	2.5
2	H	109	PRO	2.5
1	A	500	THR	2.4
2	H	219	VAL	2.4
3	L	36	TYR	2.4
3	L	124	LEU	2.4
1	A	381	GLY	2.4
3	L	131	VAL	2.4
1	A	502	GLY	2.3
3	L	200	SER	2.3
2	H	134	PRO	2.3
1	A	434	ILE	2.2
1	A	477	SER	2.2
2	H	195	PRO	2.2
2	H	133	ALA	2.2
1	A	517	LEU	2.1
2	H	96	CYS	2.1
3	L	34	ALA	2.1
2	H	166	SER	2.1
1	A	481	ASN	2.1
1	A	446	GLY	2.1
1	A	483	VAL	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	435	ALA	2.1
1	A	375	SER	2.0
1	A	510	VAL	2.0
3	L	110	ALA	2.0
3	L	152	SER	2.0
3	L	196	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

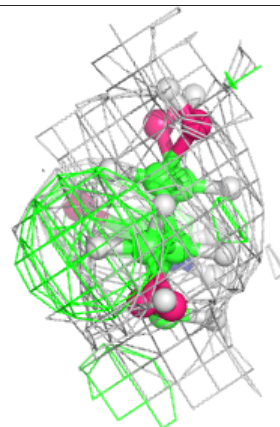
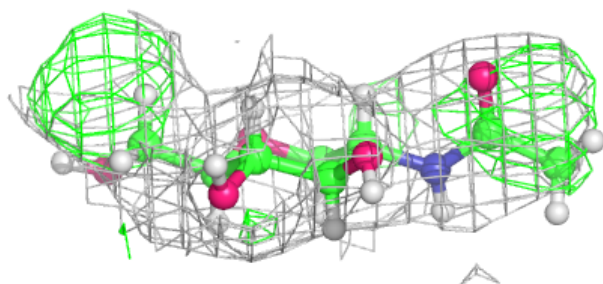
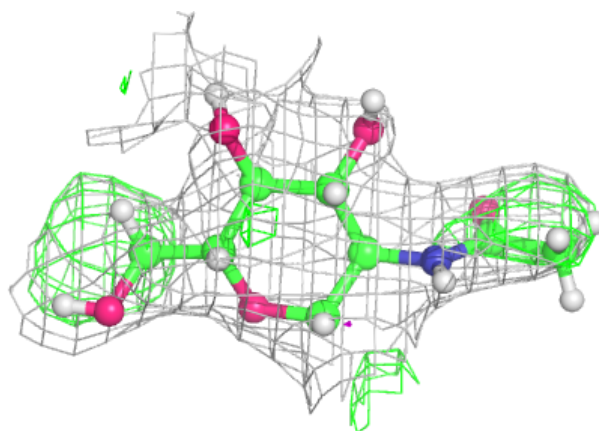
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	601	14/15	0.70	0.22	100,123,161,161	0

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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.