



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2024 – 02:49 PM JST

PDB ID : 8HC0  
Title : Crystal structure of the extracellular domains of GPR110  
Authors : Wang, F.F.; Song, G.J.  
Deposited on : 2022-11-01  
Resolution : 2.90 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)

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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>.

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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 : 2.36.2  
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) : 2.36.2

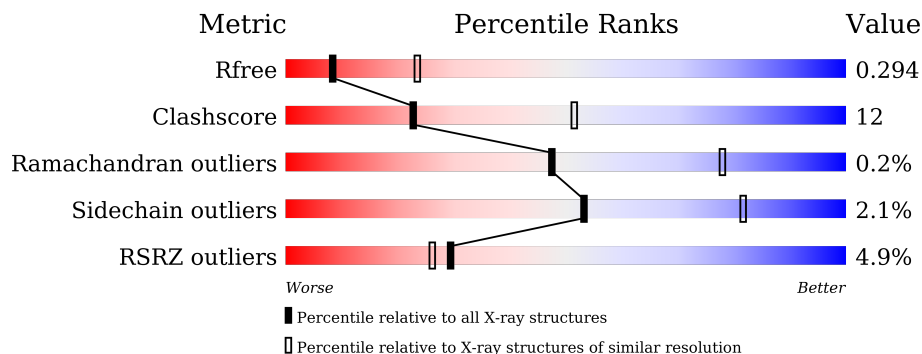
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	360	 5% 72% 27%
2	C	21	 57% 5% 38%
3	B	57	 4% 81% 18%
4	D	6	 17% 67% 17%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	602	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3524 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 Adhesion G-protein coupled receptor F1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	360	2744	1734	459	538	13	0	1	0

- Molecule 2 is a protein called Adhesion G-protein coupled receptor F1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	13	98	66	13	18	1	0	0	0

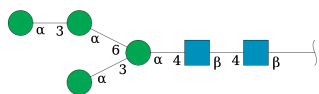
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	581	HIS	-	expression tag	UNP Q5T601
C	582	HIS	-	expression tag	UNP Q5T601
C	583	HIS	-	expression tag	UNP Q5T601
C	584	HIS	-	expression tag	UNP Q5T601
C	585	HIS	-	expression tag	UNP Q5T601
C	586	HIS	-	expression tag	UNP Q5T601
C	587	ALA	-	expression tag	UNP Q5T601

- Molecule 3 is a protein called Adhesion G-protein coupled receptor F1.

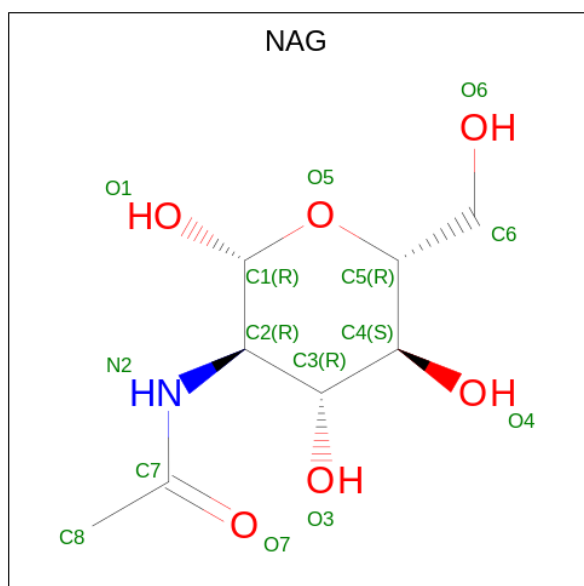
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	B	57	467	298	81	88	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	6	72	40	2	30	0	0	0

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

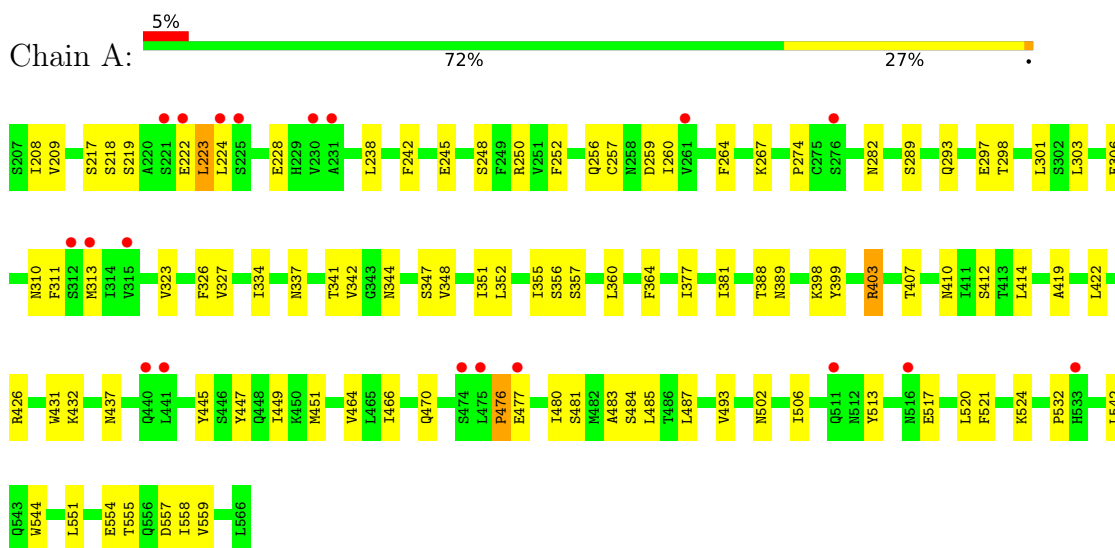
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	36	Total O 36 36	0	0
6	C	1	Total O 1 1	0	0
6	B	8	Total O 8 8	0	0

### 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.

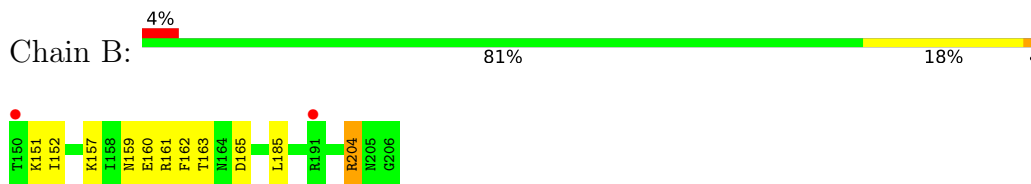
- Molecule 1: Adhesion G-protein coupled receptor F1



- Molecule 2: Adhesion G-protein coupled receptor F1



- Molecule 3: Adhesion G-protein coupled receptor F1



- Molecule 4: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose







## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.82Å 47.99Å 87.02Å 90.00° 127.35° 90.00°	Depositor
Resolution (Å)	19.80 – 2.90 43.80 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.7 (19.80-2.90) 90.2 (43.80-2.90)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.05 (at 2.90Å)	Xtrriage
Refinement program	PHENIX phenix-1.19.2-4158	Depositor
R, $R_{free}$	0.233 , 0.292 0.236 , 0.294	Depositor DCC
$R_{free}$ test set	491 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.8	Xtrriage
Anisotropy	0.279	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 64.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.016 for -h-2*1,-k,l	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3524	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.56% 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: MAN, 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	0.26	0/2797	0.47	1/3811 (0.0%)
2	C	0.28	0/101	0.55	0/137
3	B	0.28	0/475	0.46	0/637
All	All	0.26	0/3373	0.47	1/4585 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	223	LEU	CB-CG-CD2	6.52	122.08	111.00

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	2744	0	2671	72	1
2	C	98	0	98	1	0
3	B	467	0	462	13	0
4	D	72	0	61	1	0
5	A	84	0	78	9	0
5	B	14	0	13	0	0
6	A	36	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	8	0	0	0	0
6	C	1	0	0	0	0
All	All	3524	0	3383	79	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 12.

All (79) 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:310:ASN:O	1:A:313:MET:HG2	1.69	0.93
1:A:310:ASN:HA	1:A:313:MET:CE	2.06	0.85
1:A:301:LEU:HD21	1:A:337:ASN:HD22	1.47	0.80
3:B:163:THR:HG22	3:B:165:ASP:H	1.47	0.77
1:A:310:ASN:HA	1:A:313:MET:HE3	1.66	0.75
1:A:412:SER:HB3	1:A:480:ILE:HG21	1.69	0.72
1:A:310:ASN:HA	1:A:313:MET:HE2	1.73	0.68
1:A:245:GLU:HB2	3:B:159:ASN:HD21	1.59	0.68
1:A:419:ALA:HA	5:A:602:NAG:HN2	1.59	0.67
1:A:470:GLN:HE21	1:A:517:GLU:HB3	1.61	0.66
6:A:702:HOH:O	3:B:159:ASN:ND2	2.29	0.65
1:A:306:GLU:HB3	5:A:605:NAG:H61	1.80	0.64
1:A:432:LYS:HB2	1:A:447:TYR:HE1	1.63	0.63
1:A:348:VAL:HG11	1:A:381:ILE:HG21	1.82	0.61
1:A:360:LEU:HD11	1:A:410:ASN:HB3	1.82	0.60
1:A:419:ALA:HA	5:A:602:NAG:N2	2.16	0.60
1:A:398:LYS:NZ	6:A:705:HOH:O	2.34	0.60
1:A:422:LEU:HB3	1:A:431:TRP:HZ3	1.67	0.60
1:A:451:MET:HE2	1:A:485:LEU:HD12	1.85	0.59
1:A:449:ILE:HD12	1:A:483:ALA:HB3	1.86	0.58
1:A:403:ARG:NH1	5:A:601:NAG:H62	2.20	0.57
1:A:323:VAL:O	1:A:327:VAL:HG23	2.05	0.56
1:A:524:LYS:HD2	1:A:559:VAL:HG23	1.86	0.56
1:A:218:SER:OG	1:A:219:SER:N	2.38	0.56
1:A:344:ASN:O	1:A:348:VAL:HG12	2.05	0.55
1:A:419:ALA:CA	5:A:602:NAG:HN2	2.19	0.55
1:A:464:VAL:HG22	1:A:520:LEU:HD23	1.88	0.55
1:A:521:PHE:HB3	1:A:558:ILE:HD12	1.89	0.55
1:A:256:GLN:HE21	1:A:289:SER:HA	1.71	0.55
1:A:422:LEU:CD1	5:A:602:NAG:H5	2.37	0.54
1:A:250:ARG:HD3	1:A:252:PHE:CD1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:PRO:HA	1:A:282:ASN:HD22	1.75	0.52
1:A:399:TYR:HB3	1:A:542:LEU:HD11	1.90	0.52
1:A:502:ASN:HB3	2:C:573:MET:HG3	1.91	0.52
3:B:151:LYS:O	3:B:152:ILE:HD13	2.09	0.52
1:A:224:LEU:O	1:A:228:GLU:HG3	2.09	0.52
1:A:311:PHE:HB2	1:A:326:PHE:CE1	2.45	0.52
1:A:334:ILE:HD12	1:A:377:ILE:HG23	1.92	0.52
1:A:493:VAL:HG22	1:A:544:TRP:CD1	2.45	0.51
3:B:161:ARG:HD3	3:B:162:PHE:N	2.25	0.51
1:A:445:TYR:HH	1:A:481:SER:HG	1.59	0.51
1:A:297:GLU:OE1	1:A:342:VAL:HB	2.11	0.51
1:A:483:ALA:HB2	1:A:506:ILE:HD13	1.94	0.50
1:A:341:THR:HG23	1:A:344:ASN:H	1.77	0.50
1:A:208:ILE:HD13	3:B:160:GLU:HB2	1.93	0.49
1:A:342:VAL:HG22	1:A:389:ASN:O	2.13	0.48
1:A:238:LEU:HD11	3:B:185:LEU:HD21	1.96	0.47
1:A:347:SER:O	1:A:351:ILE:HG13	2.14	0.47
1:A:326:PHE:CD2	1:A:355:ILE:HD11	2.49	0.47
1:A:303:LEU:HD22	5:A:605:NAG:H62	1.97	0.47
1:A:364:PHE:O	1:A:414:LEU:HD13	2.15	0.47
3:B:151:LYS:HE3	3:B:151:LYS:HB2	1.64	0.47
1:A:298:THR:HG22	1:A:298:THR:O	2.16	0.46
1:A:437:ASN:N	1:A:437:ASN:OD1	2.49	0.46
1:A:403:ARG:HH12	5:A:601:NAG:H62	1.80	0.46
1:A:532:PRO:HG2	1:A:551:LEU:HD22	1.98	0.45
1:A:422:LEU:HD12	5:A:602:NAG:H5	1.99	0.44
1:A:470:GLN:NE2	1:A:517:GLU:HB3	2.27	0.44
1:A:351:ILE:O	1:A:355:ILE:HG13	2.17	0.44
1:A:257:CYS:O	1:A:264:PHE:HA	2.17	0.44
1:A:476:PRO:HB2	1:A:477:GLU:H	1.68	0.44
1:A:555:THR:HG22	1:A:557:ASP:H	1.83	0.43
1:A:248:SER:HB2	3:B:157:LYS:H	1.81	0.43
1:A:259:ASP:OD1	1:A:260:ILE:N	2.52	0.43
1:A:432:LYS:HB2	1:A:447:TYR:CE1	2.49	0.43
1:A:445:TYR:HB3	1:A:466:ILE:HB	2.01	0.43
1:A:356:SER:HB2	1:A:407:THR:HG23	2.00	0.43
1:A:209:VAL:HB	3:B:204:ARG:HB2	2.00	0.42
1:A:218:SER:OG	1:A:222:GLU:HB3	2.20	0.42
1:A:256:GLN:NE2	1:A:289:SER:HA	2.33	0.42
1:A:352:LEU:HB3	1:A:407:THR:HG21	2.02	0.42
6:A:735:HOH:O	4:D:5:MAN:O6	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:GLU:CD	3:B:157:LYS:HE3	2.40	0.42
1:A:445:TYR:OH	1:A:481:SER:OG	2.29	0.42
1:A:256:GLN:NE2	1:A:267:LYS:HD2	2.34	0.41
1:A:303:LEU:HD23	1:A:303:LEU:HA	1.83	0.41
1:A:223:LEU:HD22	3:B:152:ILE:HG12	2.02	0.41
3:B:161:ARG:HD3	3:B:162:PHE:H	1.84	0.41
1:A:484:SER:HB3	1:A:487:LEU:HD12	2.02	0.41

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:388:THR:OG1	1:A:554:GLU:OE1[4_445]	2.18	0.02

## 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	359/360 (100%)	348 (97%)	10 (3%)	1 (0%)	41	71
2	C	11/21 (52%)	10 (91%)	1 (9%)	0	100	100
3	B	55/57 (96%)	54 (98%)	1 (2%)	0	100	100
All	All	425/438 (97%)	412 (97%)	12 (3%)	1 (0%)	47	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	476	PRO

### 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	313/321 (98%)	306 (98%)	7 (2%)	52	81
2	C	13/20 (65%)	13 (100%)	0	100	100
3	B	50/50 (100%)	49 (98%)	1 (2%)	55	82
All	All	376/391 (96%)	368 (98%)	8 (2%)	53	81

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

Mol	Chain	Res	Type
1	A	217	SER
1	A	242	PHE
1	A	293	GLN
1	A	357	SER
1	A	403	ARG
1	A	426	ARG
1	A	513	TYR
3	B	204	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
1	A	470	GLN
1	A	531	GLN
3	B	159	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

6 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	D	1	4,1	14,14,15	0.66	1 (7%)	17,19,21	0.65	0
4	NAG	D	2	4	14,14,15	0.24	0	17,19,21	0.35	0
4	MAN	D	3	4	11,11,12	0.79	0	15,15,17	1.04	1 (6%)
4	MAN	D	4	4	11,11,12	1.05	1 (9%)	15,15,17	1.04	1 (6%)
4	MAN	D	5	4	11,11,12	0.81	1 (9%)	15,15,17	1.24	2 (13%)
4	MAN	D	6	4	11,11,12	0.91	0	15,15,17	0.96	1 (6%)

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	D	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	D	2	4	-	1/6/23/26	0/1/1/1
4	MAN	D	3	4	-	0/2/19/22	1/1/1/1
4	MAN	D	4	4	-	2/2/19/22	0/1/1/1
4	MAN	D	5	4	-	0/2/19/22	0/1/1/1
4	MAN	D	6	4	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5	MAN	C1-C2	2.35	1.57	1.52
4	D	4	MAN	C4-C3	2.11	1.57	1.52
4	D	1	NAG	C1-C2	2.09	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	5	MAN	C1-O5-C5	2.59	115.70	112.19
4	D	3	MAN	C1-O5-C5	2.47	115.55	112.19
4	D	4	MAN	C1-O5-C5	2.42	115.47	112.19
4	D	5	MAN	O2-C2-C3	-2.25	105.62	110.14
4	D	6	MAN	O2-C2-C3	-2.12	105.88	110.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	4	MAN	C4-C5-C6-O6
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	4	MAN	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

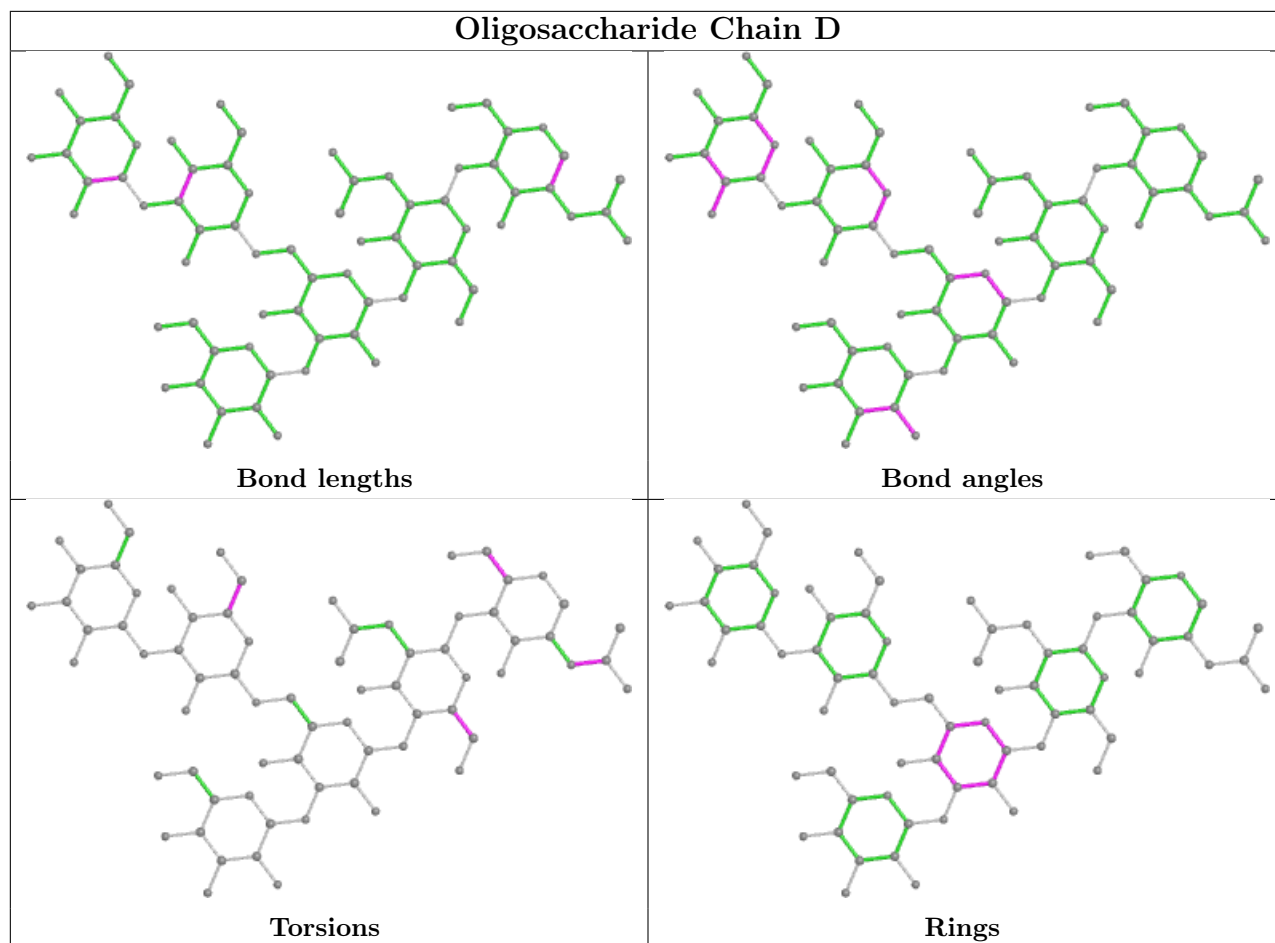
Mol	Chain	Res	Type	Atoms
4	D	3	MAN	C1-C2-C3-C4-C5-O5

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	5	MAN	1	0

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





## 5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	NAG	A	606	1	14,14,15	0.28	0	17,19,21	0.53	0
5	NAG	A	601	1	14,14,15	0.50	0	17,19,21	1.21	4 (23%)
5	NAG	A	605	1	14,14,15	0.42	0	17,19,21	0.46	0
5	NAG	A	602	1	14,14,15	0.39	0	17,19,21	0.80	1 (5%)
5	NAG	A	603	1	14,14,15	1.00	1 (7%)	17,19,21	1.06	1 (5%)
5	NAG	A	604	1	14,14,15	0.22	0	17,19,21	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	B	301	3	14,14,15	0.24	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
5	NAG	A	606	1	-	2/6/23/26	0/1/1/1
5	NAG	A	601	1	-	2/6/23/26	0/1/1/1
5	NAG	A	605	1	-	3/6/23/26	0/1/1/1
5	NAG	A	602	1	-	4/6/23/26	0/1/1/1
5	NAG	A	603	1	-	3/6/23/26	0/1/1/1
5	NAG	A	604	1	-	1/6/23/26	0/1/1/1
5	NAG	B	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)
5	A	603	NAG	O5-C1	3.23	1.48	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	603	NAG	C1-O5-C5	4.16	117.82	112.19
5	A	602	NAG	O5-C1-C2	-3.03	106.50	111.29
5	A	601	NAG	C1-O5-C5	2.38	115.41	112.19
5	A	601	NAG	C1-C2-N2	2.14	114.15	110.49
5	A	601	NAG	C3-C4-C5	2.07	113.93	110.24
5	A	601	NAG	C2-N2-C7	2.00	125.75	122.90

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	602	NAG	C8-C7-N2-C2
5	A	602	NAG	O7-C7-N2-C2
5	A	605	NAG	C8-C7-N2-C2
5	A	605	NAG	O7-C7-N2-C2
5	A	606	NAG	O5-C5-C6-O6

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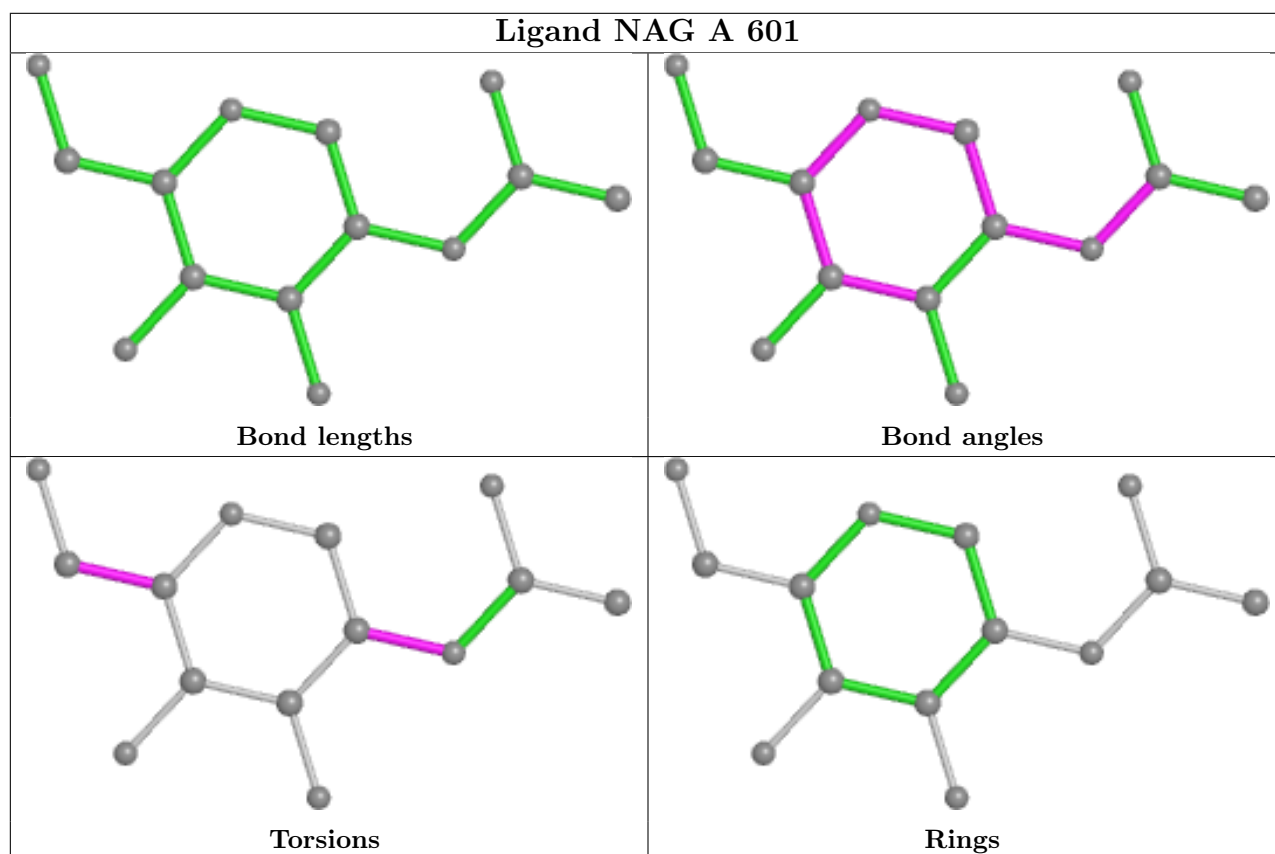
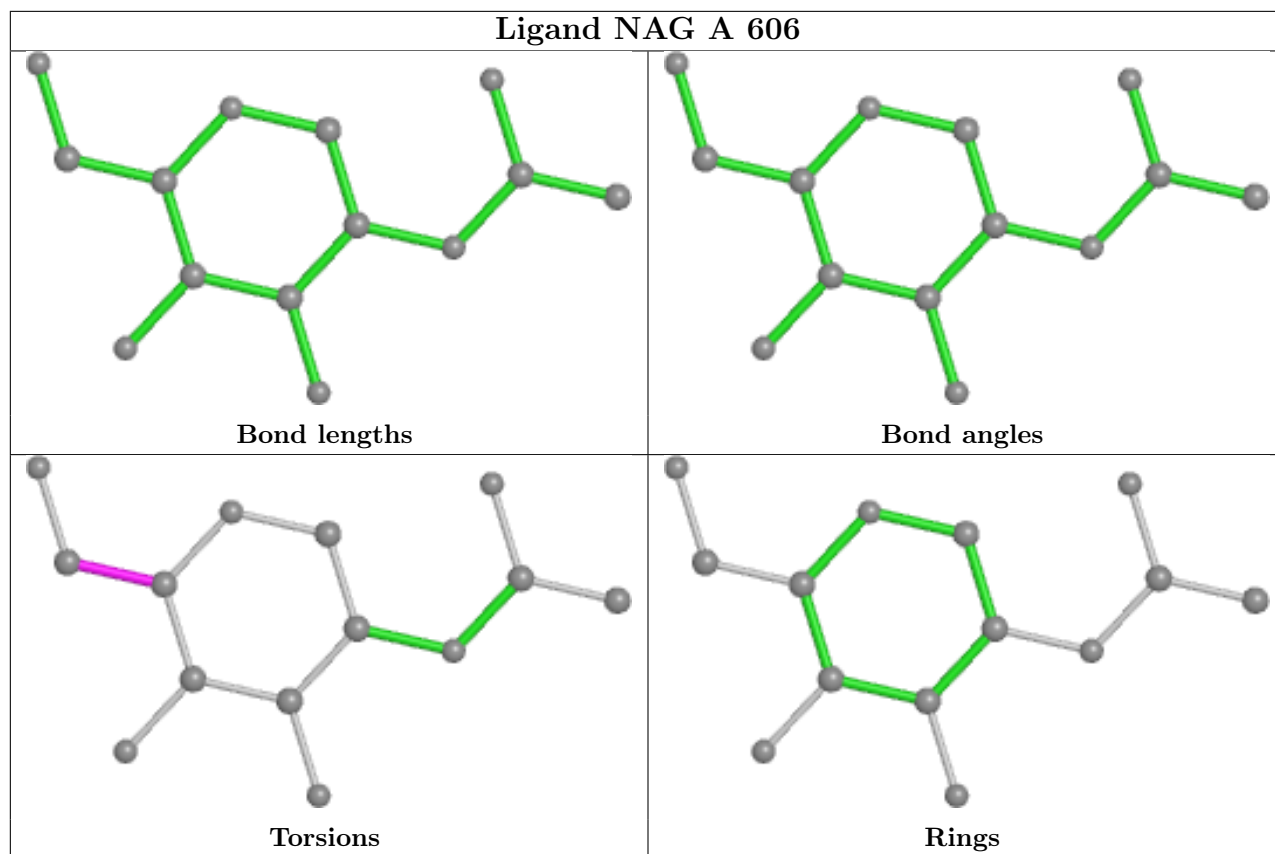
Mol	Chain	Res	Type	Atoms
5	A	606	NAG	C4-C5-C6-O6
5	B	301	NAG	O5-C5-C6-O6
5	A	603	NAG	O5-C5-C6-O6
5	A	603	NAG	C4-C5-C6-O6
5	A	602	NAG	C4-C5-C6-O6
5	B	301	NAG	C4-C5-C6-O6
5	A	601	NAG	C3-C2-N2-C7
5	A	601	NAG	O5-C5-C6-O6
5	A	604	NAG	O5-C5-C6-O6
5	A	605	NAG	O5-C5-C6-O6
5	A	602	NAG	O5-C5-C6-O6
5	A	603	NAG	C3-C2-N2-C7

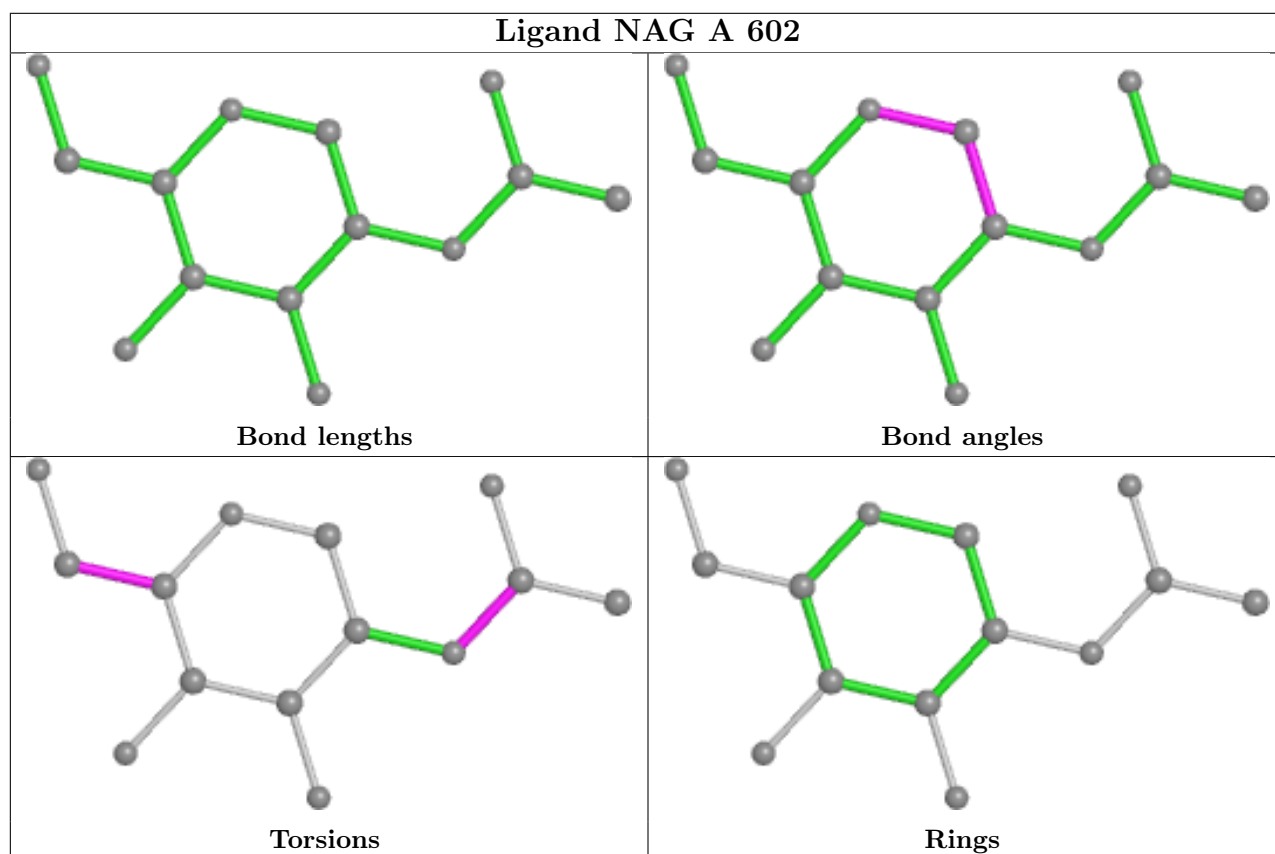
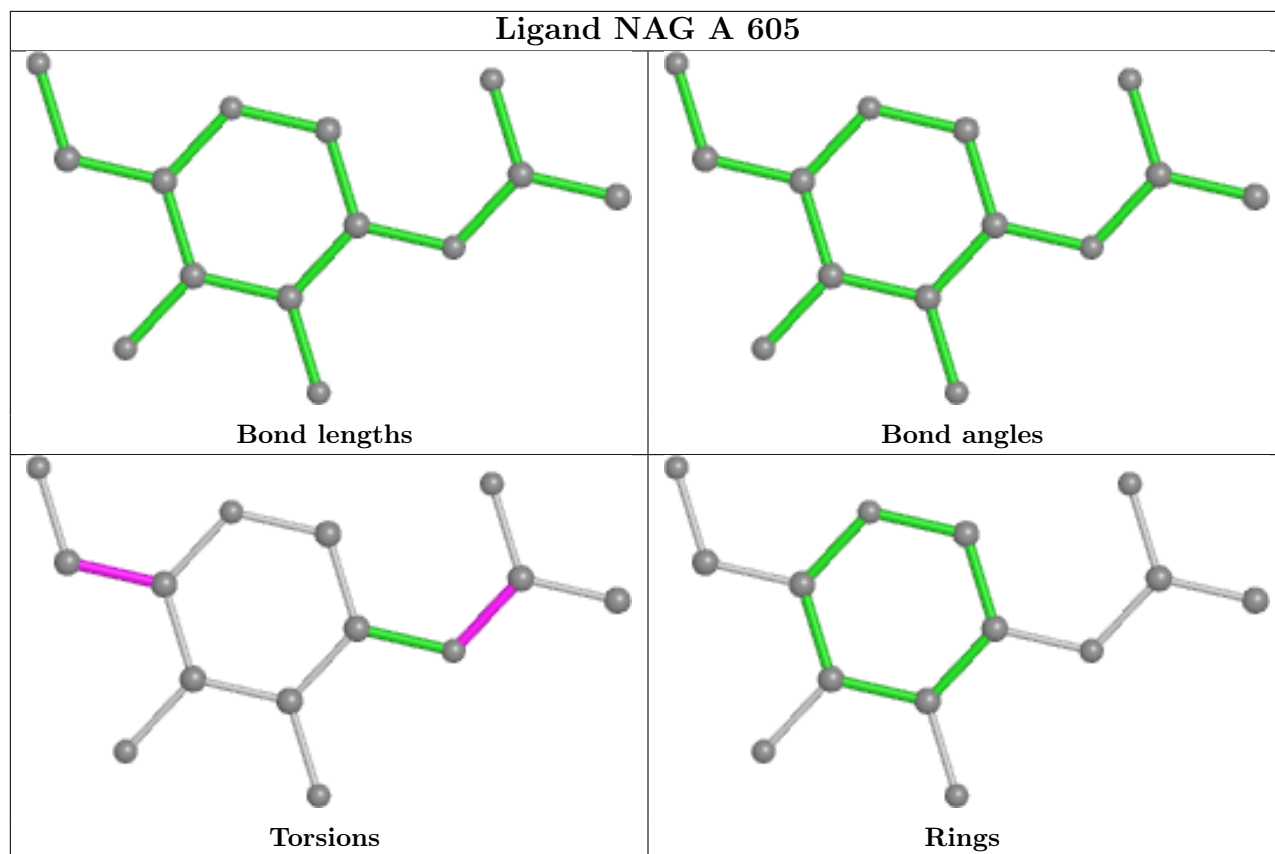
There are no ring outliers.

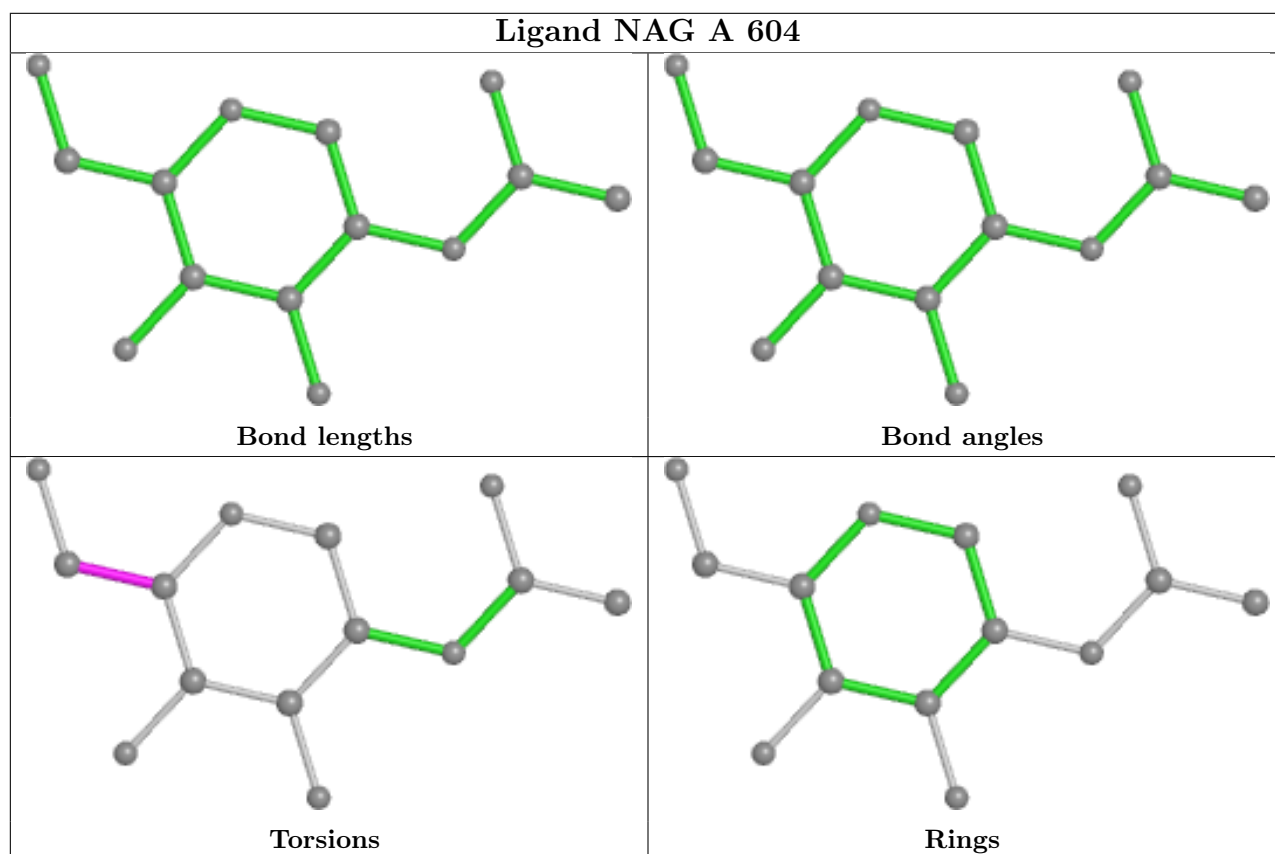
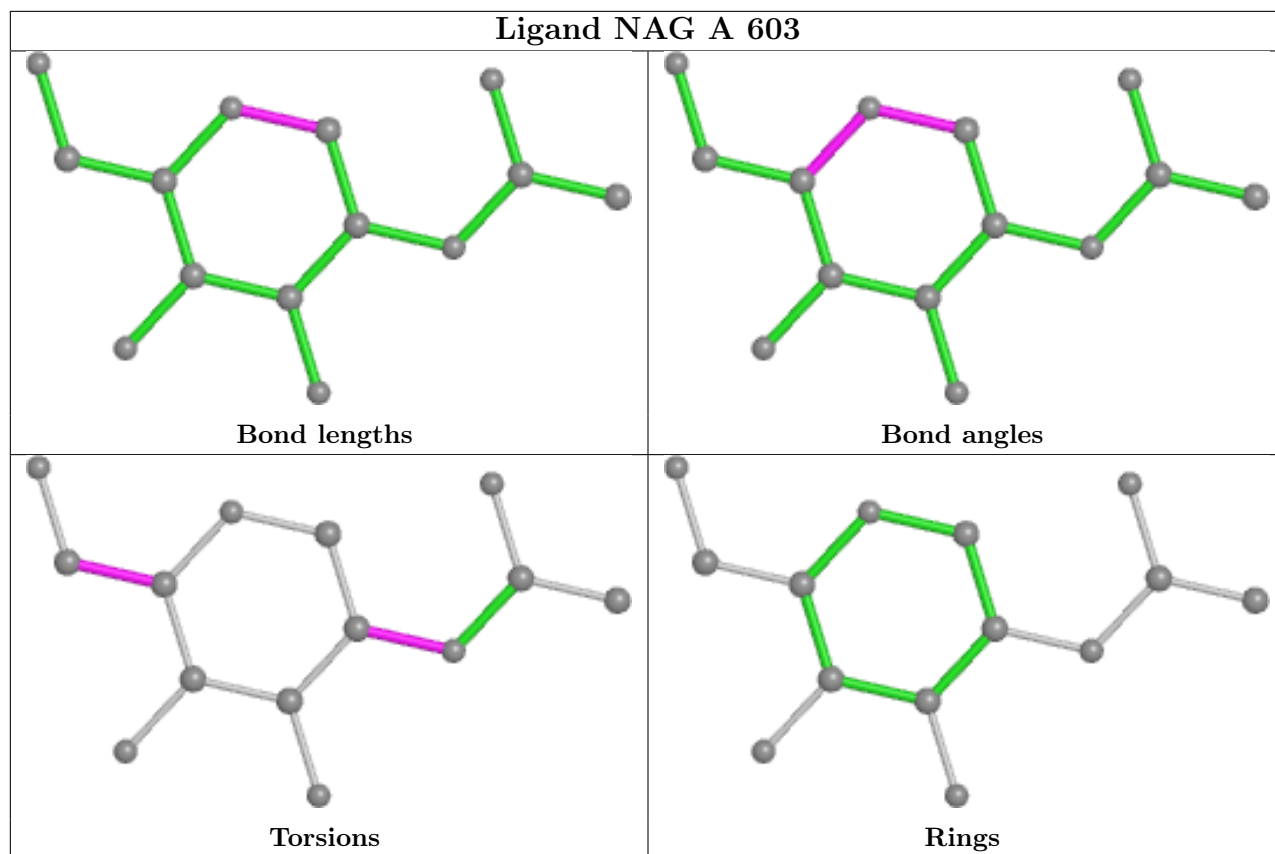
3 monomers are involved in 9 short contacts:

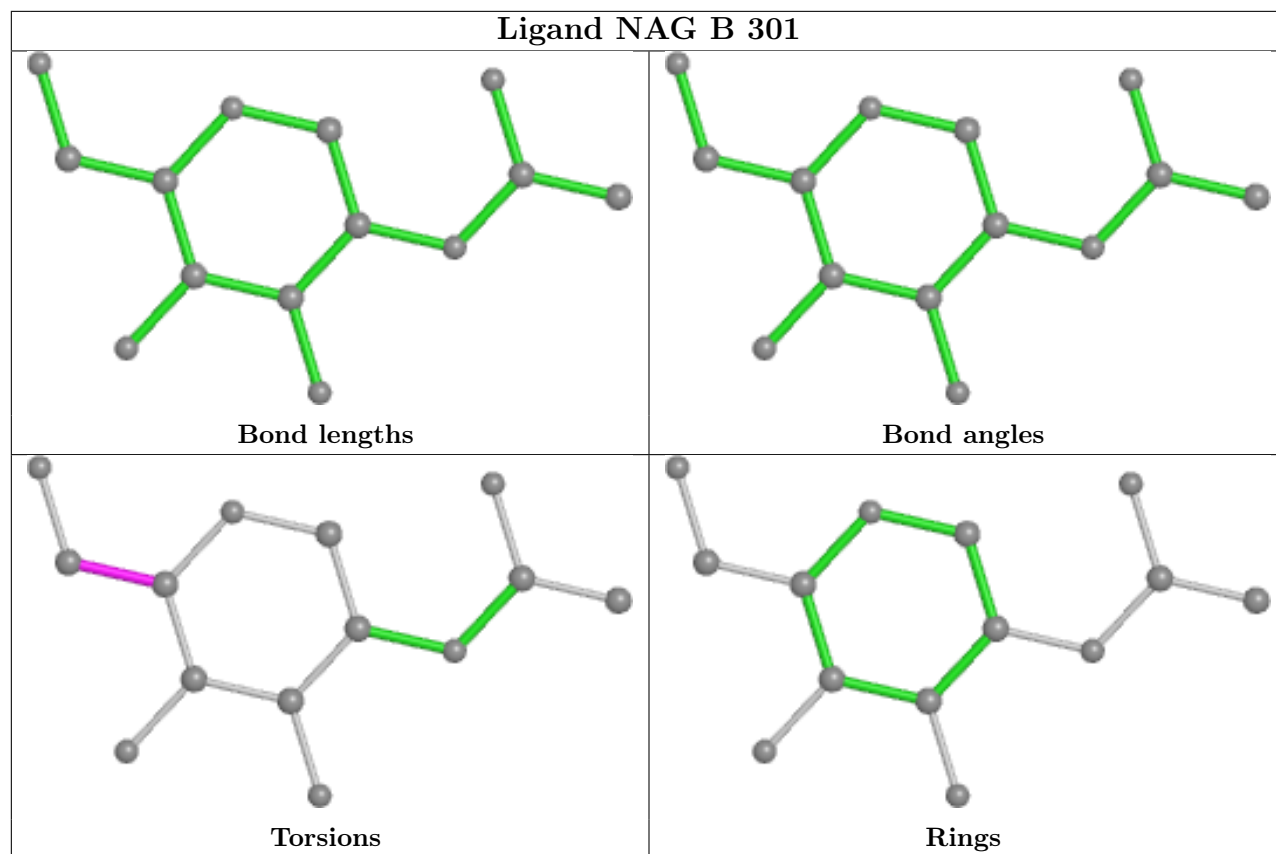
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	NAG	2	0
5	A	605	NAG	2	0
5	A	602	NAG	5	0

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.









## 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	360/360 (100%)	0.43	19 (5%) 26 22	44, 65, 111, 159	0
2	C	13/21 (61%)	0.21	0 100 100	49, 57, 71, 73	0
3	B	57/57 (100%)	0.36	2 (3%) 44 38	53, 71, 105, 131	0
All	All	430/438 (98%)	0.41	21 (4%) 29 26	44, 66, 111, 159	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	440	GLN	4.6
1	A	441	LEU	4.4
1	A	313	MET	3.7
1	A	474	SER	3.2
1	A	231	ALA	3.2
3	B	150	THR	3.2
1	A	315	VAL	3.0
1	A	261	VAL	2.9
1	A	475	LEU	2.8
1	A	516	ASN	2.8
1	A	221	SER	2.8
1	A	533[A]	HIS	2.4
1	A	225	SER	2.4
1	A	477	GLU	2.3
1	A	511	GLN	2.2
1	A	224	LEU	2.2
1	A	312	SER	2.1
1	A	276	SER	2.1
3	B	191	ARG	2.1
1	A	230	VAL	2.0
1	A	222	GLU	2.0



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

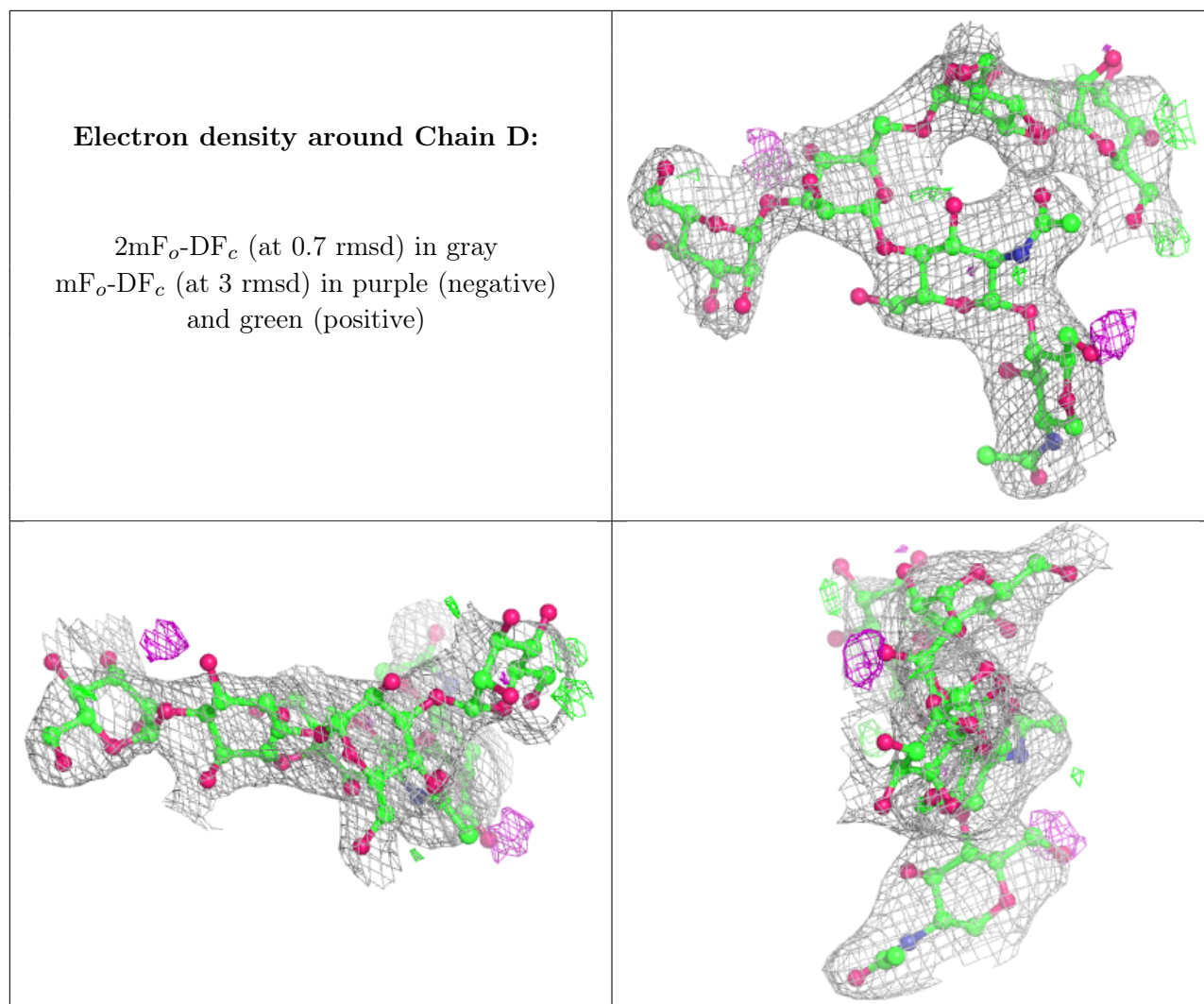
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	MAN	D	6	11/12	0.69	0.30	77,86,110,111	0
4	MAN	D	5	11/12	0.77	0.28	61,78,92,99	0
4	NAG	D	2	14/15	0.87	0.22	57,71,81,83	0
4	MAN	D	3	11/12	0.90	0.22	60,72,82,88	0
4	MAN	D	4	11/12	0.93	0.17	56,64,74,90	0
4	NAG	D	1	14/15	0.94	0.21	50,61,72,90	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



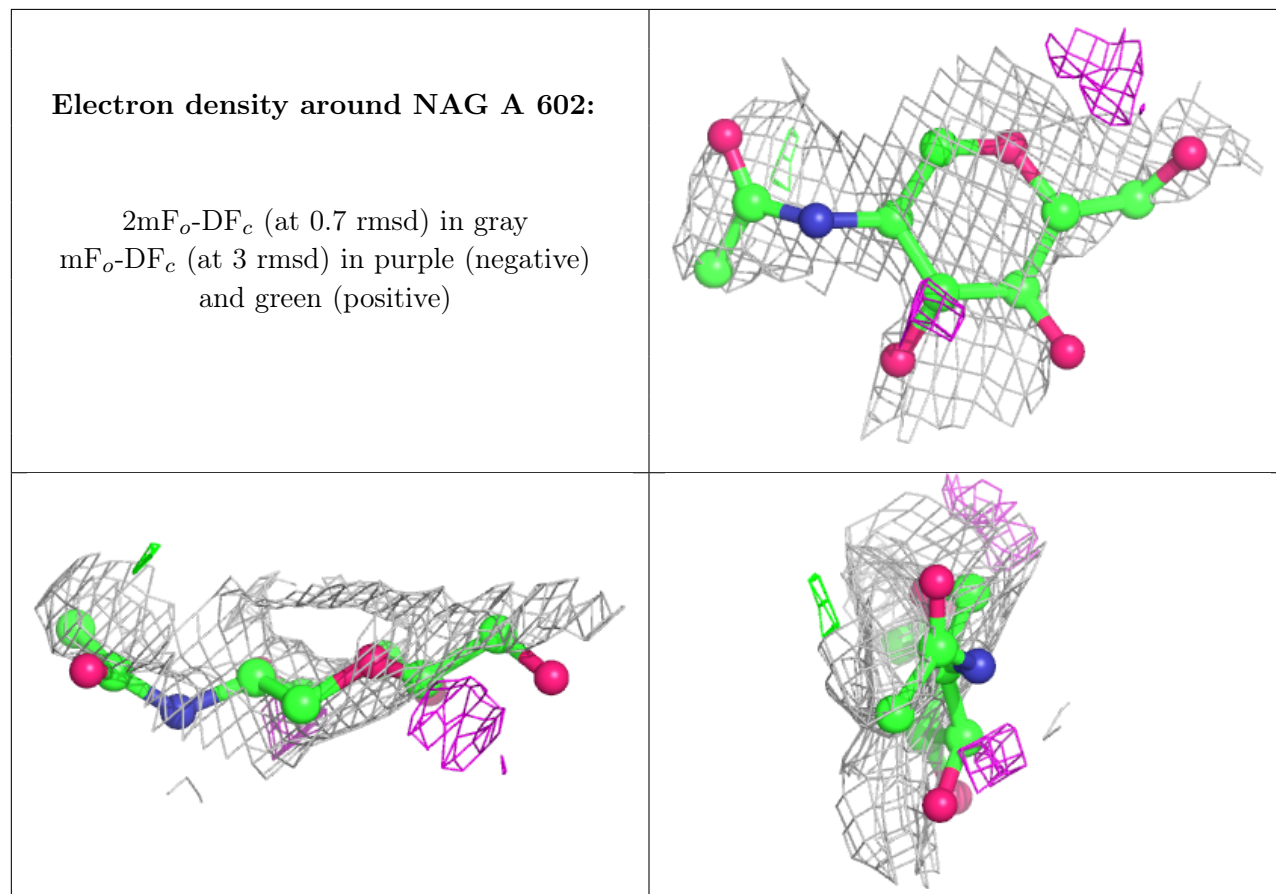
## 6.4 Ligands [i](#)

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
5	NAG	A	602	14/15	0.35	0.55	105,113,127,130	0
5	NAG	A	605	14/15	0.69	0.37	82,98,107,117	0
5	NAG	A	601	14/15	0.74	0.22	83,92,107,114	0
5	NAG	B	301	14/15	0.75	0.34	112,128,137,145	0
5	NAG	A	603	14/15	0.77	0.31	68,91,102,103	0
5	NAG	A	606	14/15	0.86	0.25	70,84,96,103	0
5	NAG	A	604	14/15	0.90	0.20	52,68,90,92	0

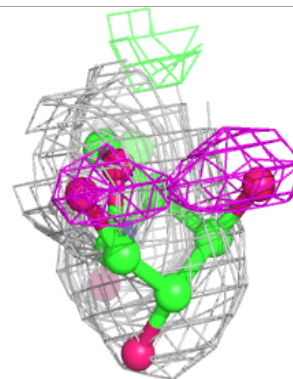
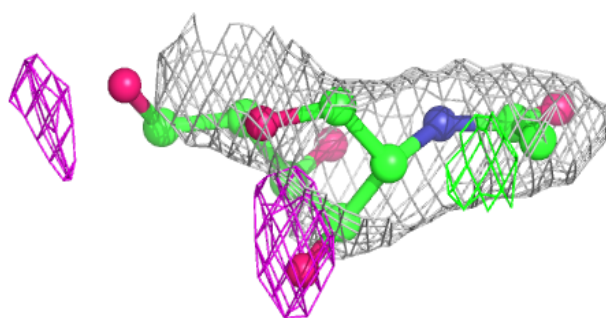
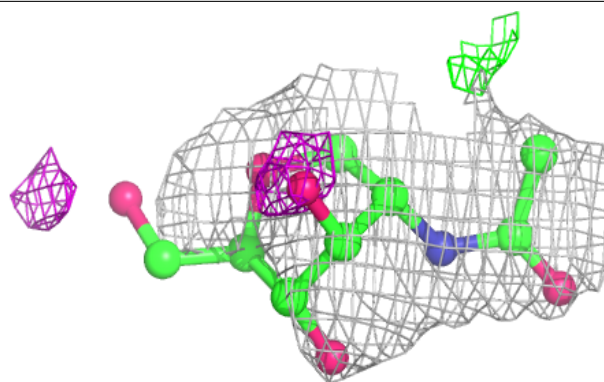
The following is a graphical depiction of the model fit to experimental electron density of all

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.

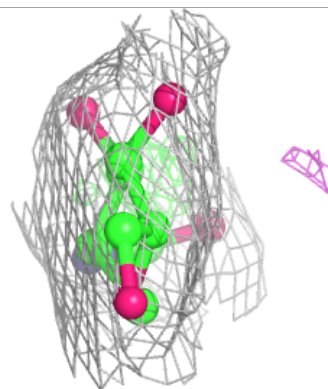
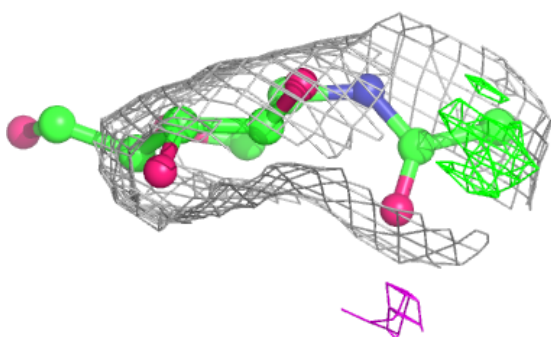
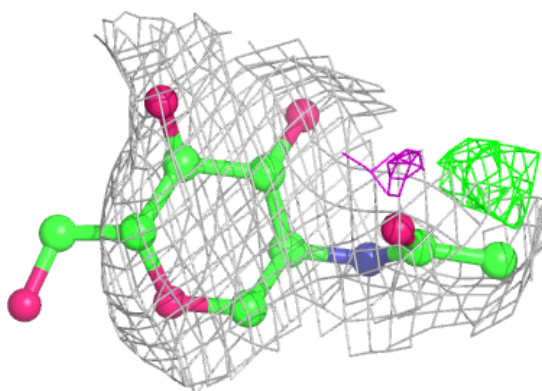


**Electron density around NAG A 605:**

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

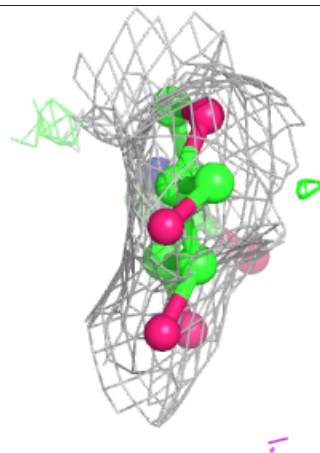
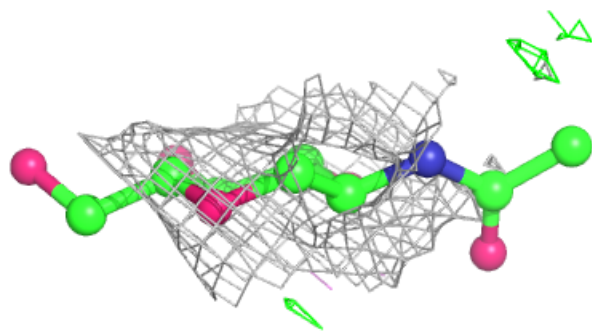
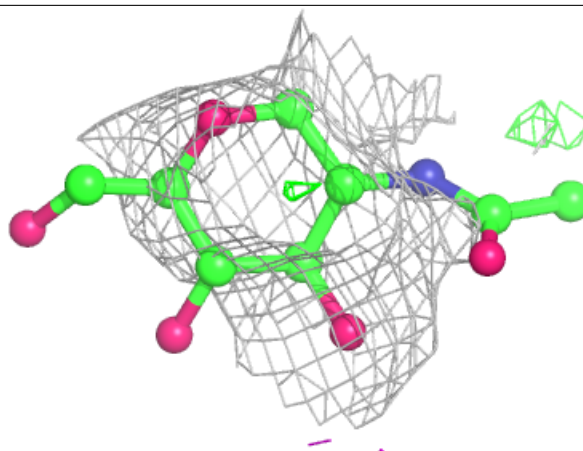
**Electron density around NAG A 601:**

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



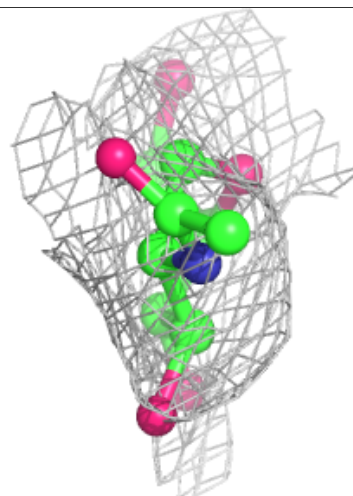
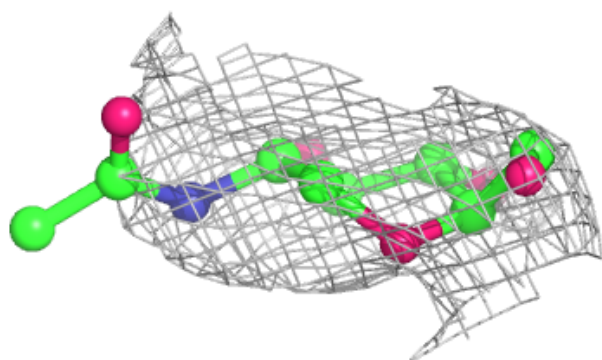
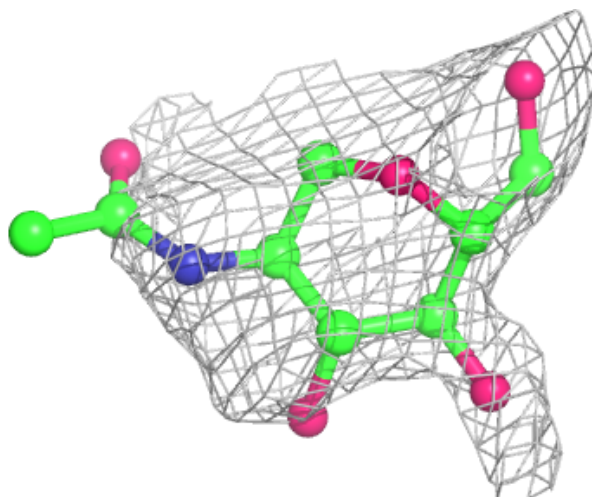
**Electron density around NAG B 301:**

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



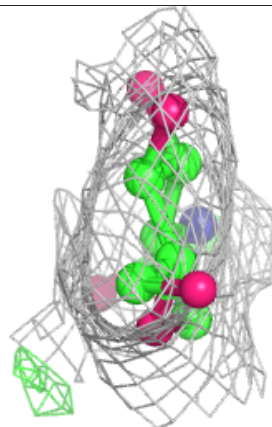
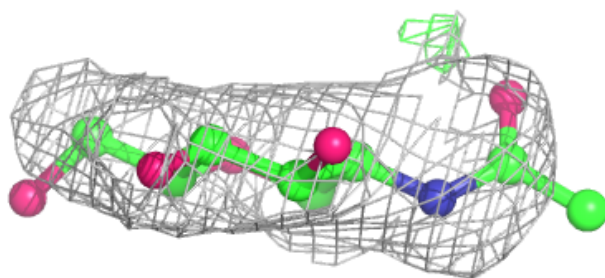
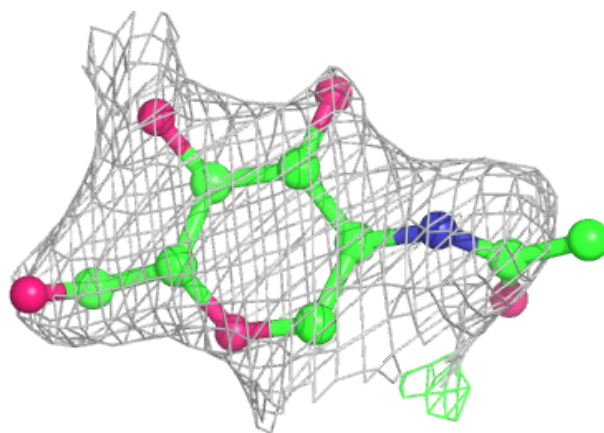
**Electron density around NAG A 603:**

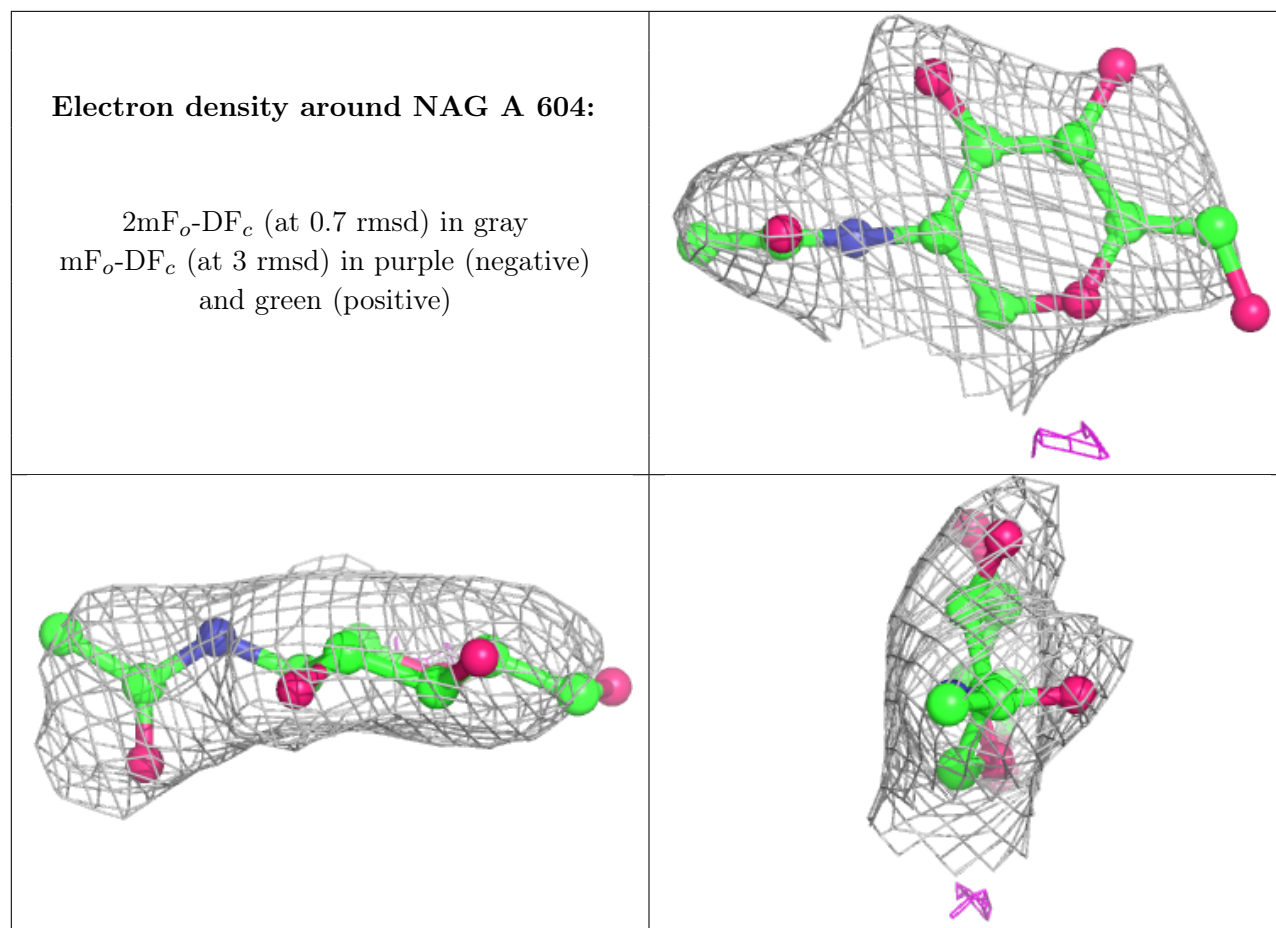
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around NAG A 606:**

$2mF_o-DF_c$  (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.