



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2022 – 06:04 PM EDT

PDB ID : 6WAS  
Title : Structure of D19.PA8 Fab in complex with 1FD6 16055 V1V2 scaffold  
Authors : Singh, S.; Liban, T.J.; Pancera, M.  
Deposited on : 2020-03-26  
Resolution : 1.90 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 : 2.27  
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) : 2.27

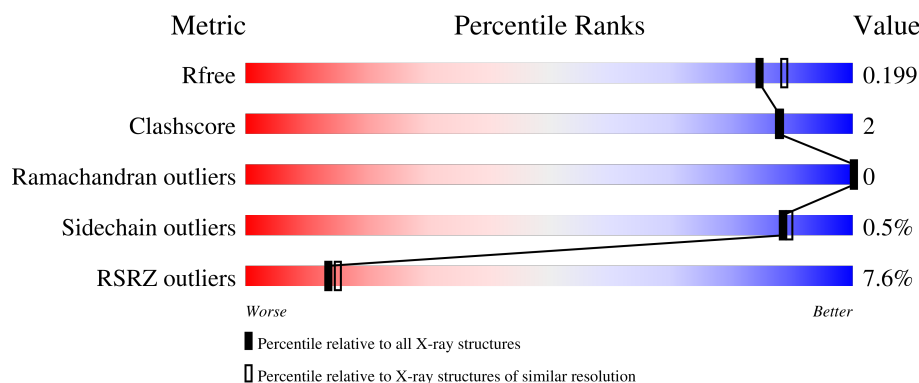
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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>25%</div> <div> <div></div> <div>91%</div> <div>7%</div> </div> </div>
1	H	223	<div> <div>3%</div> <div> <div></div> <div>95%</div> </div> </div>
2	B	217	<div> <div>%</div> <div> <div></div> <div>97%</div> </div> </div>
2	L	217	<div> <div></div> <div> <div></div> <div>95%</div> </div> </div>
3	G	151	<div> <div>3%</div> <div> <div>31%</div> <div>66%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	J	151	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>31%</div><div>.</div><div>68%</div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15419 atoms, of which 7032 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 GN1\_PA8 Fab Heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	H	219	Total	C	H	N	O	S	0	4	0
			3207	1033	1569	276	322	7			
1	A	219	Total	C	H	N	O	S	0	4	0
			3215	1035	1573	277	323	7			

- Molecule 2 is a protein called GN1\_PA8 Fab Light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	215	Total	C	H	N	O	S	0	14	0
			3272	1038	1598	285	346	5			
2	B	215	Total	C	H	N	O	S	0	0	0
			3180	1012	1550	278	336	4			

- Molecule 3 is a protein called 1FD6 16055 V1V2 scaffold.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	G	51	Total	C	H	N	O	S	0	0	0
			768	258	360	71	75	4			
3	J	48	Total	C	H	N	O	S	0	0	0
			739	243	354	68	70	4			

- Molecule 4 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 depositor).



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

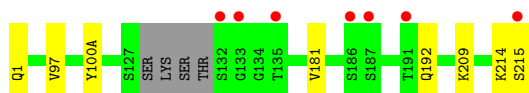
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	213	Total	O	0	0
			213	213		
5	L	275	Total	O	0	0
			275	275		
5	A	181	Total	O	0	0
			181	181		
5	B	192	Total	O	0	0
			192	192		
5	G	50	Total	O	0	0
			50	50		
5	J	43	Total	O	0	0
			43	43		

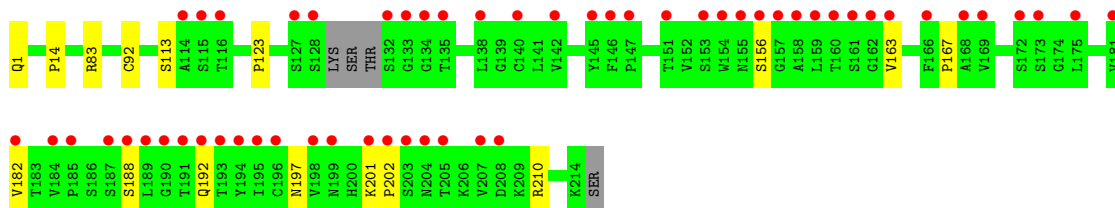
### 3 Residue-property plots

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: GN1\_PA8 Fab Heavy chain



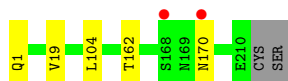
- Molecule 1: GN1\_PA8 Fab Heavy chain



- Molecule 2: GN1\_PA8 Fab Light chain

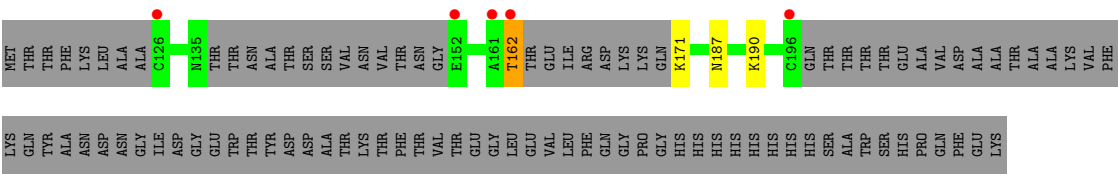


- Molecule 2: GN1\_PA8 Fab Light chain

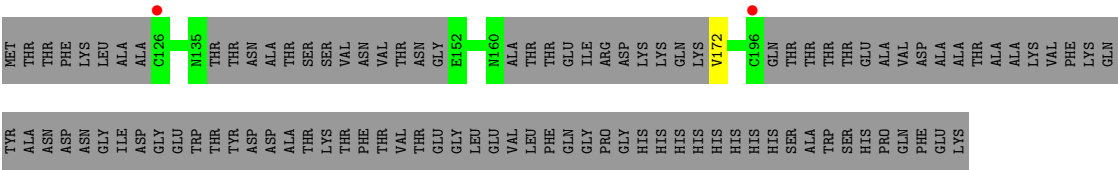


- Molecule 3: 1FD6 16055 V1V2 scaffold





● Molecule 3: 1FD6 16055 V1V2 scaffold



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.70Å 97.89Å 168.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.90 – 1.90 31.90 – 1.90	Depositor EDS
% Data completeness (in resolution range)	88.2 (31.90-1.90) 88.2 (31.90-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.189 , 0.221 0.189 , 0.199	Depositor DCC
$R_{free}$ test set	4155 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.4	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 51.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15419	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PCA, 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	0.30	0/1693	0.53	0/2312
1	H	0.30	0/1686	0.52	0/2303
2	B	0.30	0/1663	0.51	0/2273
2	L	0.30	0/1763	0.52	0/2411
3	G	0.30	0/411	0.55	0/549
3	J	0.29	0/388	0.50	0/519
All	All	0.30	0/7604	0.52	0/10367

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 [i](#)

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	1642	1573	1562	10	0
1	H	1638	1569	1545	5	0
2	B	1630	1550	1550	2	0
2	L	1674	1598	1538	6	0
3	G	408	360	400	7	0
3	J	385	354	372	1	0
4	G	28	28	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	28	0	26	0	0
5	A	181	0	0	3	0
5	B	192	0	0	0	0
5	G	50	0	0	2	0
5	H	213	0	0	2	0
5	J	43	0	0	1	0
5	L	275	0	0	3	0
All	All	8387	7032	7019	29	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 2.

All (29) 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:J:172:VAL:N	5:J:401:HOH:O	2.10	0.83
2:L:123:GLU:OE2	5:L:301:HOH:O	2.00	0.80
1:H:192:GLN:OE1	5:H:301:HOH:O	2.03	0.74
3:G:162:THR:HG23	3:G:190:LYS:NZ	2.06	0.70
2:L:54:ARG:NH2	5:L:302:HOH:O	2.24	0.70
3:G:162:THR:HG21	5:G:440:HOH:O	1.95	0.66
3:G:187:ASN:HD21	4:G:302:NAG:C1	2.15	0.60
1:A:123:PRO:O	5:A:301:HOH:O	2.17	0.59
3:G:171:LYS:N	5:G:401:HOH:O	2.38	0.57
3:G:162:THR:HG23	3:G:190:LYS:HZ1	1.69	0.56
2:L:149:LYS:NZ	5:L:307:HOH:O	2.41	0.53
1:A:188:SER:HB2	1:A:192:GLN:HG3	1.89	0.53
1:A:83:ARG:NH1	5:A:304:HOH:O	2.43	0.51
1:A:156:SER:N	1:A:197:ASN:OD1	2.38	0.51
3:G:187:ASN:OD1	4:G:302:NAG:C1	2.59	0.51
2:B:19:VAL:HG21	2:B:104:LEU:HD11	1.94	0.49
3:G:162:THR:HG23	3:G:190:LYS:HZ3	1.75	0.48
1:H:181:VAL:HB	2:L:135:LEU:HD13	1.95	0.47
2:L:61:ARG:HD2	2:L:76[B]:SER:O	2.15	0.46
1:H:209:LYS:NZ	5:H:313:HOH:O	2.48	0.46
2:L:61:ARG:HD2	2:L:76[A]:SER:O	2.16	0.45
1:A:210:ARG:HD3	5:A:358:HOH:O	2.16	0.44
1:A:210:ARG:O	1:A:210:ARG:HG3	2.19	0.42
1:H:97:VAL:HG12	1:H:100(A):TYR:OH	2.20	0.42
1:A:14:PRO:HD2	1:A:113:SER:HB3	2.01	0.42
1:A:167:PRO:HG2	2:B:162:THR:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:214:LYS:O	1:H:215:SER:CB	2.67	0.41
1:A:201:LYS:N	1:A:202:PRO:CD	2.83	0.41
1:A:163:VAL:HG12	1:A:182:VAL:HG12	2.03	0.41

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	A	219/223 (98%)	210 (96%)	9 (4%)	0	100	100
1	H	219/223 (98%)	216 (99%)	3 (1%)	0	100	100
2	B	213/217 (98%)	208 (98%)	5 (2%)	0	100	100
2	L	227/217 (105%)	221 (97%)	6 (3%)	0	100	100
3	G	45/151 (30%)	45 (100%)	0	0	100	100
3	J	42/151 (28%)	42 (100%)	0	0	100	100
All	All	965/1182 (82%)	942 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	181/186 (97%)	179 (99%)	2 (1%)	73	73
1	H	178/186 (96%)	178 (100%)	0	100	100
2	B	186/189 (98%)	185 (100%)	1 (0%)	88	89
2	L	198/189 (105%)	197 (100%)	1 (0%)	88	89
3	G	45/131 (34%)	44 (98%)	1 (2%)	52	47
3	J	43/131 (33%)	43 (100%)	0	100	100
All	All	831/1012 (82%)	826 (99%)	5 (1%)	88	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	34	ARG
1	A	92[A]	CYS
1	A	92[B]	CYS
2	B	170	ASN
3	G	162	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
2	PCA	L	1	2	7,8,9	2.18	2 (28%)	9,10,12	2.41	5 (55%)
1	PCA	H	1	1	7,8,9	2.22	2 (28%)	9,10,12	2.13	5 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PCA	B	1	2	7,8,9	2.22	2 (28%)	9,10,12	2.09	5 (55%)
1	PCA	A	1	1	7,8,9	1.76	1 (14%)	9,10,12	1.92	5 (55%)

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
2	PCA	L	1	2	-	0/0/11/13	0/1/1/1
1	PCA	H	1	1	-	0/0/11/13	0/1/1/1
2	PCA	B	1	2	-	0/0/11/13	0/1/1/1
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	1	PCA	CD-N	4.79	1.47	1.34
2	L	1	PCA	CD-N	4.73	1.47	1.34
2	B	1	PCA	CD-N	4.63	1.46	1.34
1	A	1	PCA	CD-N	4.54	1.46	1.34
2	B	1	PCA	CA-N	3.46	1.50	1.46
1	H	1	PCA	CA-N	3.22	1.50	1.46
2	L	1	PCA	CA-N	3.10	1.50	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1	PCA	CB-CA-C	-3.86	107.40	112.70
2	L	1	PCA	CA-N-CD	-3.44	101.80	113.58
1	H	1	PCA	CA-N-CD	-3.14	102.83	113.58
1	H	1	PCA	OE-CD-CG	-3.05	121.44	126.76
2	L	1	PCA	OE-CD-CG	-3.04	121.45	126.76
2	B	1	PCA	CA-N-CD	-3.02	103.24	113.58
2	B	1	PCA	OE-CD-CG	-2.97	121.59	126.76
1	A	1	PCA	CB-CA-N	2.89	111.59	103.30
1	A	1	PCA	CA-N-CD	-2.75	104.17	113.58
1	A	1	PCA	OE-CD-CG	-2.64	122.15	126.76
2	B	1	PCA	CB-CA-N	2.63	110.86	103.30
1	H	1	PCA	CB-CA-C	-2.61	109.11	112.70
2	B	1	PCA	CB-CA-C	-2.52	109.24	112.70
2	L	1	PCA	CB-CA-N	2.50	110.47	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	PCA	CG-CD-N	2.44	114.71	108.39
2	L	1	PCA	CG-CD-N	2.41	114.63	108.39
1	H	1	PCA	CG-CD-N	2.31	114.37	108.39
1	A	1	PCA	O-C-CA	-2.27	118.82	124.78
1	H	1	PCA	CB-CA-N	2.22	109.67	103.30
1	A	1	PCA	CG-CD-N	2.17	114.02	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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	$\# Z  > 2$
4	NAG	G	302	-	14,14,15	1.93	1 (7%)	17,19,21	0.97	1 (5%)
4	NAG	J	301	3	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	J	302	3	14,14,15	0.22	0	17,19,21	0.60	0
4	NAG	G	301	3	14,14,15	0.27	0	17,19,21	0.93	1 (5%)

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	G	302	-	-	2/6/23/26	0/1/1/1
4	NAG	J	301	3	-	4/6/23/26	0/1/1/1
4	NAG	J	302	3	-	0/6/23/26	0/1/1/1
4	NAG	G	301	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	302	NAG	O5-C1	-7.09	1.32	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	301	NAG	C1-O5-C5	2.90	116.12	112.19
4	G	302	NAG	C1-C2-N2	2.76	115.21	110.49

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	301	NAG	O5-C5-C6-O6
4	J	301	NAG	O5-C5-C6-O6
4	J	301	NAG	C4-C5-C6-O6
4	G	301	NAG	C4-C5-C6-O6
4	G	302	NAG	C1-C2-N2-C7
4	J	301	NAG	C1-C2-N2-C7
4	J	301	NAG	C3-C2-N2-C7
4	G	302	NAG	C3-C2-N2-C7

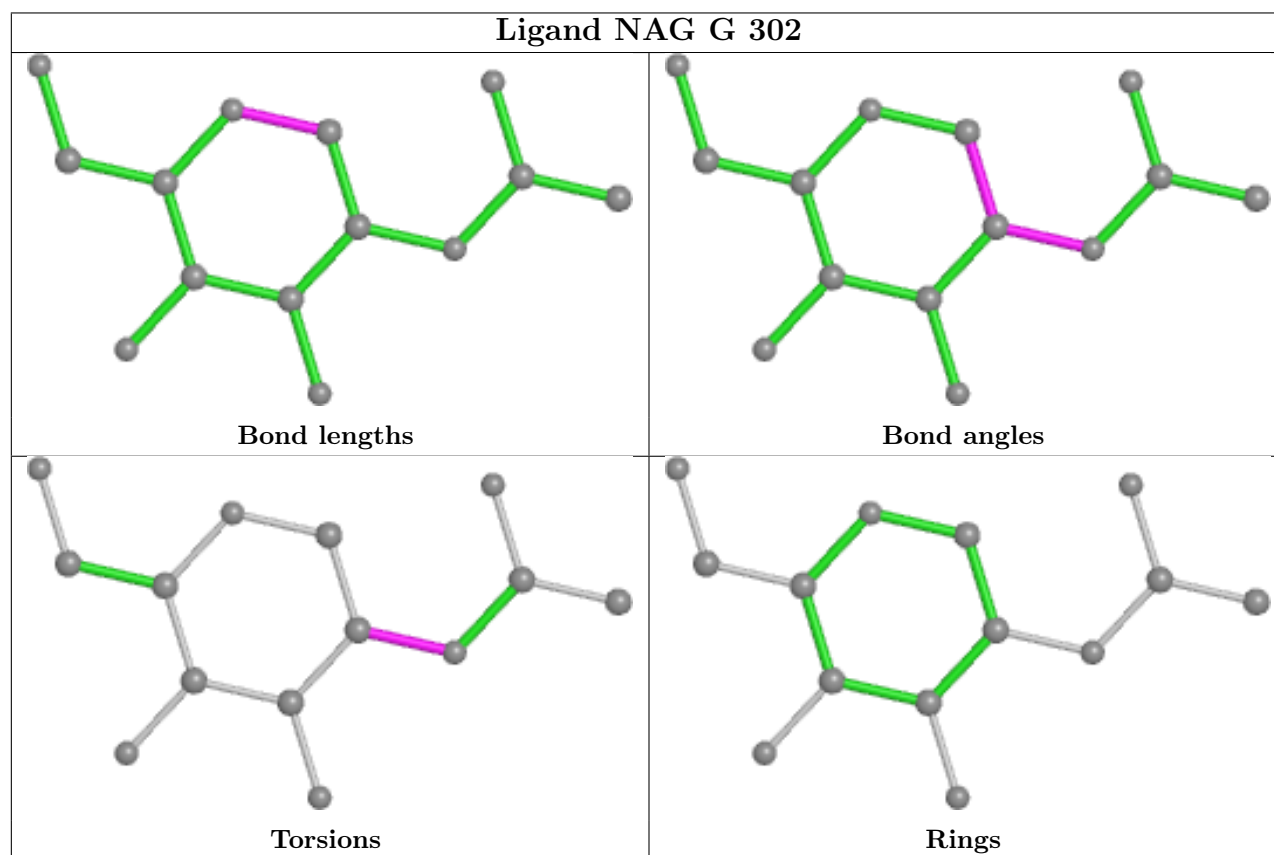
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	302	NAG	2	0

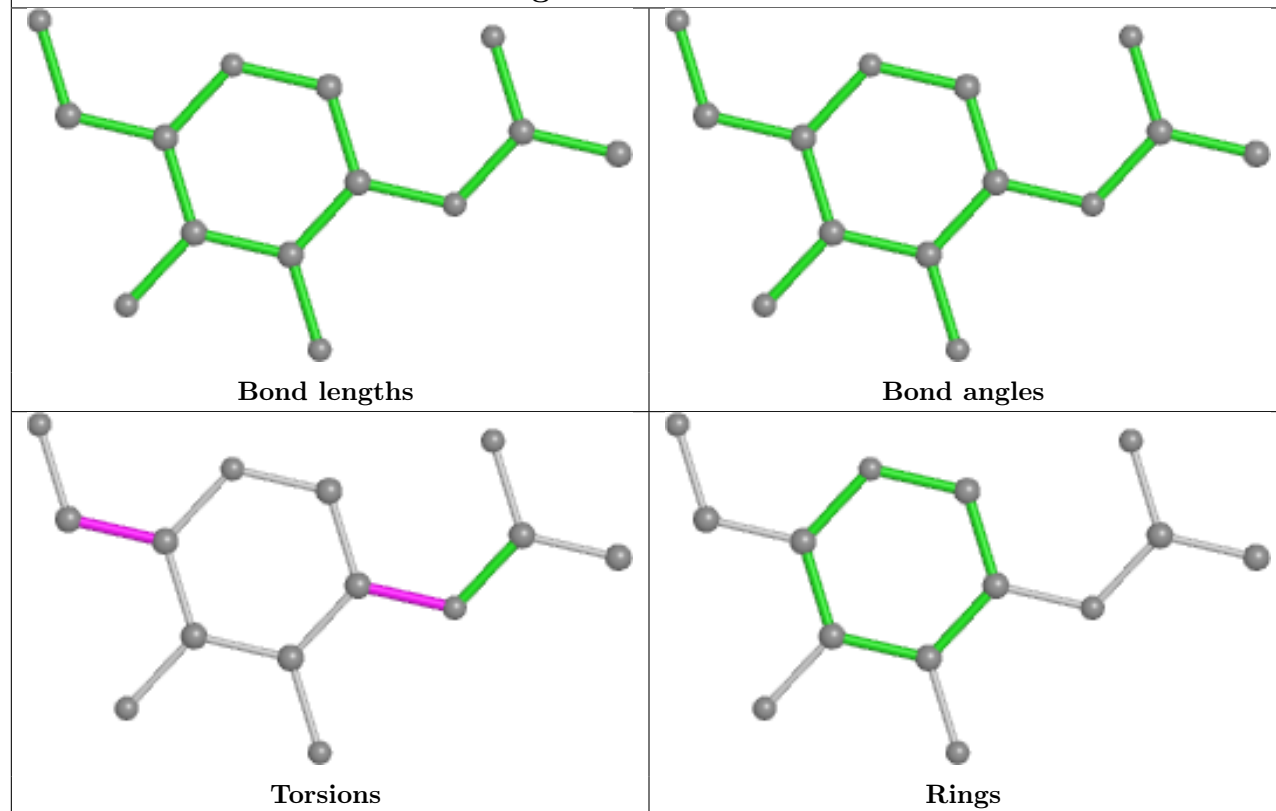
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

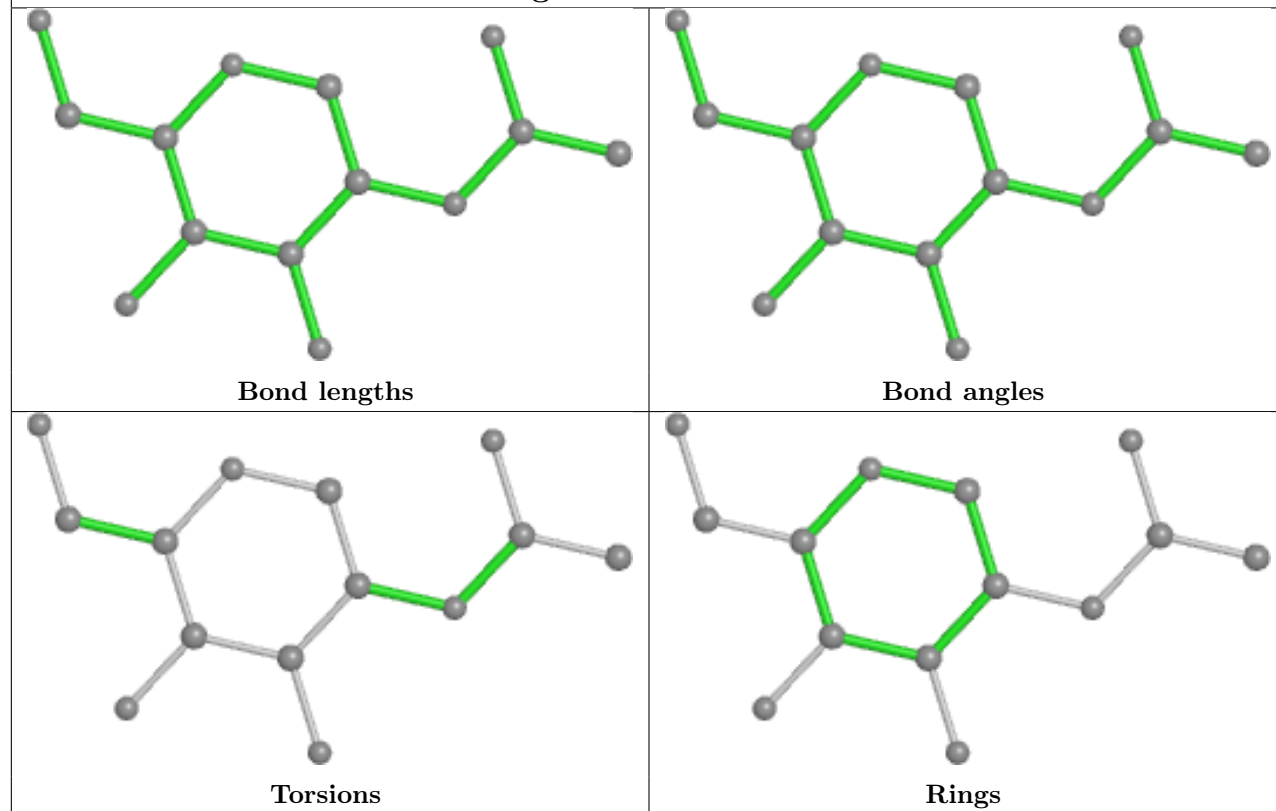


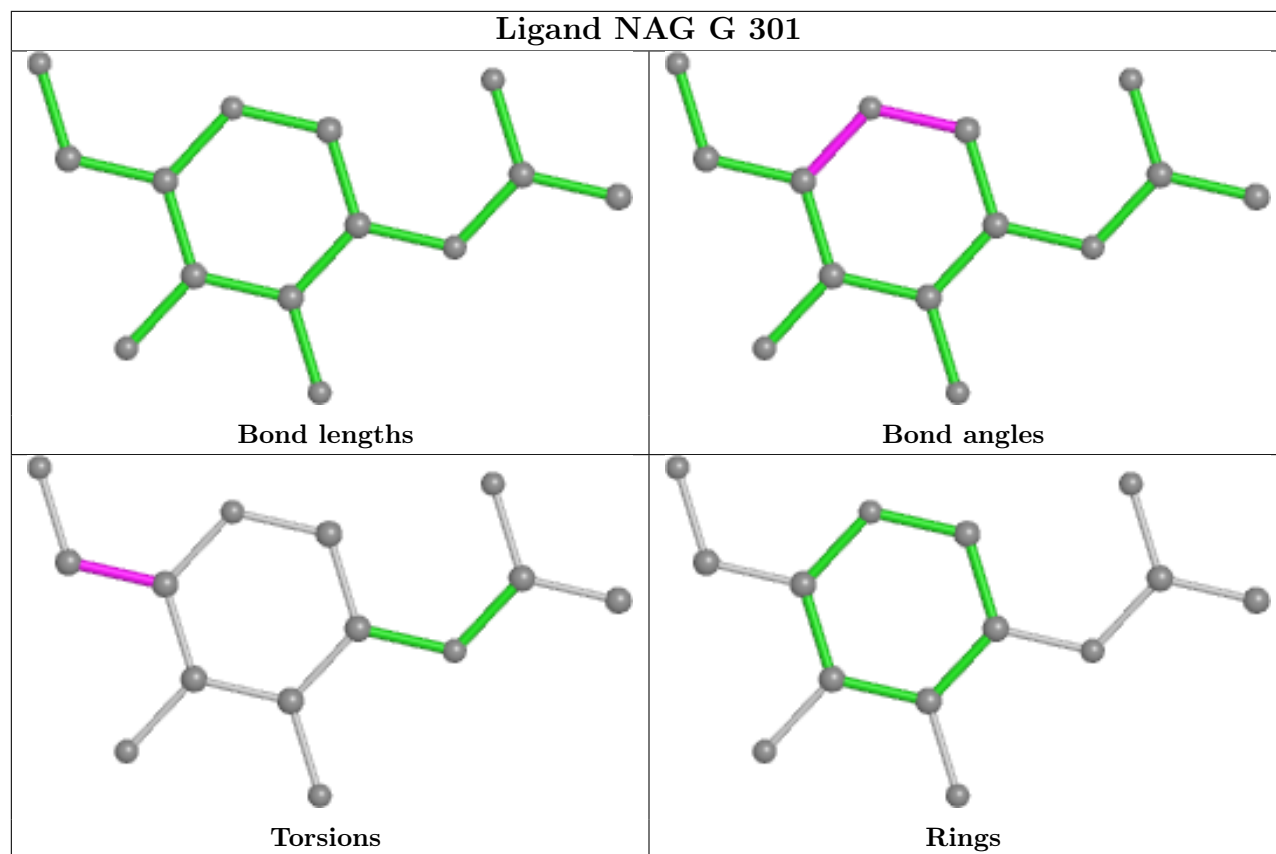


## Ligand NAG J 301



## Ligand NAG J 302





## 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	218/223 (97%)	1.05	56 (25%) 0 0	10, 34, 79, 98	0
1	H	218/223 (97%)	0.03	7 (3%) 47 50	10, 25, 53, 87	0
2	B	214/217 (98%)	-0.03	2 (0%) 84 85	12, 26, 44, 68	0
2	L	214/217 (98%)	-0.23	1 (0%) 91 92	10, 22, 38, 64	0
3	G	51/151 (33%)	0.35	5 (9%) 7 8	15, 26, 58, 60	0
3	J	48/151 (31%)	0.15	2 (4%) 36 39	13, 25, 54, 69	0
All	All	963/1182 (81%)	0.21	73 (7%) 13 15	10, 25, 66, 98	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	189	LEU	7.1
1	A	188	SER	6.4
1	H	132	SER	6.1
1	A	192	GLN	5.8
1	A	161	SER	5.6
1	A	187	SER	5.2
1	A	157	GLY	5.1
1	A	159	LEU	4.9
1	A	133	GLY	4.7
1	A	194	TYR	4.6
1	A	191	THR	4.5
1	A	146	PHE	4.3
2	B	168	SER	4.2
1	A	160	THR	4.1
1	A	158	ALA	4.0
1	A	190	GLY	3.8
1	A	135	THR	3.7
1	A	203	SER	3.7
1	H	187	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	162	GLY	3.6
1	A	202	PRO	3.6
1	A	127	SER	3.5
3	G	126	CYS	3.5
1	A	205	THR	3.5
1	A	173	SER	3.4
1	A	154	TRP	3.4
1	H	133	GLY	3.3
1	A	134	GLY	3.2
1	A	151	THR	3.2
1	A	115	SER	3.2
1	A	156	SER	3.1
1	A	116	THR	3.0
1	A	196	CYS	3.0
1	A	172	SER	3.0
3	G	162	THR	2.9
1	A	184	VAL	2.9
1	H	215	SER	2.9
1	A	147	PRO	2.8
1	A	182	VAL	2.8
1	A	204	ASN	2.8
3	J	196	CYS	2.8
1	H	135	THR	2.8
3	G	152	GLU	2.7
1	A	163	VAL	2.6
1	A	193	THR	2.6
1	H	191	THR	2.6
1	H	186	SER	2.6
3	G	161	ALA	2.6
1	A	114	ALA	2.5
1	A	128	SER	2.5
1	A	142	VAL	2.5
1	A	155	ASN	2.5
1	A	195	ILE	2.5
2	B	170	ASN	2.5
1	A	145	TYR	2.4
1	A	199	ASN	2.4
3	G	196	CYS	2.4
1	A	169	VAL	2.3
1	A	198	VAL	2.3
1	A	201	LYS	2.3
1	A	207	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	168	ALA	2.3
1	A	132	SER	2.3
2	L	183	GLU	2.2
1	A	153	SER	2.2
1	A	208	ASP	2.2
3	J	126	CYS	2.2
1	A	166	PHE	2.2
1	A	140[A]	CYS	2.2
1	A	138	LEU	2.1
1	A	175	LEU	2.1
1	A	185	PRO	2.1
1	A	181	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
2	PCA	B	1	8/9	0.78	0.33	54,69,82,87	0
2	PCA	L	1	8/9	0.81	0.30	46,72,87,87	0
1	PCA	A	1	8/9	0.85	0.23	33,57,92,92	0
1	PCA	H	1	8/9	0.87	0.28	45,65,81,81	0

## 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.

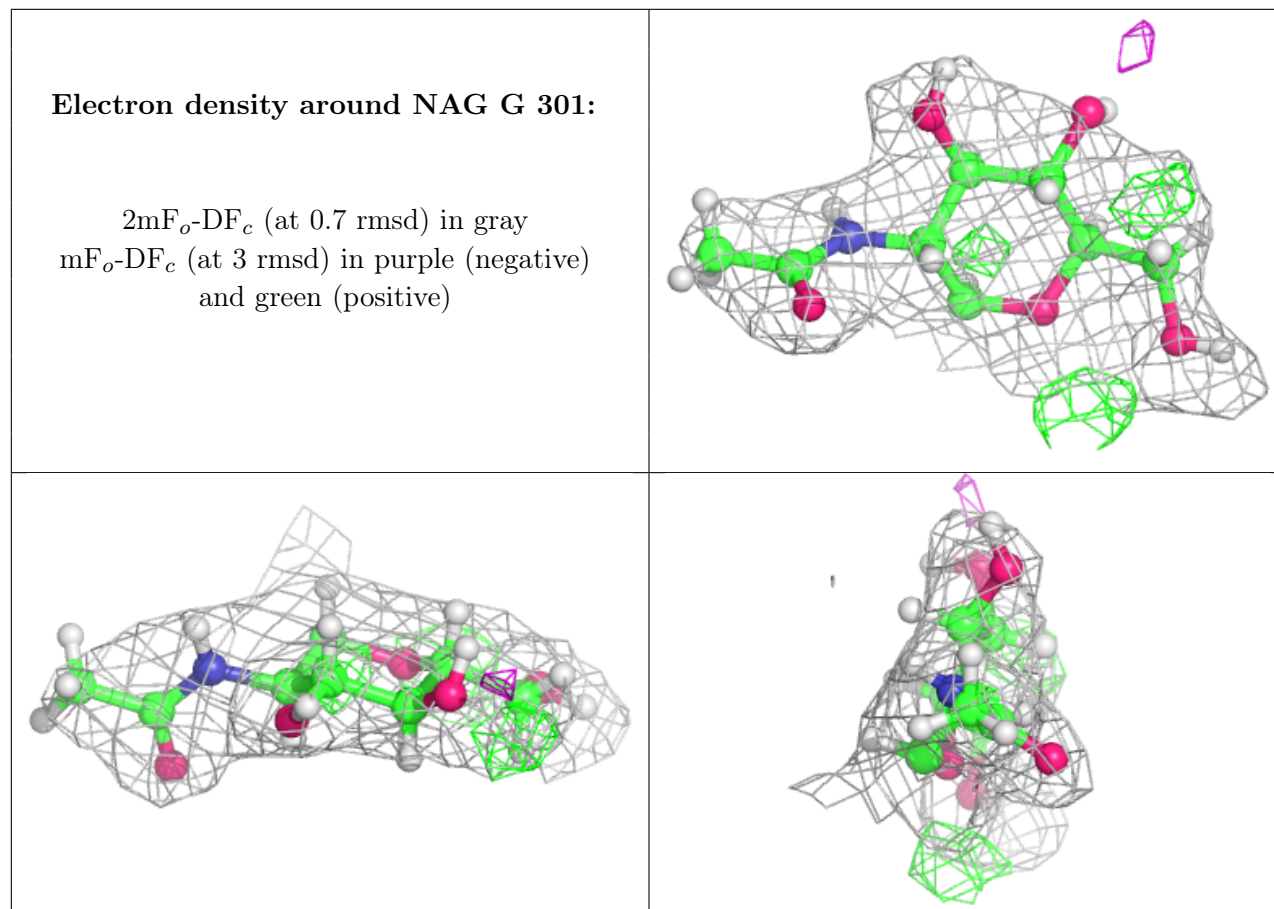
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	G	301	14/15	0.86	0.17	34,48,63,76	0
4	NAG	J	302	14/15	0.88	0.16	35,46,50,60	0

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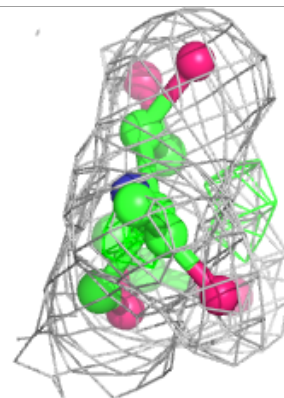
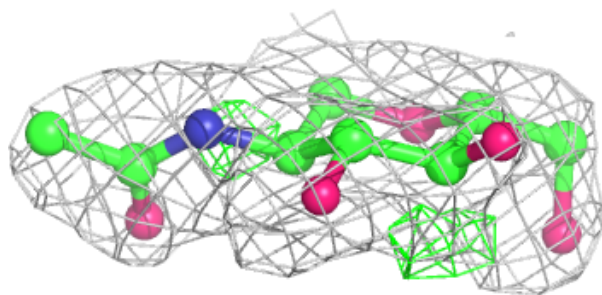
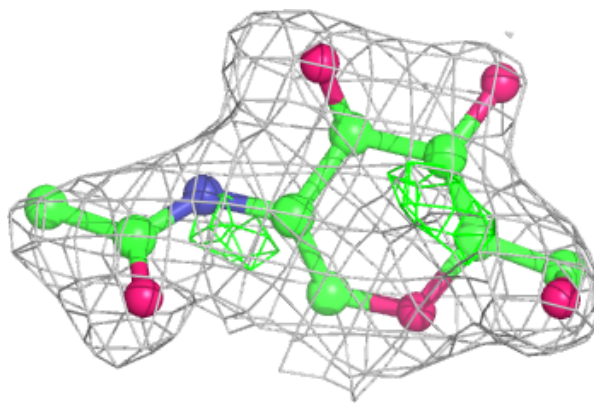
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	G	302	14/15	0.89	0.21	33,48,67,72	0
4	NAG	J	301	14/15	0.95	0.10	17,25,44,50	0

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.



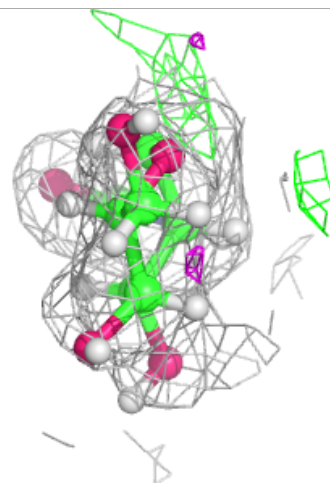
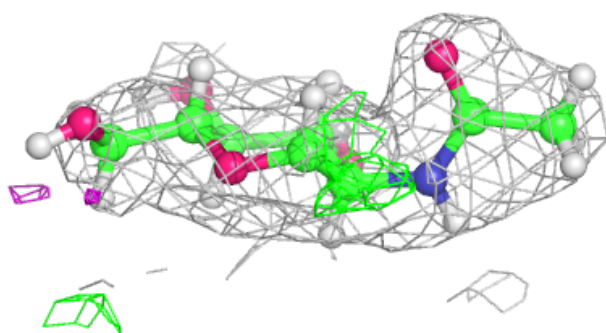
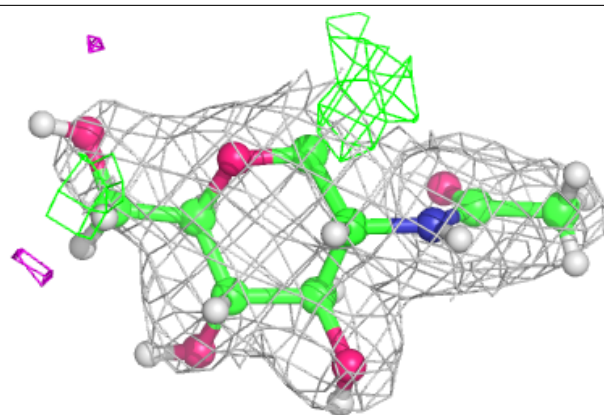
**Electron density around NAG J 302:**

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

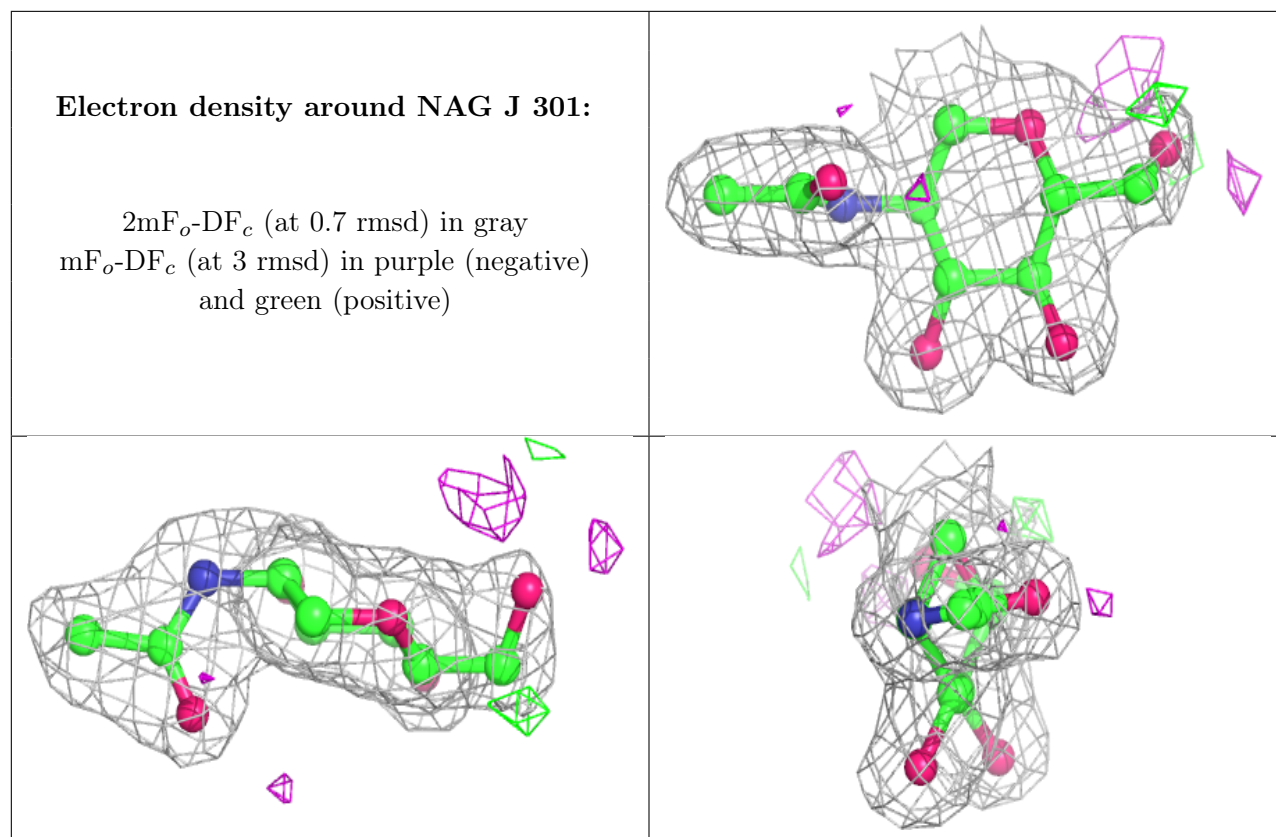


**Electron density around NAG G 302:**

$2mF_o-DF_c$  (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.