



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 02:26 PM BST

PDB ID : 6YJS  
Title : Crystal structure of MGAT5 (alpha-1,6-mannosylglycoprotein 6-beta-N-acetylglucosaminyltransferase V) luminal domain with a Lys329-Ile345 loop truncation, in complex with biantennary pentasaccharide M592  
Authors : Wu, L.; Darby, J.F.; Gilio, A.K.; Davies, G.J.  
Deposited on : 2020-04-04  
Resolution : 1.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.13.1  
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

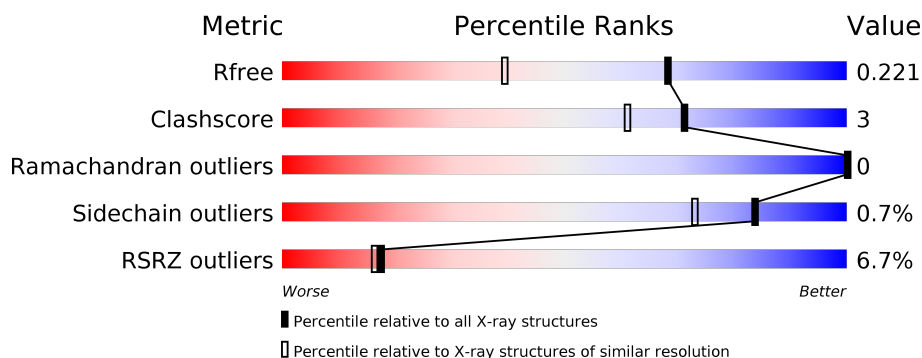
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	AAA	515	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>9%</div> </div> </div>
1	BBB	515	<div> <div>8%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>6%</div> </div> </div>
2	A	5	<div> <div>20%</div> <div>80%</div> </div>
2	B	5	<div> <div>20%</div> <div>60%</div> <div>20%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	AAA	812	-	-	X	-
5	SO4	BBB	818	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16416 atoms, of which 7961 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 Alpha-1,6-mannosylglycoprotein 6-beta-N-acetylglucosaminyl transferase A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	470	Total	C	H	N	O	S	190	1	0
			7613	2453	3806	654	675	25			
1	BBB	486	Total	C	H	N	O	S	197	0	0
			7879	2534	3943	678	698	26			

There are 32 discrepancies between the modelled and reference sequences:

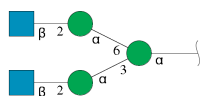
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	?	-	LYS	deletion	UNP Q09328
AAA	?	-	LYS	deletion	UNP Q09328
AAA	?	-	VAL	deletion	UNP Q09328
AAA	?	-	VAL	deletion	UNP Q09328
AAA	?	-	GLY	deletion	UNP Q09328
AAA	?	-	ASN	deletion	UNP Q09328
AAA	?	-	ARG	deletion	UNP Q09328
AAA	?	-	SER	deletion	UNP Q09328
AAA	?	-	GLY	deletion	UNP Q09328
AAA	?	-	CYS	deletion	UNP Q09328
AAA	?	-	PRO	deletion	UNP Q09328
AAA	?	-	THR	deletion	UNP Q09328
AAA	?	-	VAL	deletion	UNP Q09328
AAA	330	GLY	ASP	conflict	UNP Q09328
AAA	331	GLY	ARG	conflict	UNP Q09328
AAA	332	GLY	ILE	conflict	UNP Q09328
BBB	?	-	LYS	deletion	UNP Q09328
BBB	?	-	LYS	deletion	UNP Q09328
BBB	?	-	VAL	deletion	UNP Q09328
BBB	?	-	VAL	deletion	UNP Q09328
BBB	?	-	GLY	deletion	UNP Q09328
BBB	?	-	ASN	deletion	UNP Q09328
BBB	?	-	ARG	deletion	UNP Q09328
BBB	?	-	SER	deletion	UNP Q09328

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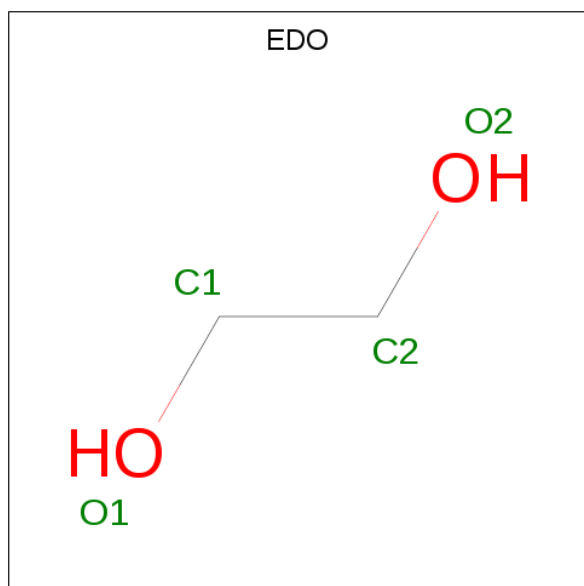
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	?	-	GLY	deletion	UNP Q09328
BBB	?	-	CYS	deletion	UNP Q09328
BBB	?	-	PRO	deletion	UNP Q09328
BBB	?	-	THR	deletion	UNP Q09328
BBB	?	-	VAL	deletion	UNP Q09328
BBB	330	GLY	ASP	conflict	UNP Q09328
BBB	331	GLY	ARG	conflict	UNP Q09328
BBB	332	GLY	ILE	conflict	UNP Q09328

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



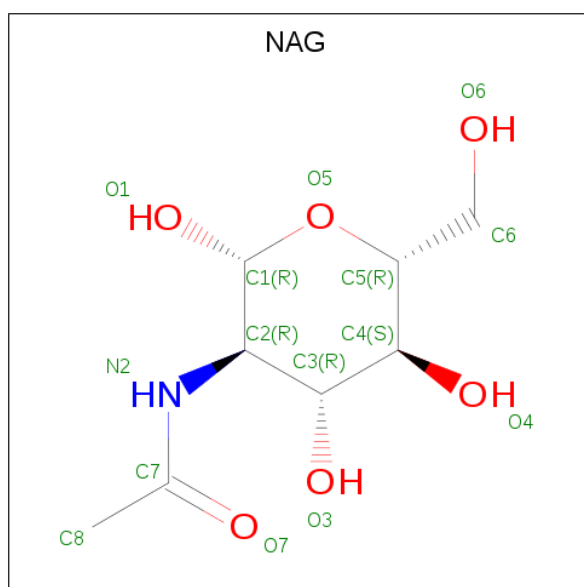
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	5	Total	C	H	N	O	15	0	0
			121	34	59	2	26			
2	B	5	Total	C	H	N	O	15	0	0
			121	34	59	2	26			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



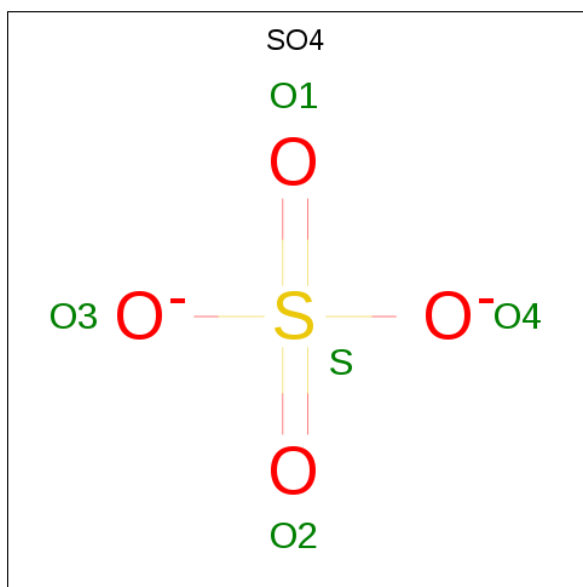
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
3	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
3	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
3	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
3	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
3	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
3	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
3	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
3	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
3	BBB	1	Total	C	H	O	1	0
			10	2	6	2		

- 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 author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	AAA	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
4	BBB	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	O	S	0	0
			5	4	1		
5	AAA	1	Total	O	S	0	0
			5	4	1		
5	AAA	1	Total	O	S	0	0
			5	4	1		
5	AAA	1	Total	O	S	0	0
			5	4	1		
5	BBB	1	Total	O	S	0	0
			5	4	1		
5	BBB	1	Total	O	S	0	0
			5	4	1		
5	BBB	1	Total	O	S	0	0
			5	4	1		
5	BBB	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

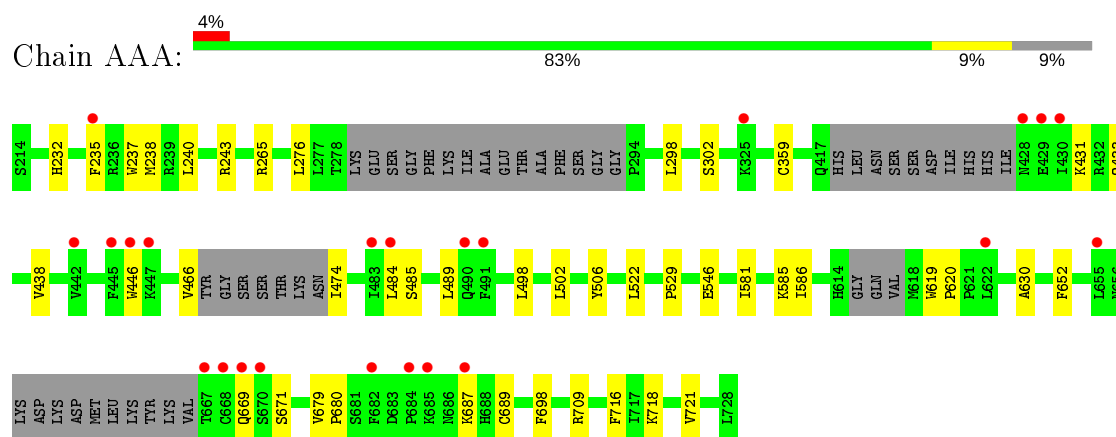
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	224	Total 224	O 224	0	0
6	BBB	242	Total 242	O 242	0	0



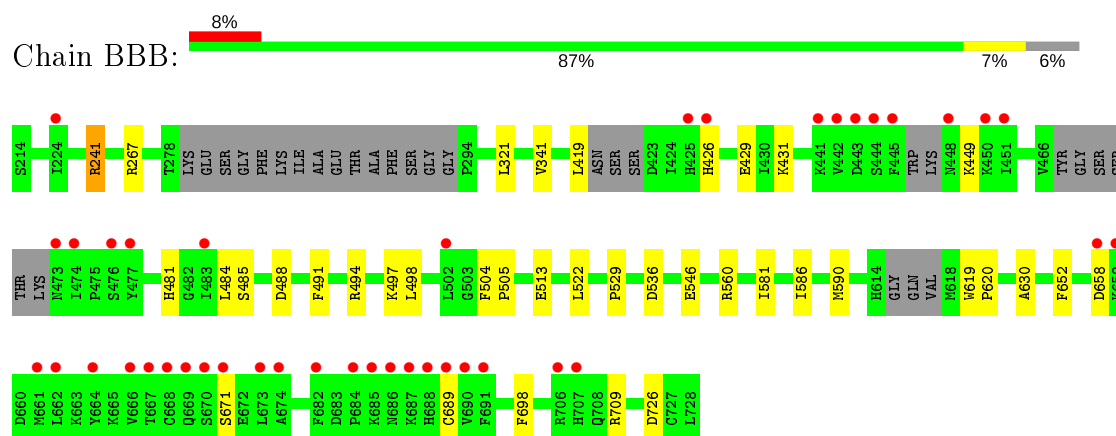
### 3 Residue-property plots [i](#)

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: Alpha-1,6-mannosylglycoprotein 6-beta-N-acetylglucosaminyltransferase A



- Molecule 1: Alpha-1,6-mannosylglycoprotein 6-beta-N-acetylglucosaminyltransferase A



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



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

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.28Å 67.37Å 91.05Å 108.81° 92.20° 106.72°	Depositor
Resolution (Å)	42.52 – 1.60 42.52 – 1.60	Depositor EDS
% Data completeness (in resolution range)	96.2 (42.52-1.60) 96.2 (42.52-1.60)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.184 , 0.214 0.193 , 0.221	Depositor DCC
$R_{free}$ test set	3770 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.4	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 58.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	16416	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.61% 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: SO4, NAG, EDO, MAN

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	AAA	0.69	0/3907	0.82	1/5276 (0.0%)
1	BBB	0.69	0/4035	0.85	1/5446 (0.0%)
All	All	0.69	0/7942	0.84	2/10722 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	241	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	AAA	265	ARG	NE-CZ-NH1	5.16	122.88	120.30

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	AAA	3807	3806	3782	27	1
1	BBB	3936	3943	3915	27	1
2	A	62	59	54	0	0
2	B	62	59	54	1	0
3	AAA	12	18	18	4	0
3	BBB	32	48	48	4	1
4	AAA	14	14	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	BBB	14	14	13	0	0
5	AAA	25	0	0	2	1
5	BBB	25	0	0	2	0
6	AAA	224	0	0	1	0
6	BBB	242	0	0	5	0
All	All	8455	7961	7897	55	2

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 3.

The worst 5 of 55 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:BBB:497:LYS:HE3	1:BBB:586:ILE:CD1	2.13	0.78
1:BBB:449:LYS:HA	6:BBB:1086:HOH:O	1.86	0.75
1:AAA:506:TYR:HH	3:AAA:807:EDO:HO2	1.34	0.73
1:BBB:513:GLU:OE2	6:BBB:901:HOH:O	2.09	0.71
1:AAA:466:VAL:HG11	1:AAA:474:ILE:CD1	2.24	0.67

All (2) 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:AAA:359:CYS:H	3:BBB:809:EDO:HO1[1_556]	1.29	0.31
1:BBB:560:ARG:H	5:AAA:813:SO4:O2[1_565]	1.54	0.06

## 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	AAA	459/515 (89%)	449 (98%)	10 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BBB	474/515 (92%)	461 (97%)	13 (3%)	0	100	100
All	All	933/1030 (91%)	910 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	AAA	419/456 (92%)	417 (100%)	2 (0%)	88	80
1	BBB	434/456 (95%)	430 (99%)	4 (1%)	78	65
All	All	853/912 (94%)	847 (99%)	6 (1%)	84	73

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	431	LYS
1	BBB	658	ASP
1	BBB	536	ASP
1	AAA	431	LYS
1	BBB	590	MET

Some 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 ⓘ

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

## 5.5 Carbohydrates ⓘ

10 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$
2	MAN	A	1	2	12,12,12	0.90	1 (8%)	17,17,17	1.00	0
2	MAN	A	2	2	11,11,12	0.55	0	15,15,17	0.76	0
2	NAG	A	3	2	14,14,15	0.44	0	17,19,21	1.57	4 (23%)
2	MAN	A	4	2	11,11,12	0.83	0	15,15,17	2.20	7 (46%)
2	NAG	A	5	2	14,14,15	0.92	1 (7%)	17,19,21	1.49	3 (17%)
2	MAN	B	1	2	12,12,12	0.85	0	17,17,17	1.64	5 (29%)
2	MAN	B	2	2	11,11,12	0.54	0	15,15,17	1.32	2 (13%)
2	NAG	B	3	2	14,14,15	0.65	0	17,19,21	1.56	4 (23%)
2	MAN	B	4	2	11,11,12	0.42	0	15,15,17	1.26	1 (6%)
2	NAG	B	5	2	14,14,15	0.79	0	17,19,21	0.89	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
2	MAN	A	1	2	-	0/2/22/22	0/1/1/1
2	MAN	A	2	2	-	0/2/19/22	0/1/1/1
2	NAG	A	3	2	-	2/6/23/26	0/1/1/1
2	MAN	A	4	2	-	1/2/19/22	0/1/1/1
2	NAG	A	5	2	-	2/6/23/26	0/1/1/1
2	MAN	B	1	2	-	0/2/22/22	0/1/1/1
2	MAN	B	2	2	-	0/2/19/22	0/1/1/1
2	NAG	B	3	2	-	0/6/23/26	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	NAG	B	5	2	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5	NAG	C1-C2	2.17	1.55	1.52
2	A	1	MAN	O1-C1	2.16	1.46	1.39

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4	MAN	O4-C4-C5	3.95	119.11	109.30
2	A	4	MAN	C1-C2-C3	3.53	114.00	109.67
2	B	1	MAN	O3-C3-C4	-3.25	102.83	110.35
2	A	3	NAG	O5-C5-C6	3.23	112.27	107.20
2	A	4	MAN	O2-C2-C3	-3.21	103.70	110.14

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3	NAG	C4-C5-C6-O6
2	A	3	NAG	O5-C5-C6-O6
2	A	4	MAN	O5-C5-C6-O6
2	A	5	NAG	C3-C2-N2-C7
2	B	5	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3	NAG	1	0

## 5.6 Ligand geometry [i](#)

23 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	EDO	AAA	806	-	3,3,3	0.24	0	2,2,2	0.49	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	BBB	817	-	4,4,4	0.34	0	6,6,6	0.21	0
5	SO4	BBB	818	-	4,4,4	0.44	0	6,6,6	0.22	0
3	EDO	BBB	814	-	3,3,3	0.07	0	2,2,2	0.18	0
3	EDO	BBB	808	-	3,3,3	0.33	0	2,2,2	0.50	0
5	SO4	BBB	816	-	4,4,4	0.37	0	6,6,6	0.23	0
5	SO4	BBB	815	-	4,4,4	0.40	0	6,6,6	0.32	0
4	NAG	BBB	810	1	14,14,15	0.97	1 (7%)	17,19,21	1.79	6 (35%)
3	EDO	BBB	812	-	3,3,3	0.13	0	2,2,2	0.28	0
5	SO4	BBB	819	-	4,4,4	0.37	0	6,6,6	0.11	0
3	EDO	BBB	809	-	3,3,3	0.06	0	2,2,2	0.12	0
3	EDO	BBB	813	-	3,3,3	0.28	0	2,2,2	0.40	0
3	EDO	BBB	806	-	3,3,3	0.12	0	2,2,2	0.17	0
4	NAG	AAA	809	1	14,14,15	0.81	0	17,19,21	1.39	1 (5%)
3	EDO	BBB	807	-	3,3,3	0.30	0	2,2,2	0.58	0
3	EDO	BBB	811	-	3,3,3	0.32	0	2,2,2	0.69	0
3	EDO	AAA	808	-	3,3,3	0.22	0	2,2,2	0.29	0
5	SO4	AAA	810	-	4,4,4	0.40	0	6,6,6	0.09	0
3	EDO	AAA	807	-	3,3,3	0.19	0	2,2,2	0.07	0
5	SO4	AAA	813	-	4,4,4	0.50	0	6,6,6	0.15	0
5	SO4	AAA	814	-	4,4,4	0.40	0	6,6,6	0.23	0
5	SO4	AAA	812	-	4,4,4	0.38	0	6,6,6	0.15	0
5	SO4	AAA	811	-	4,4,4	0.41	0	6,6,6	0.14	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	EDO	AAA	806	-	-	0/1/1/1	-
3	EDO	BBB	814	-	-	1/1/1/1	-
3	EDO	BBB	812	-	-	1/1/1/1	-
3	EDO	AAA	807	-	-	0/1/1/1	-
3	EDO	BBB	809	-	-	1/1/1/1	-
3	EDO	BBB	813	-	-	1/1/1/1	-
3	EDO	BBB	807	-	-	1/1/1/1	-
3	EDO	BBB	806	-	-	0/1/1/1	-
3	EDO	BBB	808	-	-	0/1/1/1	-
3	EDO	BBB	811	-	-	1/1/1/1	-
3	EDO	AAA	808	-	-	0/1/1/1	-
4	NAG	BBB	810	1	-	2/6/23/26	0/1/1/1
4	NAG	AAA	809	1	-	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	BBB	810	NAG	C3-C2	2.01	1.56	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AAA	809	NAG	C1-O5-C5	3.63	117.11	112.19
4	BBB	810	NAG	C1-O5-C5	3.23	116.57	112.19
4	BBB	810	NAG	C4-C3-C2	2.90	115.27	111.02
4	BBB	810	NAG	O7-C7-N2	2.70	126.92	121.95
4	BBB	810	NAG	C2-N2-C7	2.52	126.50	122.90

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	809	NAG	O5-C5-C6-O6
4	AAA	809	NAG	C4-C5-C6-O6
3	BBB	814	EDO	O1-C1-C2-O2
3	BBB	811	EDO	O1-C1-C2-O2
4	BBB	810	NAG	C4-C5-C6-O6

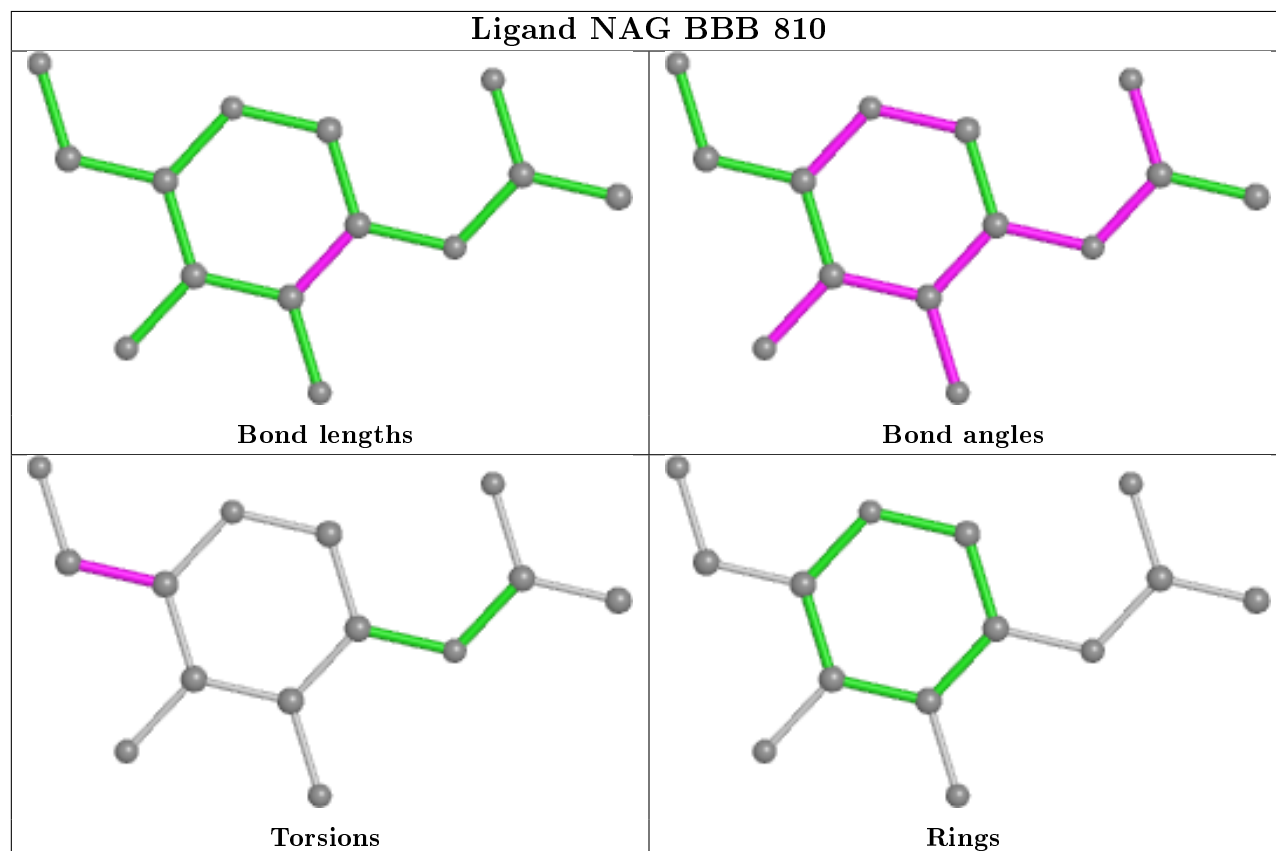
There are no ring outliers.

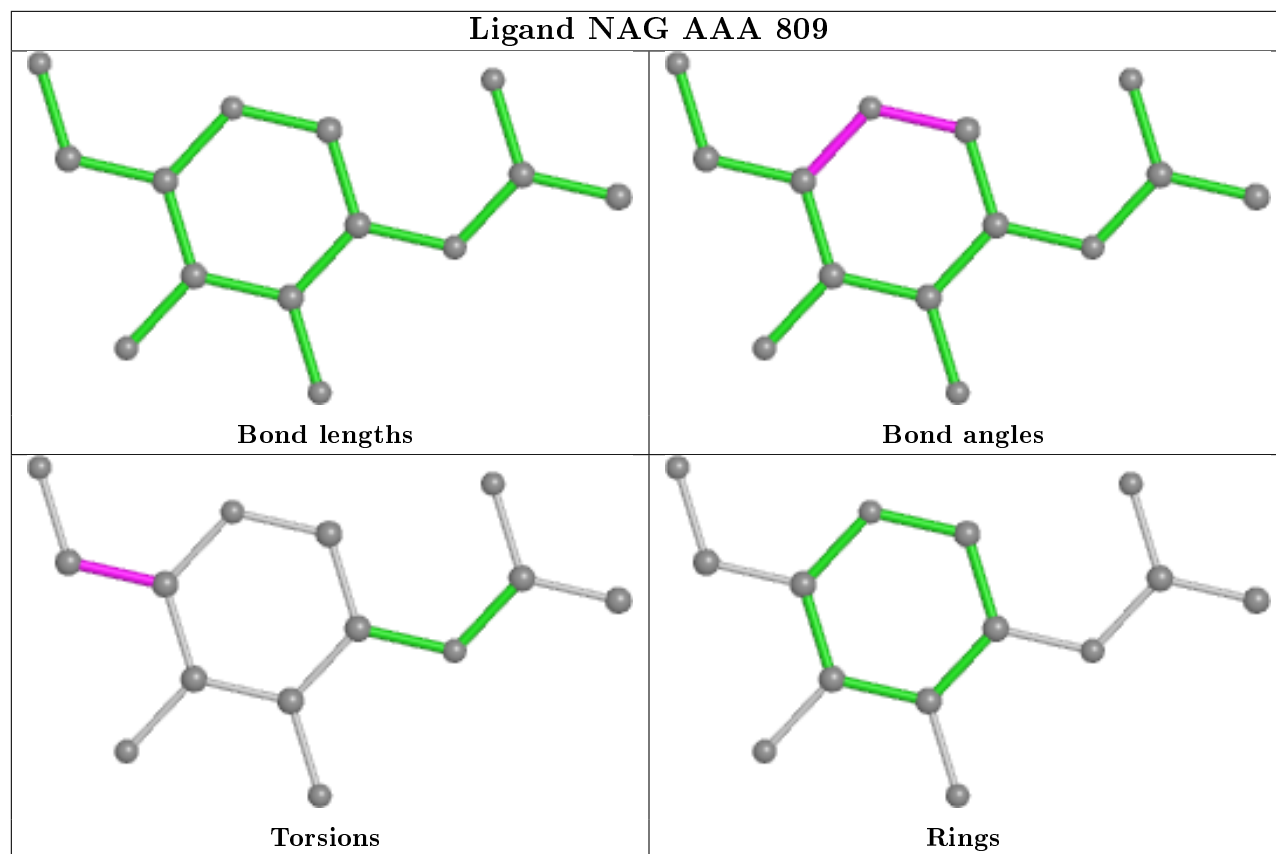
8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	806	EDO	1	0
5	BBB	818	SO4	2	0
3	BBB	808	EDO	2	0
3	BBB	809	EDO	0	1
3	BBB	811	EDO	2	0
3	AAA	807	EDO	3	0
5	AAA	813	SO4	0	1
5	AAA	812	SO4	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.





## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	AAA	470/515 (91%)	0.14	23 (4%) 29 27	21, 33, 69, 111	0
1	BBB	486/515 (94%)	0.25	41 (8%) 11 9	20, 31, 65, 114	0
All	All	956/1030 (92%)	0.20	64 (6%) 17 16	20, 31, 67, 114	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	445	PHE	8.8
1	BBB	442	VAL	5.6
1	BBB	685	LYS	5.3
1	BBB	669	GLN	5.1
1	BBB	666	VAL	4.9

### 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
2	NAG	B	3	14/15	0.83	0.23	61,68,75,76	3
2	MAN	B	2	11/12	0.85	0.19	57,67,73,82	3
2	MAN	A	2	11/12	0.88	0.19	69,85,91,98	3
2	MAN	A	1	12/12	0.89	0.11	44,56,59,64	3
2	NAG	A	3	14/15	0.89	0.17	69,77,82,87	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MAN	B	1	12/12	0.90	0.14	35,50,54,56	3
2	MAN	A	4	11/12	0.95	0.08	30,45,56,59	3
2	MAN	B	4	11/12	0.97	0.07	26,33,41,49	3
2	NAG	A	5	14/15	0.97	0.09	23,25,34,38	3
2	NAG	B	5	14/15	0.98	0.07	20,22,28,29	3

## 6.4 Ligands ⓘ

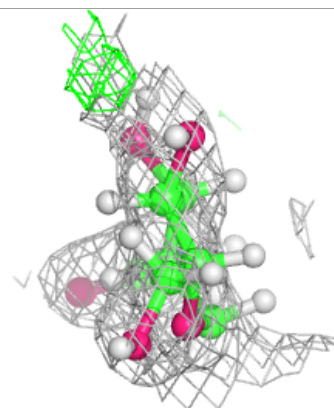
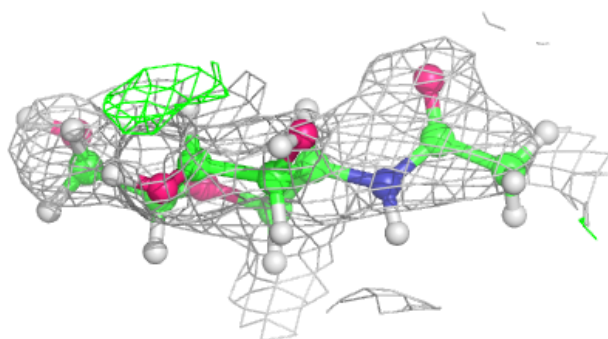
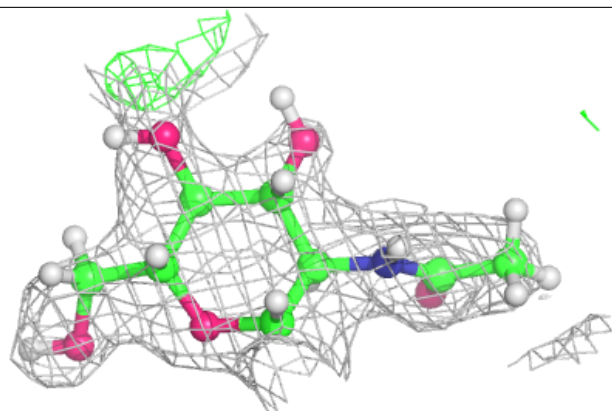
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	AAA	809	14/15	0.78	0.21	67,76,80,83	3
3	EDO	BBB	814	4/4	0.80	0.09	63,65,69,70	1
3	EDO	BBB	813	4/4	0.81	0.12	55,57,59,59	1
5	SO4	BBB	817	5/5	0.85	0.14	42,47,51,52	5
4	NAG	BBB	810	14/15	0.85	0.18	46,61,70,70	3
3	EDO	AAA	808	4/4	0.85	0.12	51,53,61,62	1
3	EDO	BBB	811	4/4	0.86	0.09	38,42,43,44	1
3	EDO	BBB	808	4/4	0.86	0.13	42,50,53,54	1
3	EDO	BBB	812	4/4	0.88	0.18	43,50,56,57	1
5	SO4	AAA	813	5/5	0.88	0.20	51,51,62,69	5
5	SO4	AAA	812	5/5	0.92	0.12	47,48,49,52	5
3	EDO	AAA	806	4/4	0.93	0.26	40,46,49,49	1
5	SO4	BBB	818	5/5	0.94	0.08	44,49,54,57	5
5	SO4	BBB	819	5/5	0.94	0.24	56,62,62,62	5
5	SO4	AAA	811	5/5	0.94	0.12	56,57,61,67	5
3	EDO	AAA	807	4/4	0.95	0.10	41,48,50,51	1
3	EDO	BBB	807	4/4	0.95	0.09	44,44,45,45	1
5	SO4	BBB	816	5/5	0.95	0.09	51,52,54,57	5
3	EDO	BBB	809	4/4	0.95	0.11	40,45,46,47	1
3	EDO	BBB	806	4/4	0.96	0.08	33,42,50,52	1
5	SO4	AAA	810	5/5	0.96	0.12	54,59,62,67	5
5	SO4	AAA	814	5/5	0.97	0.17	29,38,44,46	5
5	SO4	BBB	815	5/5	0.99	0.06	39,40,42,46	0

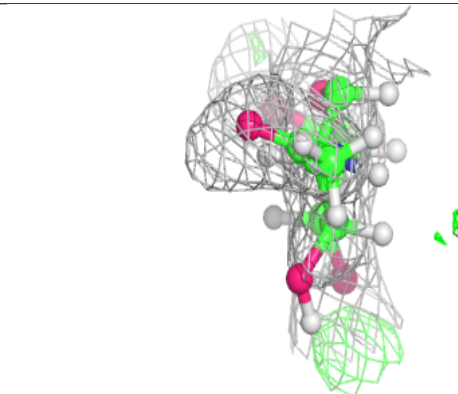
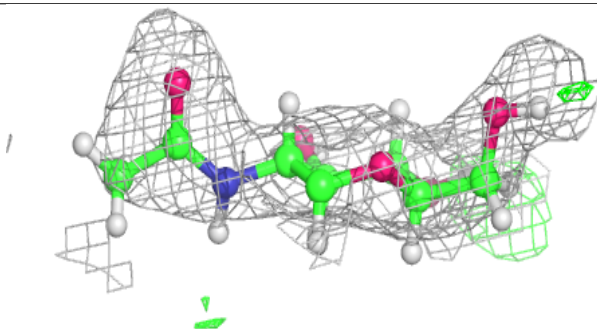
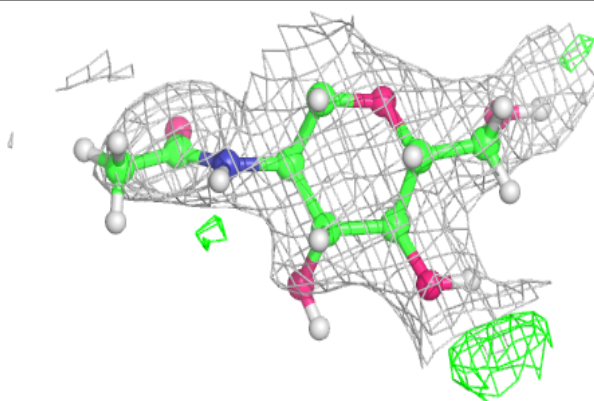
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around NAG AAA 809:**

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

**Electron density around NAG BBB 810:**

$2mF_o-DF_c$  (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.