



# Full wwPDB X-ray Structure Validation Report ⓘ

May 30, 2022 – 07:30 pm BST

PDB ID : 7Z5S  
Title : Crystal Structure of botulinum neurotoxin A2 cell binding domain in complex with GD1a  
Authors : Gregory, K.S.; Acharya, K.R.; Liu, S.M.; Mahadeva, T.B.  
Deposited on : 2022-03-10  
Resolution : 2.10 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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.28.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.28.1

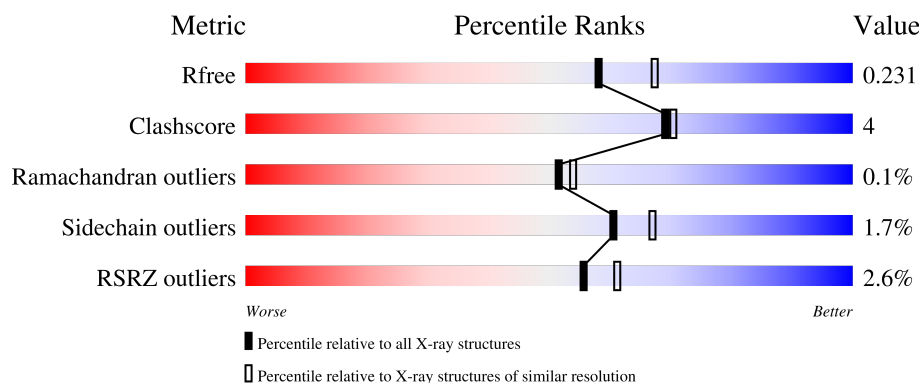
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	AAA	433	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div></div> </div> </div>
1	BBB	433	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>7%</div> </div> </div>
2	DDD	5	<div> <div></div> <div>100%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7143 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.

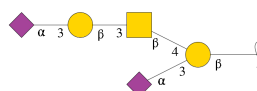
- Molecule 1 is a protein called Botulinum neurotoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	419	Total	C	N	O	S	0	0	0
			3429	2196	580	641	12			
1	BBB	403	Total	C	N	O	S	0	0	0
			3304	2121	553	618	12			

There are 14 discrepancies between the modelled and reference sequences:

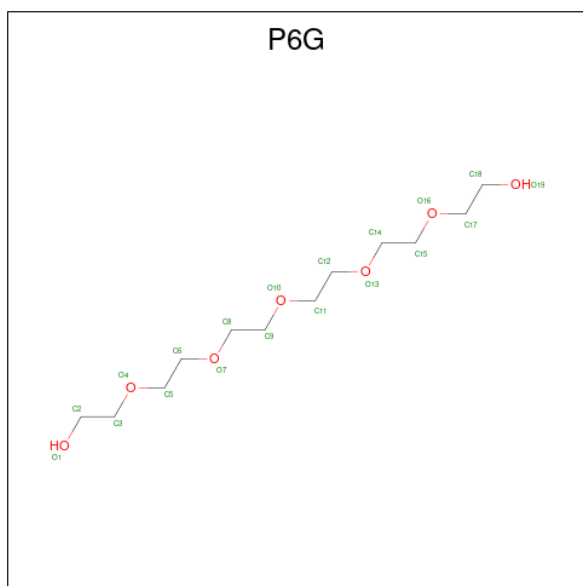
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	864	MET	-	initiating methionine	UNP K4GGE0
AAA	865	HIS	-	expression tag	UNP K4GGE0
AAA	866	HIS	-	expression tag	UNP K4GGE0
AAA	867	HIS	-	expression tag	UNP K4GGE0
AAA	868	HIS	-	expression tag	UNP K4GGE0
AAA	869	HIS	-	expression tag	UNP K4GGE0
AAA	870	HIS	-	expression tag	UNP K4GGE0
BBB	864	MET	-	initiating methionine	UNP K4GGE0
BBB	865	HIS	-	expression tag	UNP K4GGE0
BBB	866	HIS	-	expression tag	UNP K4GGE0
BBB	867	HIS	-	expression tag	UNP K4GGE0
BBB	868	HIS	-	expression tag	UNP K4GGE0
BBB	869	HIS	-	expression tag	UNP K4GGE0
BBB	870	HIS	-	expression tag	UNP K4GGE0

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	DDD	5	Total	C	N	O	0	0	0
			77	42	3	32			

- Molecule 3 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $C_{12}H_{26}O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			19	12	7		
3	BBB	1	Total	C	O	0	0
			19	12	7		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			4	2	2		

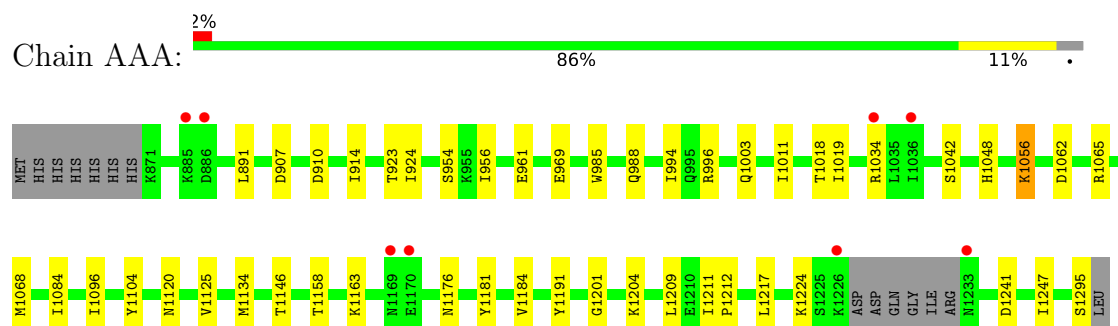
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	164	Total	O	0	0
			164	164		
5	BBB	127	Total	O	0	0
			127	127		

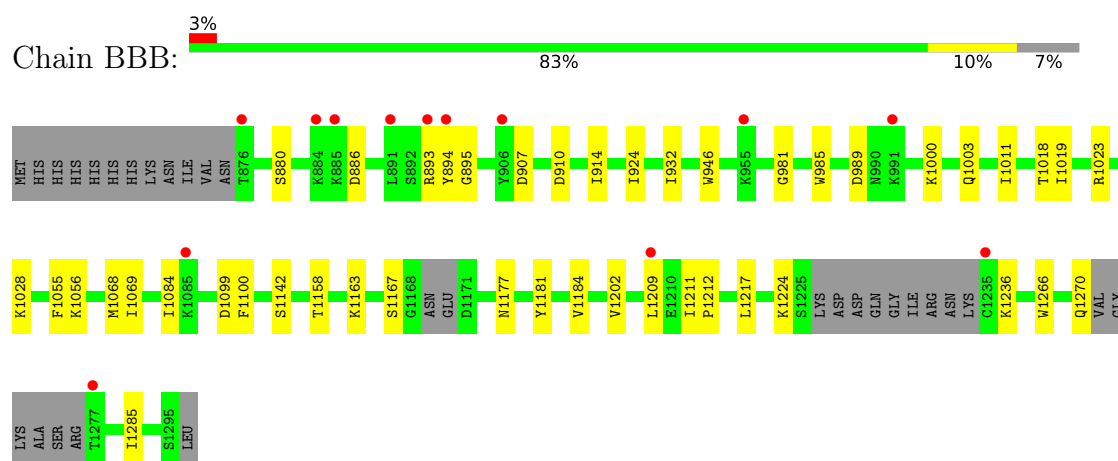
### 3 Residue-property plots [i](#)

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: Botulinum neurotoxin



#### • Molecule 1: Botulinum neurotoxin



#### • Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.07 Å   105.07 Å   132.58 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	105.07 – 2.10 105.07 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (105.07-2.10) 100.0 (105.07-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.188 , 0.226 0.195 , 0.231	Depositor DCC
$R_{free}$ test set	4166 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.0	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7143	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, EDO, SIA, NGA, P6G

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	0.72	0/3497	0.89	0/4724
1	BBB	0.71	0/3370	0.84	0/4553
All	All	0.72	0/6867	0.87	0/9277

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	3429	0	3426	30	0
1	BBB	3304	0	3287	22	0
2	DDD	77	0	65	0	0
3	AAA	19	0	26	0	0
3	BBB	19	0	26	0	0
4	AAA	4	0	6	0	0
5	AAA	164	0	0	2	0
5	BBB	127	0	0	0	0
All	All	7143	0	6836	51	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 4.



All (51) 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:AAA:961:GLU:OE1	1:AAA:996:ARG:NH2	2.26	0.68
1:AAA:1003:GLN:HA	1:AAA:1011:ILE:HD11	1.78	0.66
1:AAA:923:THR:HG22	1:AAA:1056:LYS:HB2	1.78	0.66
1:AAA:1158:THR:CG2	1:AAA:1184:VAL:HG13	2.32	0.60
1:BBB:1209:LEU:HD11	1:BBB:1217:LEU:HD13	1.85	0.59
1:AAA:1209:LEU:HD21	1:AAA:1217:LEU:CD1	2.37	0.54
1:AAA:954:SER:HB2	1:AAA:956:ILE:HG22	1.90	0.54
1:BBB:1163:LYS:HB2	1:BBB:1181:TYR:HB2	1.91	0.53
1:BBB:1158:THR:CG2	1:BBB:1184:VAL:HG13	2.39	0.53
1:BBB:1266:TRP:O	1:BBB:1270:GLN:HG2	2.09	0.53
1:AAA:1158:THR:HG21	1:AAA:1184:VAL:HG13	1.90	0.53
1:BBB:985:TRP:CD2	1:BBB:1019:ILE:HG21	2.45	0.52
1:BBB:1158:THR:HG21	1:BBB:1184:VAL:HG13	1.92	0.51
1:AAA:969:GLU:OE1	1:AAA:1048:HIS:NE2	2.33	0.51
1:AAA:985:TRP:CE3	1:AAA:1019:ILE:HD13	2.47	0.50
1:AAA:1042:SER:OG	1:BBB:893:ARG:NH1	2.44	0.50
1:BBB:1177:ASN:OD1	1:BBB:1224:LYS:HE3	2.11	0.50
1:AAA:1209:LEU:CD2	1:AAA:1217:LEU:HD12	2.42	0.49
1:BBB:1018:THR:HG21	1:BBB:1084:ILE:HG12	1.94	0.49
1:AAA:1125:VAL:HG22	1:AAA:1134:MET:HG2	1.94	0.49
1:AAA:985:TRP:CD2	1:AAA:1019:ILE:HG21	2.48	0.49
1:AAA:1209:LEU:CD2	1:AAA:1217:LEU:CD1	2.90	0.48
1:AAA:914:ILE:O	1:AAA:1068:MET:HA	2.14	0.47
1:AAA:1204:LYS:HG3	1:AAA:1247:ILE:CG2	2.46	0.46
1:BBB:1209:LEU:CD1	1:BBB:1217:LEU:HD13	2.45	0.46
1:BBB:894:TYR:CG	1:BBB:932:ILE:HG21	2.50	0.46
1:AAA:1176:ASN:ND2	1:AAA:1224:LYS:HA	2.31	0.46
1:AAA:907:ASP:HB3	1:AAA:910:ASP:O	2.16	0.46
1:AAA:988:GLN:HG2	1:AAA:994:ILE:HG12	1.97	0.46
1:AAA:1211:ILE:N	1:AAA:1212:PRO:CD	2.80	0.45
1:AAA:1241:ASP:HB3	1:AAA:1247:ILE:HD11	1.98	0.45
1:BBB:1003:GLN:HA	1:BBB:1011:ILE:HD11	1.99	0.44
1:AAA:914:ILE:HG21	1:AAA:924:ILE:HD11	1.99	0.44
1:AAA:1191:TYR:OH	5:AAA:1402:HOH:O	2.20	0.44
1:BBB:914:ILE:O	1:BBB:1068:MET:HA	2.16	0.44
1:BBB:924:ILE:HB	1:BBB:1055:PHE:HB2	1.99	0.43
1:BBB:1019:ILE:HA	1:BBB:1028:LYS:O	2.17	0.43
1:AAA:1018:THR:HG21	1:AAA:1084:ILE:HG12	2.00	0.42
1:AAA:954:SER:CB	1:AAA:956:ILE:HG22	2.50	0.42
1:BBB:981:GLY:O	1:BBB:1000:LYS:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:1201:GLY:HA3	5:AAA:1535:HOH:O	2.20	0.42
1:AAA:1096:ILE:HG21	1:AAA:1104:TYR:CD1	2.55	0.41
1:BBB:1211:ILE:N	1:BBB:1212:PRO:HD2	2.35	0.41
1:BBB:1100:PHE:CB	1:BBB:1285:ILE:HG12	2.50	0.41
1:BBB:946:TRP:O	1:BBB:1069:ILE:HA	2.20	0.41
1:AAA:891:LEU:HD23	1:AAA:891:LEU:HA	1.93	0.41
1:AAA:1062:ASP:HB3	1:AAA:1065:ARG:HG2	2.02	0.41
1:AAA:1163:LYS:HB2	1:AAA:1181:TYR:HB2	2.03	0.41
1:BBB:907:ASP:HB3	1:BBB:910:ASP:O	2.19	0.41
1:BBB:989:ASP:OD1	1:BBB:989:ASP:C	2.60	0.41
1:BBB:1099:ASP:C	1:BBB:1099:ASP:OD1	2.59	0.40

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	AAA	415/433 (96%)	393 (95%)	22 (5%)	0	100	100
1	BBB	395/433 (91%)	375 (95%)	19 (5%)	1 (0%)	41	41
All	All	810/866 (94%)	768 (95%)	41 (5%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	895	GLY

### 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	AAA	384/397 (97%)	379 (99%)	5 (1%)	69	75
1	BBB	370/397 (93%)	362 (98%)	8 (2%)	52	57
All	All	754/794 (95%)	741 (98%)	13 (2%)	60	67

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	1034	ARG
1	AAA	1056	LYS
1	AAA	1120	ASN
1	AAA	1146	THR
1	AAA	1295	SER
1	BBB	880	SER
1	BBB	886	ASP
1	BBB	1023	ARG
1	BBB	1056	LYS
1	BBB	1142	SER
1	BBB	1167	SER
1	BBB	1202	VAL
1	BBB	1236	LYS

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 ⓘ

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

## 5.5 Carbohydrates ⓘ

5 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	GAL	DDD	1	2	12,12,12	1.39	1 (8%)	17,17,17	2.37	4 (23%)
2	NGA	DDD	2	2	14,14,15	0.94	1 (7%)	17,19,21	0.95	0
2	GAL	DDD	3	2	11,11,12	0.68	0	15,15,17	1.13	1 (6%)
2	SIA	DDD	4	2	17,20,21	0.31	0	21,28,31	1.49	5 (23%)
2	SIA	DDD	5	2	17,20,21	0.36	0	21,28,31	2.03	6 (28%)

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	GAL	DDD	1	2	-	0/2/22/22	0/1/1/1
2	NGA	DDD	2	2	-	0/6/23/26	0/1/1/1
2	GAL	DDD	3	2	-	0/2/19/22	0/1/1/1
2	SIA	DDD	4	2	-	7/14/34/38	0/1/1/1
2	SIA	DDD	5	2	-	8/14/34/38	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DDD	1	GAL	O4-C4	-3.77	1.34	1.43
2	DDD	2	NGA	O3-C3	-3.15	1.35	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DDD	1	GAL	O3-C3-C2	7.36	127.38	110.35
2	DDD	5	SIA	C6-C5-N5	4.61	118.58	110.91
2	DDD	5	SIA	O6-C2-C3	4.38	117.56	109.87
2	DDD	5	SIA	C6-O6-C2	3.60	119.05	111.34
2	DDD	5	SIA	C3-C4-C5	-3.51	107.21	111.46
2	DDD	1	GAL	O4-C4-C3	-3.16	103.05	110.35
2	DDD	4	SIA	C3-C2-C1	-3.10	105.15	111.93
2	DDD	1	GAL	O4-C4-C5	3.02	116.78	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DDD	4	SIA	C3-C4-C5	-3.01	107.82	111.46
2	DDD	1	GAL	C3-C4-C5	3.01	115.61	110.24
2	DDD	5	SIA	C4-C3-C2	2.65	114.56	109.81
2	DDD	5	SIA	C4-C5-N5	2.29	114.91	110.38
2	DDD	4	SIA	C6-C5-N5	2.23	114.62	110.91
2	DDD	4	SIA	C4-C5-N5	2.23	114.78	110.38
2	DDD	4	SIA	C8-C7-C6	2.19	117.19	113.03
2	DDD	3	GAL	O6-C6-C5	-2.18	103.80	111.29

There are no chirality outliers.

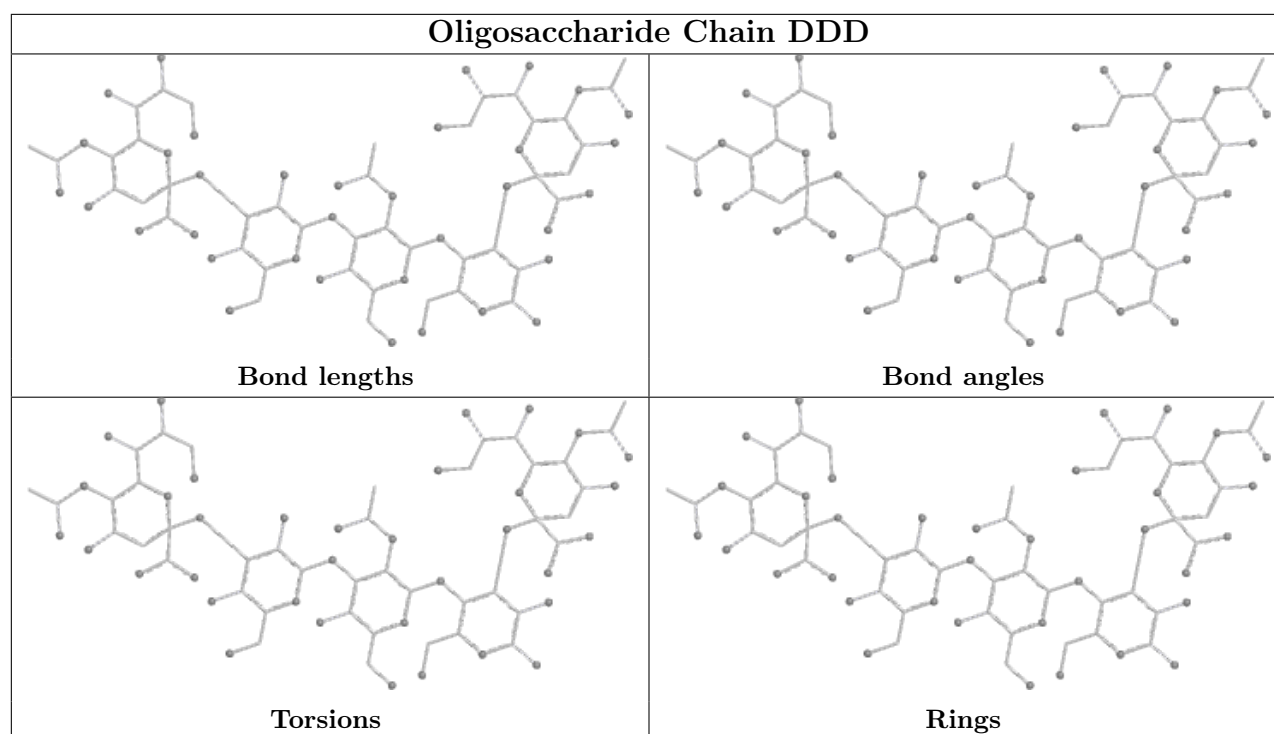
All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	DDD	4	SIA	C7-C8-C9-O9
2	DDD	4	SIA	O8-C8-C9-O9
2	DDD	4	SIA	C11-C10-N5-C5
2	DDD	4	SIA	O10-C10-N5-C5
2	DDD	5	SIA	C5-C6-C7-C8
2	DDD	5	SIA	C5-C6-C7-O7
2	DDD	5	SIA	O6-C6-C7-C8
2	DDD	5	SIA	O6-C6-C7-O7
2	DDD	5	SIA	O8-C8-C9-O9
2	DDD	5	SIA	C11-C10-N5-C5
2	DDD	5	SIA	O10-C10-N5-C5
2	DDD	5	SIA	C7-C8-C9-O9
2	DDD	4	SIA	C6-C7-C8-C9
2	DDD	4	SIA	O7-C7-C8-O8
2	DDD	4	SIA	C6-C7-C8-O8

There are no ring outliers.

No monomer is involved in short contacts.

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



## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	EDO	AAA	1302	-	3,3,3	0.28	0	2,2,2	0.51	0
3	P6G	BBB	1301	-	18,18,18	0.29	0	17,17,17	0.18	0
3	P6G	AAA	1301	-	18,18,18	0.34	0	17,17,17	0.20	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	AAA	1302	-	-	1/1/1/1	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	P6G	BBB	1301	-	-	7/16/16/16	-
3	P6G	AAA	1301	-	-	9/16/16/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

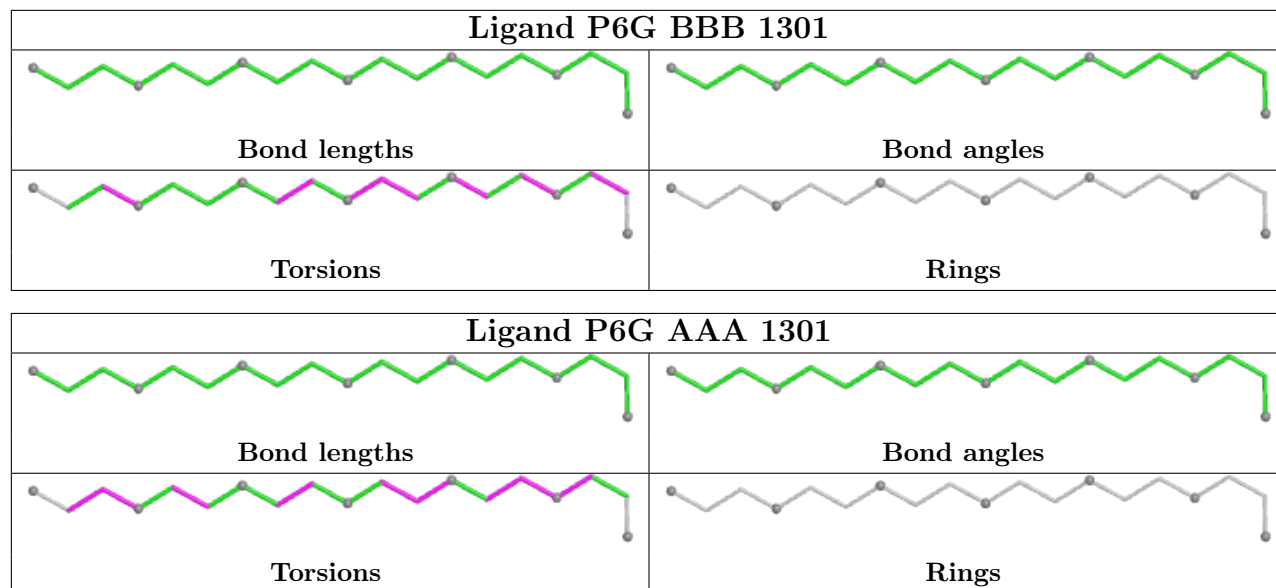
Mol	Chain	Res	Type	Atoms
3	AAA	1301	P6G	O4-C5-C6-O7
3	AAA	1301	P6G	O13-C14-C15-O16
3	BBB	1301	P6G	O1-C2-C3-O4
3	AAA	1301	P6G	O16-C17-C18-O19
4	AAA	1302	EDO	O1-C1-C2-O2
3	AAA	1301	P6G	O7-C8-C9-O10
3	BBB	1301	P6G	O7-C8-C9-O10
3	BBB	1301	P6G	O10-C11-C12-O13
3	BBB	1301	P6G	C8-C9-O10-C11
3	AAA	1301	P6G	C9-C8-O7-C6
3	AAA	1301	P6G	C18-C17-O16-C15
3	BBB	1301	P6G	C18-C17-O16-C15
3	BBB	1301	P6G	C5-C6-O7-C8
3	AAA	1301	P6G	C2-C3-O4-C5
3	AAA	1301	P6G	C6-C5-O4-C3
3	BBB	1301	P6G	C6-C5-O4-C3
3	AAA	1301	P6G	O10-C11-C12-O13

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [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	419/433 (96%)	0.55	8 (1%) 66 71	26, 43, 70, 110	0
1	BBB	403/433 (93%)	0.55	13 (3%) 47 54	29, 48, 74, 105	0
All	All	822/866 (94%)	0.55	21 (2%) 56 61	26, 45, 73, 110	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	893	ARG	5.1
1	AAA	885	LYS	3.8
1	AAA	1233	ASN	3.4
1	BBB	885	LYS	3.1
1	AAA	886	ASP	3.1
1	AAA	1036	ILE	3.1
1	BBB	1235	CYS	2.4
1	BBB	955	LYS	2.4
1	AAA	1170	GLU	2.3
1	BBB	1085	LYS	2.3
1	AAA	1169	ASN	2.3
1	BBB	876	THR	2.2
1	BBB	891	LEU	2.2
1	AAA	1226	LYS	2.2
1	BBB	906	TYR	2.2
1	AAA	1034	ARG	2.1
1	BBB	1277	THR	2.1
1	BBB	1209	LEU	2.1
1	BBB	894	TYR	2.1
1	BBB	884	LYS	2.0
1	BBB	991	LYS	2.0

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

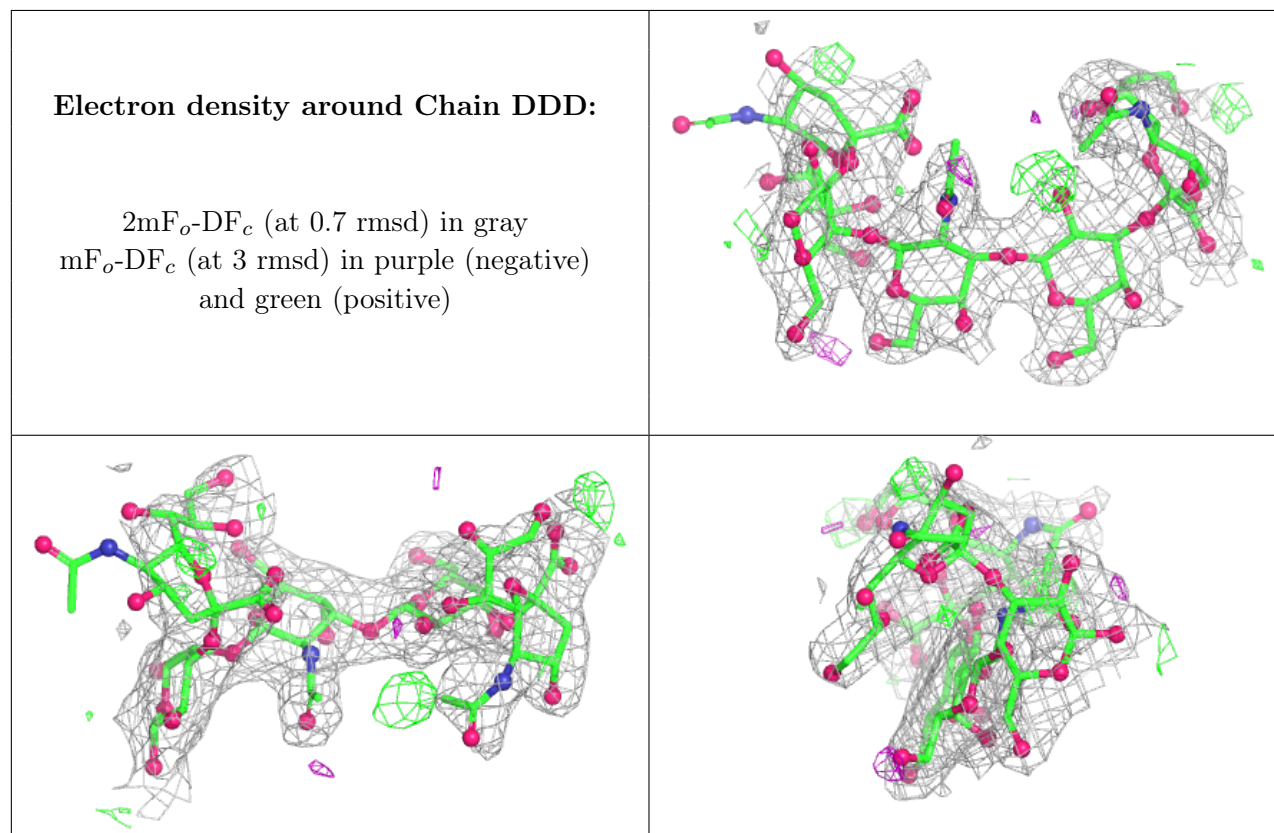
There are no non-standard protein/DNA/RNA residues in this entry.

## 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( $\text{\AA}^2$ )	Q<0.9
2	SIA	DDD	5	20/21	0.82	0.27	89,118,133,134	0
2	GAL	DDD	1	12/12	0.90	0.10	82,83,90,102	0
2	SIA	DDD	4	20/21	0.93	0.18	51,72,96,107	0
2	NGA	DDD	2	14/15	0.96	0.12	57,68,75,79	0
2	GAL	DDD	3	11/12	0.97	0.12	46,55,57,57	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

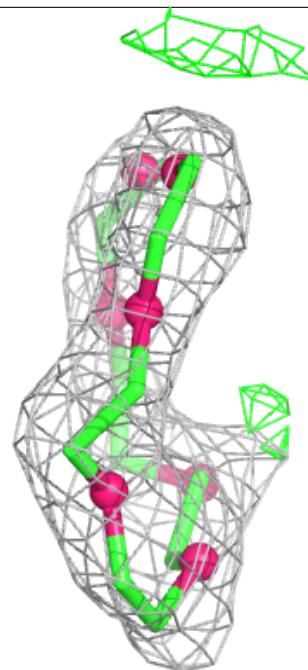
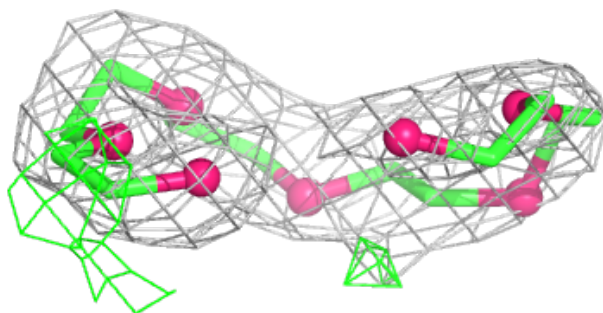
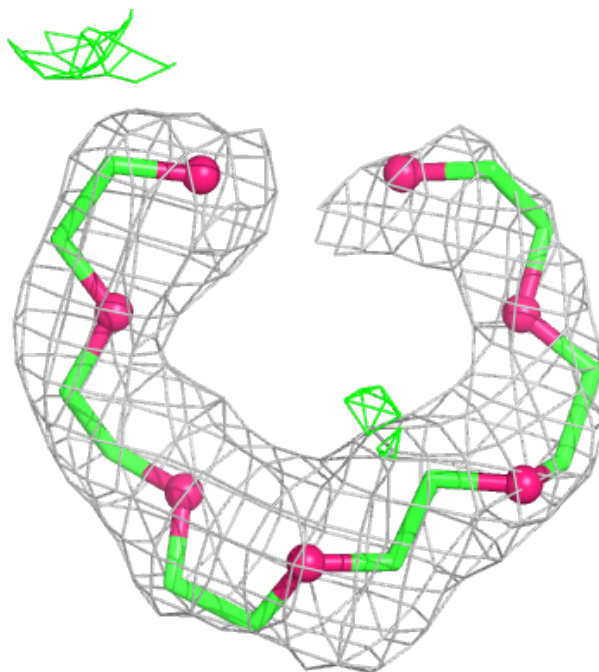
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

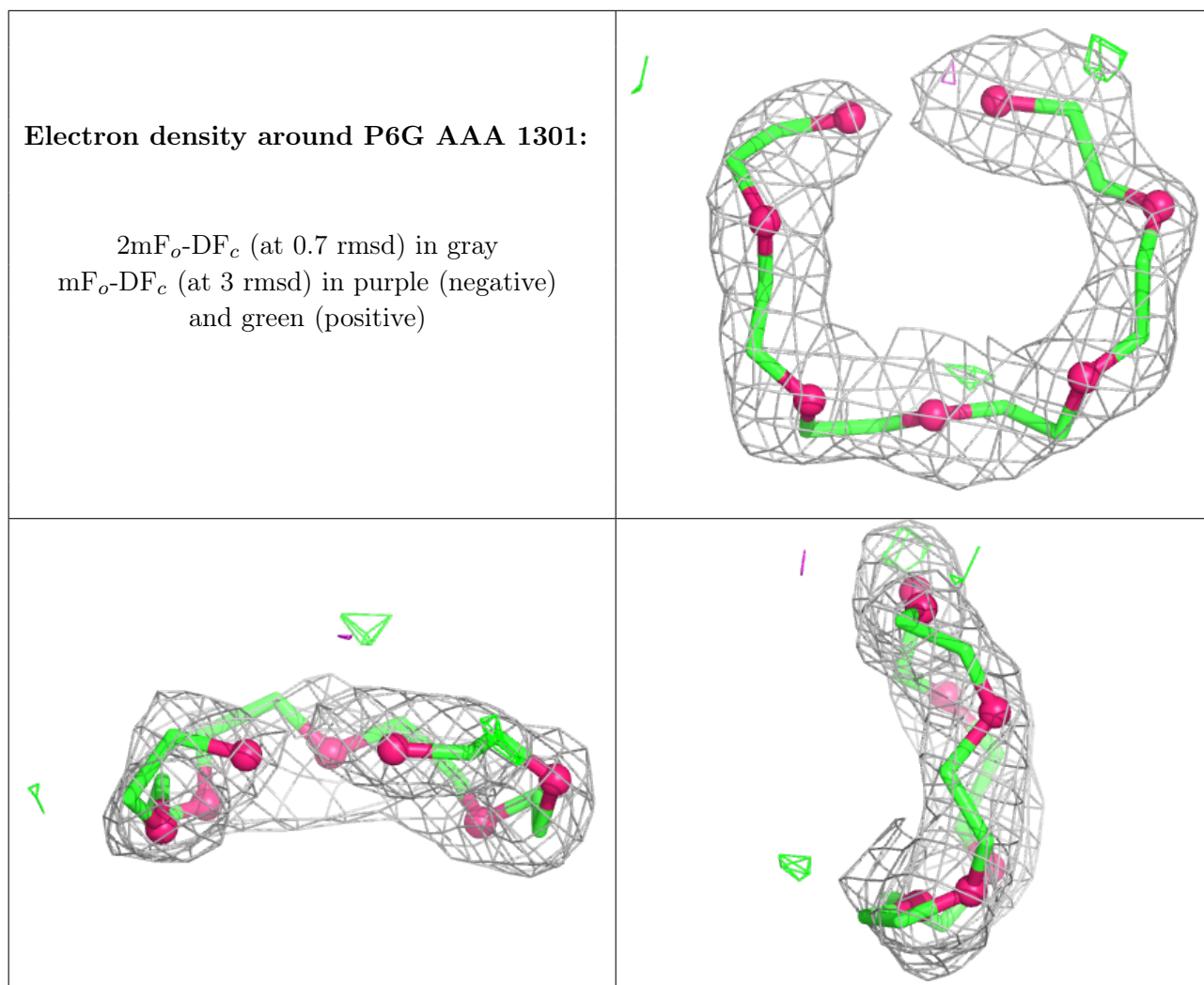
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	AAA	1302	4/4	0.81	0.20	61,64,73,74	0
3	P6G	BBB	1301	19/19	0.86	0.22	84,93,103,104	0
3	P6G	AAA	1301	19/19	0.86	0.24	63,84,96,98	0

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

**Electron density around P6G BBB 1301:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.