



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 23, 2021 – 06:12 pm GMT

PDB ID : 7P1P  
Title : Crystal structure of human acetylcholinesterase in complex with (E)-3-hydroxy-6-(3-(4-(4-(((2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)oxy)butyl)-1H-1,2,3-triazol-1-yl)propyl)picolinaldehyde oxime  
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Deposited on : 2021-07-02  
Resolution : 3.03 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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.24  
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) : 2.24

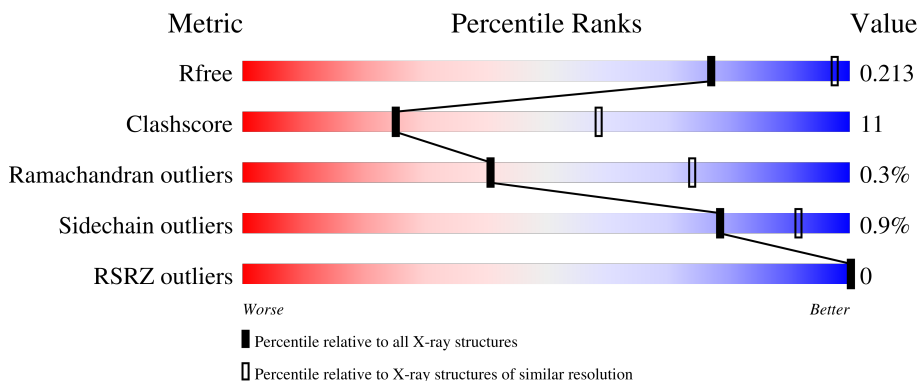
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.03 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.



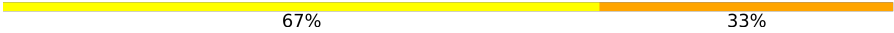

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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	aa	257	98% (green)
1	bb	257	96% (green)
2	A	282	83% (green), 17% (yellow)
2	B	282	77% (green), 21% (yellow)
3	C	4	50% (green), 50% (yellow)

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Mol	Chain	Length	Quality of chain
4	D	3	 67% 33%
5	E	3	 33% 67%

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 8784 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.

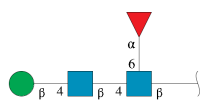
- Molecule 1 is a protein called Acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	aa	254	Total	C	N	O	S	0	0	0
			1936	1241	338	349	8			
1	bb	254	Total	C	N	O	S	0	0	0
			1936	1241	338	349	8			

- Molecule 2 is a protein called Acetylcholinesterase.

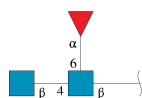
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	282	Total	C	N	O	S	0	0	0
			2229	1431	390	403	5			
2	B	279	Total	C	N	O	S	0	0	0
			2214	1423	387	399	5			

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



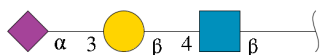
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



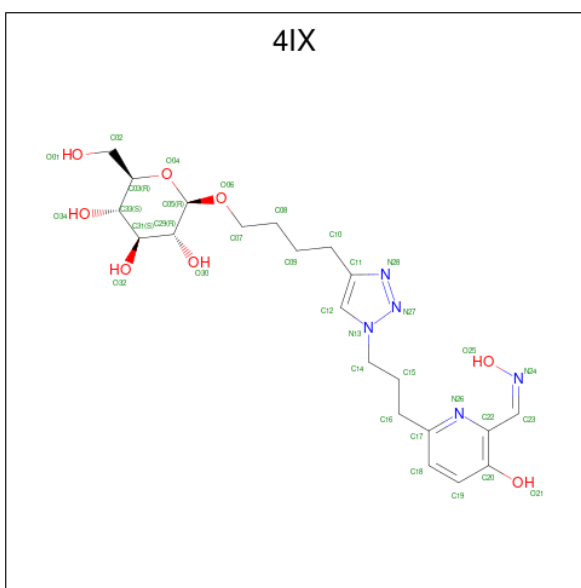
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	3	38	22	2	14	0	0	0

- Molecule 5 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	E	3	46	25	2	19	0	0	0

- Molecule 6 is (2R,3R,4S,5S,6R)-2-[4-[1-[3-[6-[(Z)-hydroxyiminomethyl]-5-oxidanyl-pyridin-2-yl]propyl]-1,2,3-triazol-4-yl]butoxy]-6-(hydroxymethyl)oxane-3,4,5-triol (three-letter code: 4IX) (formula: C<sub>21</sub>H<sub>31</sub>N<sub>5</sub>O<sub>8</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	aa	1	34	21	5	8	1	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	aa	1	Total	O	S	0	0
			5	4	1		
7	aa	1	Total	O	S	0	0
			5	4	1		
7	aa	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	bb	1	Total	O	S	0	0
			5	4	1		
7	bb	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	aa	3	Total	Cl	0	0
			3	3		
8	A	6	Total	Cl	0	0
			6	6		
8	bb	3	Total	Cl	0	0
			3	3		
8	B	10	Total	Cl	0	0
			10	10		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Mg	0	0
			1	1		
9	bb	1	Total	Mg	0	0
			1	1		
9	B	2	Total	Mg	0	0
			2	2		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	aa	51	Total	O	0	0
			51	51		
10	A	57	Total	O	0	0
			57	57		
10	bb	46	Total	O	0	0
			46	46		
10	B	47	Total	O	0	0
			47	47		

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Acetylcholinesterase

Chain aa:  98%




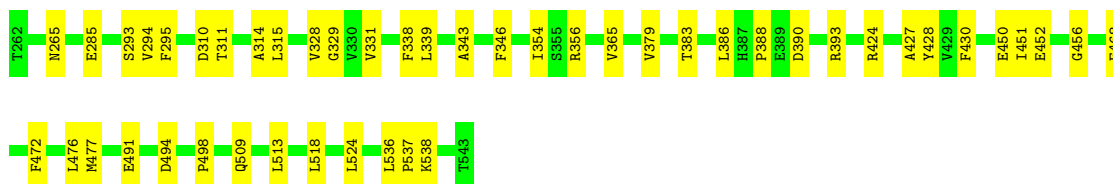
- Molecule 1: Acetylcholinesterase

Chain bb:  96%




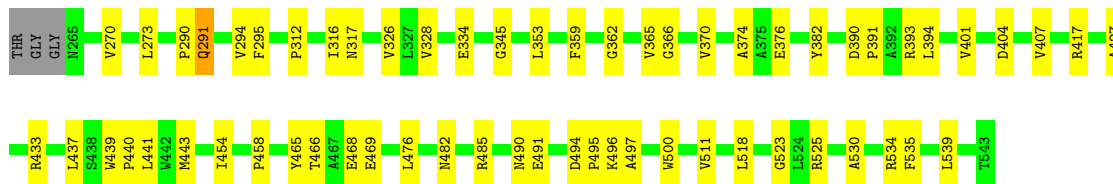
- Molecule 2: Acetylcholinesterase

Chain A:  83% 17%



- Molecule 2: Acetylcholinesterase

Chain B:  77% 21%



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

Chain C:  50% 50%





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

Chain D:  67% 33%



- Molecule 5: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  33% 67%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.86Å 211.86Å 116.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	91.74 – 3.03 183.48 – 3.03	Depositor EDS
% Data completeness (in resolution range)	99.9 (91.74-3.03) 93.3 (183.48-3.03)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.190 , 0.222 0.183 , 0.213	Depositor DCC
$R_{free}$ test set	2843 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.0	Xtrriage
Anisotropy	0.886	Xtrriage
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>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.009 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8784	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% 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: SIA, BMA, MG, FUC, GAL, NAG, CL, SO4, 4IX

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	aa	0.51	0/1996	0.75	1/2729 (0.0%)
1	bb	0.48	1/1996 (0.1%)	0.73	0/2729
2	A	0.51	0/2296	0.71	1/3137 (0.0%)
2	B	0.46	0/2281	0.70	0/3117
All	All	0.49	1/8569 (0.0%)	0.72	2/11712 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	bb	0	1
2	A	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	bb	226	VAL	CB-CG1	-5.70	1.40	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	aa	149	MET	CA-CB-CG	-7.71	100.19	113.30
2	A	524	LEU	CB-CG-CD2	-5.24	102.10	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	424	ARG	Sidechain
1	bb	257	CYS	Peptide

## 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	aa	1936	0	1892	0	0
1	bb	1936	0	1892	0	0
2	A	2229	0	2155	34	0
2	B	2214	0	2142	42	0
3	C	49	0	43	0	0
4	D	38	0	34	1	0
5	E	46	0	40	0	0
6	aa	34	0	0	0	0
7	A	30	0	0	1	0
7	B	20	0	0	0	0
7	aa	15	0	0	0	0
7	bb	10	0	0	0	0
8	A	6	0	0	0	0
8	B	10	0	0	0	0
8	aa	3	0	0	0	0
8	bb	3	0	0	0	0
9	A	1	0	0	0	0
9	B	2	0	0	0	0
9	bb	1	0	0	0	0
10	A	57	0	0	5	0
10	B	47	0	0	0	0
10	aa	51	0	0	0	0
10	bb	46	0	0	0	0
All	All	8784	0	8198	73	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 11.

The worst 5 of 73 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:356:ARG:HH22	2:A:383:THR:HG21	1.40	0.84
2:B:312:PRO:O	2:B:316:ILE:HG12	1.81	0.79
2:B:317:ASN:HB3	2:B:417:ARG:HE	1.57	0.69
2:B:362:GLY:HA2	2:B:365:VAL:HG12	1.72	0.69
2:A:343:ALA:HA	10:A:716:HOH:O	1.92	0.69

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	aa	252/257 (98%)	245 (97%)	7 (3%)	0	100	100
1	bb	252/257 (98%)	238 (94%)	14 (6%)	0	100	100
2	A	280/282 (99%)	261 (93%)	18 (6%)	1 (0%)	34	69
2	B	277/282 (98%)	256 (92%)	19 (7%)	2 (1%)	22	57
All	All	1061/1078 (98%)	1000 (94%)	58 (6%)	3 (0%)	41	74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	265	ASN
2	B	291	GLN
2	B	495	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	aa	202/204 (99%)	201 (100%)	1 (0%)	88	95
1	bb	202/204 (99%)	197 (98%)	5 (2%)	47	77
2	A	232/232 (100%)	231 (100%)	1 (0%)	91	96
2	B	231/232 (100%)	230 (100%)	1 (0%)	91	96
All	All	867/872 (99%)	859 (99%)	8 (1%)	78	91

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	295	PHE
1	bb	246	ARG
1	bb	186	ASN
1	bb	149	MET
1	bb	200	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	533	ASN
2	B	490	ASN
1	bb	186	ASN
2	A	482	ASN
2	B	413	GLN

### 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](#)

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
3	NAG	C	1	2,3	14,14,15	0.45	0	17,19,21	0.60	0
3	NAG	C	2	3	14,14,15	0.45	0	17,19,21	0.39	0
3	BMA	C	3	3	11,11,12	1.78	3 (27%)	15,15,17	0.99	1 (6%)
3	FUC	C	4	3	10,10,11	1.34	1 (10%)	14,14,16	1.47	2 (14%)
4	NAG	D	1	4,2	14,14,15	0.71	0	17,19,21	0.83	1 (5%)
4	NAG	D	2	4	14,14,15	0.61	0	17,19,21	0.78	1 (5%)
4	FUC	D	3	4	10,10,11	1.79	3 (30%)	14,14,16	1.25	2 (14%)
5	NAG	E	1	5	15,15,15	0.24	0	21,21,21	0.63	0
5	GAL	E	2	5	11,11,12	1.49	2 (18%)	15,15,17	1.59	4 (26%)
5	SIA	E	3	5	17,20,21	1.35	4 (23%)	21,28,31	1.35	3 (14%)

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	NAG	C	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	FUC	C	4	3	-	-	0/1/1/1
4	NAG	D	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
4	FUC	D	3	4	-	-	0/1/1/1
5	NAG	E	1	5	-	4/6/26/26	0/1/1/1
5	GAL	E	2	5	-	2/2/19/22	0/1/1/1
5	SIA	E	3	5	-	5/14/34/38	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	BMA	C4-C5	3.72	1.60	1.53
4	D	3	FUC	C4-C5	2.99	1.59	1.52
4	D	3	FUC	C2-C3	2.83	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3	FUC	O5-C5	2.70	1.49	1.43
5	E	3	SIA	C7-C6	2.68	1.56	1.53

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	3	SIA	C6-O6-C2	3.39	118.59	111.34
3	C	4	FUC	O5-C5-C4	3.16	115.19	109.52
5	E	2	GAL	O3-C3-C2	2.98	115.70	109.99
4	D	3	FUC	O5-C5-C4	2.94	114.80	109.52
5	E	2	GAL	O5-C1-C2	-2.91	106.27	110.77

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	2	GAL	O5-C5-C6-O6
5	E	3	SIA	C6-C7-C8-C9
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
5	E	1	NAG	C8-C7-N2-C2

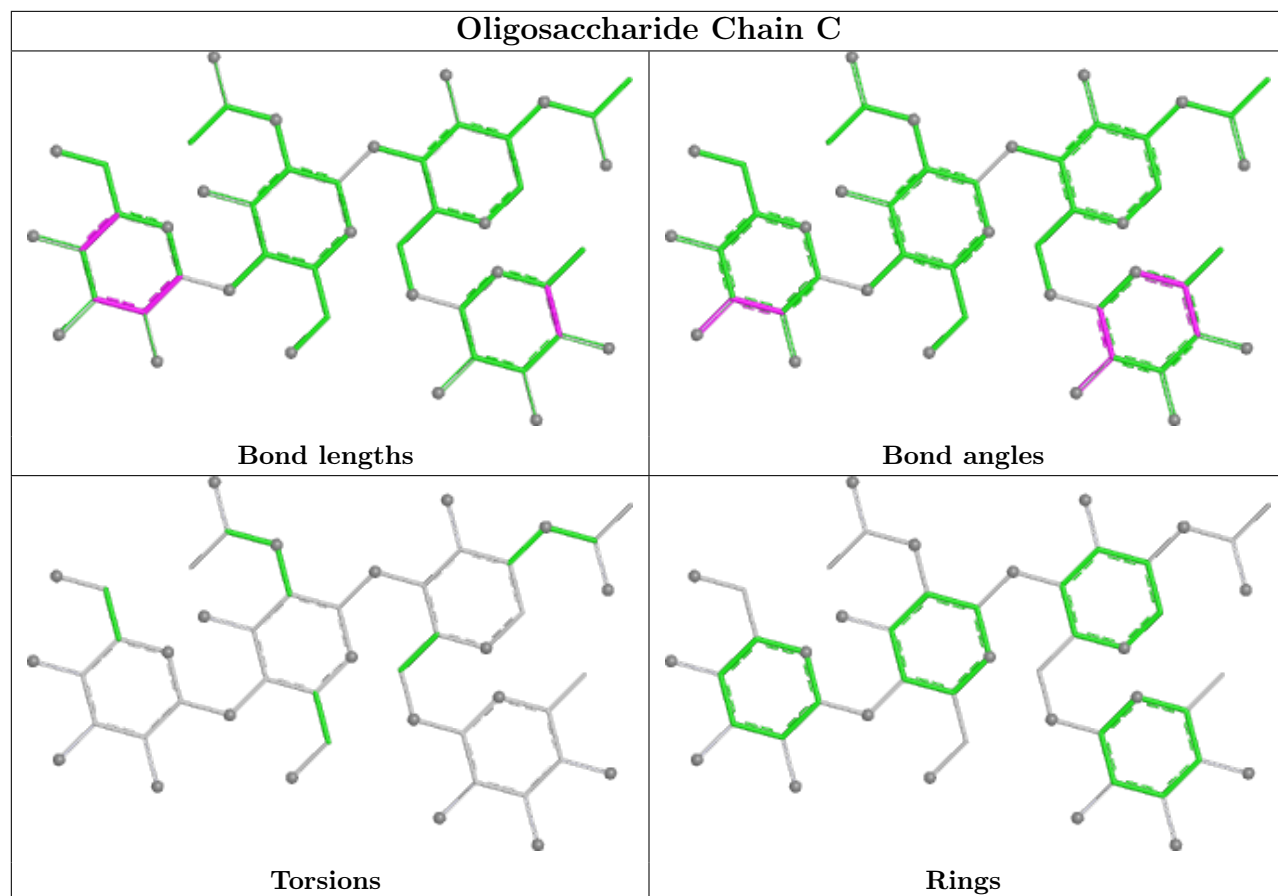
There are no ring outliers.

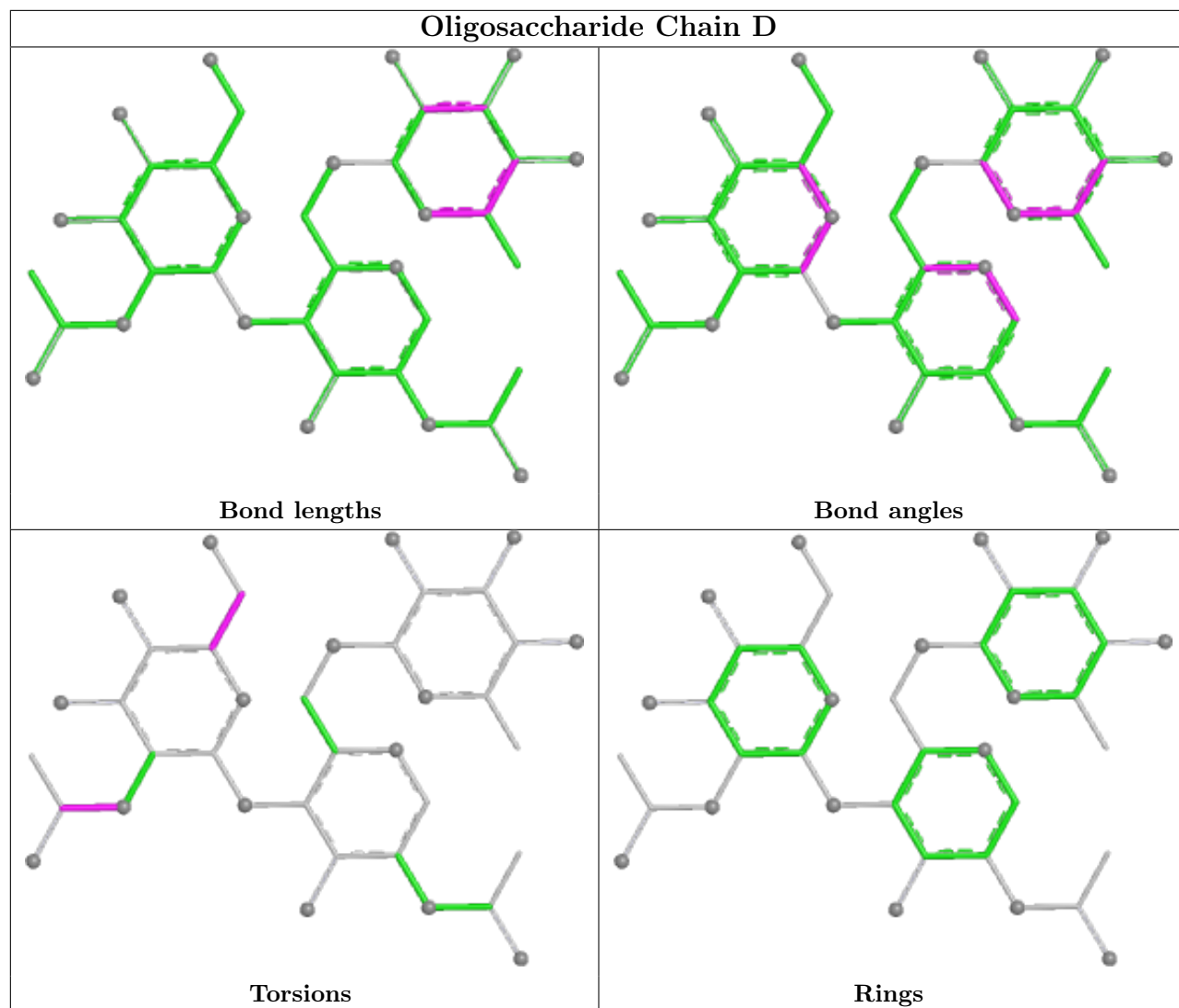
1 monomer is involved in 1 short contact:

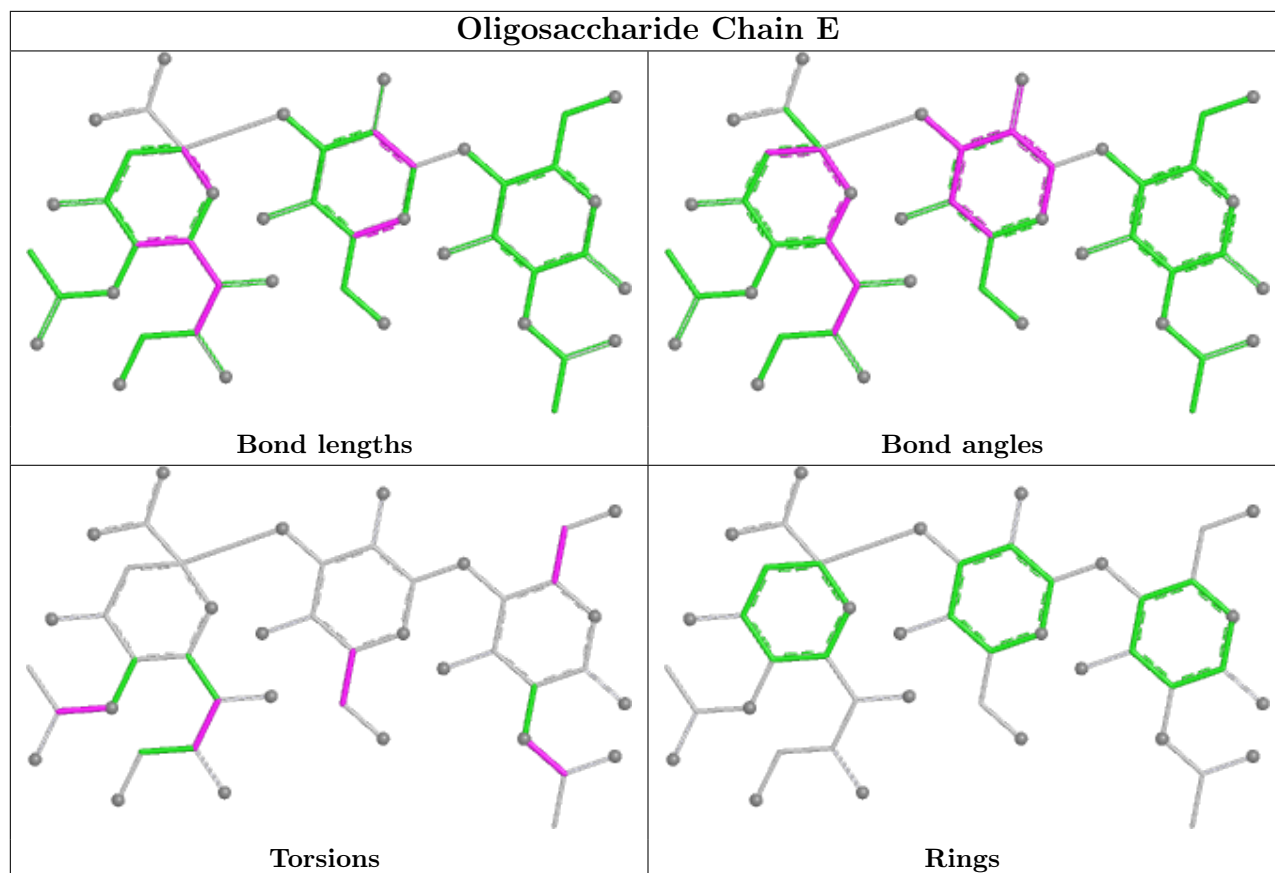
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	1	0

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](#)

Of 42 ligands modelled in this entry, 26 are monoatomic - leaving 16 for Mogul analysis.

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
7	SO4	A	606	-	4,4,4	0.27	0	6,6,6	0.24	0
7	SO4	aa	604	-	4,4,4	0.26	0	6,6,6	0.27	0
7	SO4	A	602	-	4,4,4	0.24	0	6,6,6	0.22	0
7	SO4	bb	302	-	4,4,4	0.15	0	6,6,6	0.20	0
7	SO4	B	602	9	4,4,4	0.16	0	6,6,6	0.22	0
7	SO4	aa	602	-	4,4,4	0.18	0	6,6,6	0.60	0
7	SO4	aa	603	-	4,4,4	0.17	0	6,6,6	0.25	0
7	SO4	B	601	-	4,4,4	0.23	0	6,6,6	0.63	0
7	SO4	A	604	-	4,4,4	0.19	0	6,6,6	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	SO4	A	601	-	4,4,4	0.26	0	6,6,6	0.69	0
7	SO4	B	604	-	4,4,4	0.29	0	6,6,6	0.35	0
7	SO4	A	603	-	4,4,4	0.29	0	6,6,6	0.30	0
7	SO4	bb	301	-	4,4,4	0.22	0	6,6,6	0.21	0
7	SO4	B	603	-	4,4,4	0.27	0	6,6,6	0.54	0
7	SO4	A	605	-	4,4,4	0.21	0	6,6,6	0.26	0
6	4IX	aa	601	-	36,36,36	1.82	11 (30%)	40,48,48	1.84	9 (22%)

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
6	4IX	aa	601	-	-	14/19/39/39	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	aa	601	4IX	C22-C23	5.89	1.59	1.47
6	aa	601	4IX	O04-C03	3.11	1.51	1.44
6	aa	601	4IX	C10-C11	3.11	1.57	1.51
6	aa	601	4IX	C12-C11	2.96	1.40	1.36
6	aa	601	4IX	N28-N27	2.75	1.39	1.34

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	aa	601	4IX	C22-N26-C17	5.12	123.74	117.91
6	aa	601	4IX	O25-N24-C23	4.14	119.18	111.86
6	aa	601	4IX	O04-C03-C33	3.62	116.26	109.69
6	aa	601	4IX	C12-C11-N28	-3.16	106.65	111.34
6	aa	601	4IX	C05-O04-C03	3.12	119.81	113.69

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	aa	601	4IX	C29-C05-O06-C07
6	aa	601	4IX	C09-C10-C11-N28
6	aa	601	4IX	C15-C14-N13-C12

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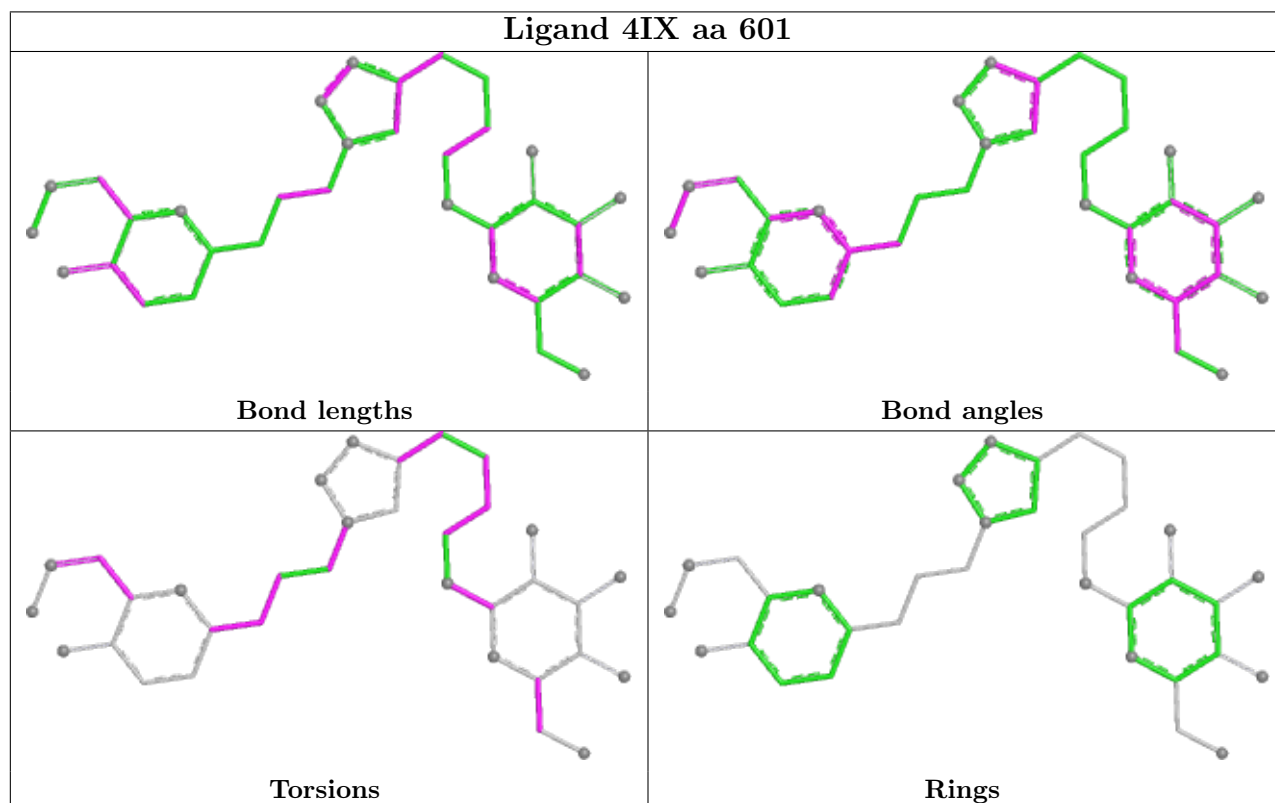
Mol	Chain	Res	Type	Atoms
6	aa	601	4IX	C15-C14-N13-N27
6	aa	601	4IX	C14-C15-C16-C17

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	603	SO4	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 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	aa	254/257 (98%)	0.18	0 100 100	59, 76, 109, 158	0
1	bb	254/257 (98%)	0.21	0 100 100	64, 89, 123, 176	0
2	A	282/282 (100%)	0.15	0 100 100	61, 79, 116, 178	0
2	B	279/282 (98%)	0.16	0 100 100	63, 87, 133, 193	0
All	All	1069/1078 (99%)	0.17	0 100 100	59, 83, 123, 193	0

There are no RSRZ outliers to report.

### 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.

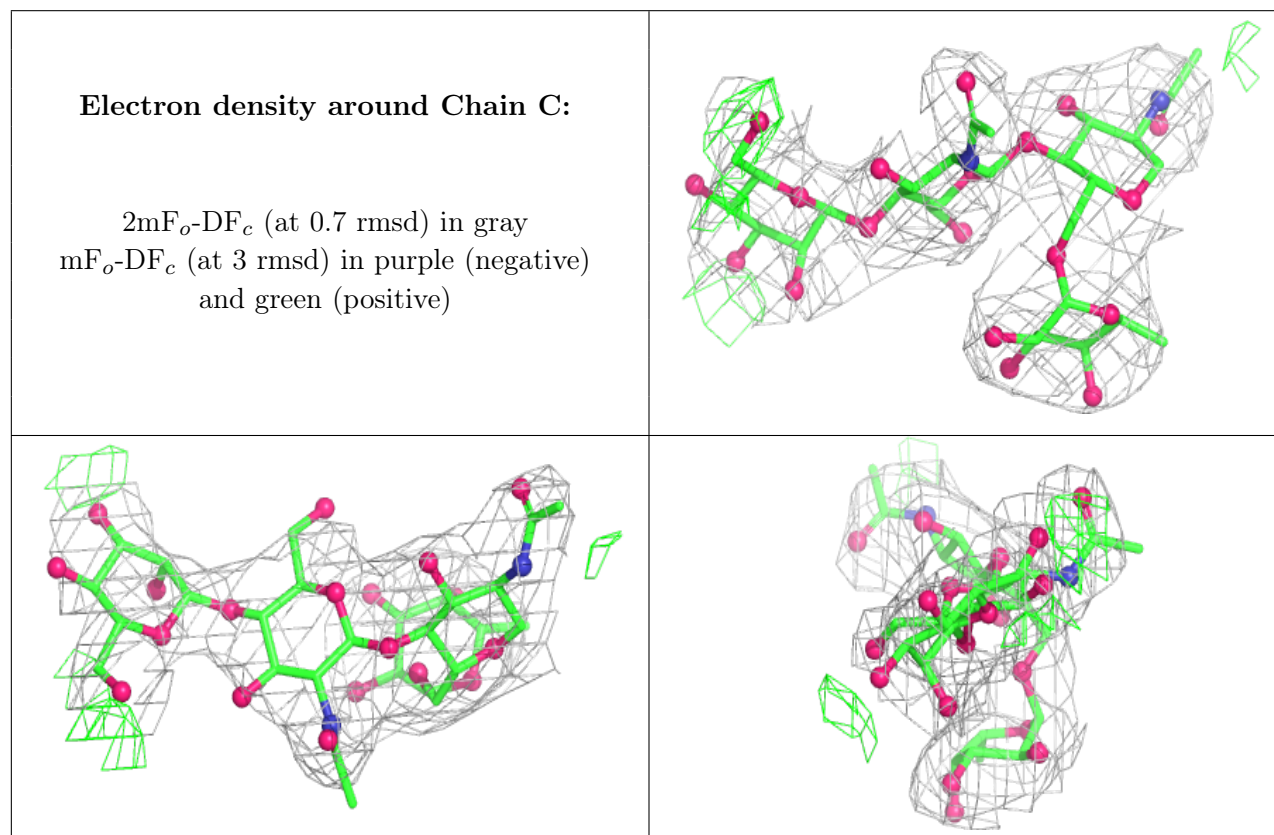
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	BMA	C	3	11/12	0.47	0.22	153,162,171,171	0
5	NAG	E	1	15/15	0.75	0.32	144,151,162,163	0
4	FUC	D	3	10/11	0.84	0.35	147,157,159,160	0
4	NAG	D	2	14/15	0.88	0.24	150,162,168,170	0
3	NAG	C	2	14/15	0.92	0.22	111,133,147,153	0
5	GAL	E	2	11/12	0.92	0.21	103,123,133,135	0
5	SIA	E	3	20/21	0.92	0.31	115,120,126,128	0
3	FUC	C	4	10/11	0.93	0.14	124,136,140,141	0
4	NAG	D	1	14/15	0.94	0.17	124,137,150,154	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	C	1	14/15	0.94	0.19	97,108,118,128	0

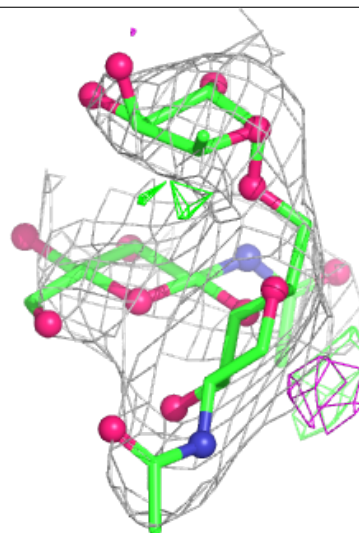
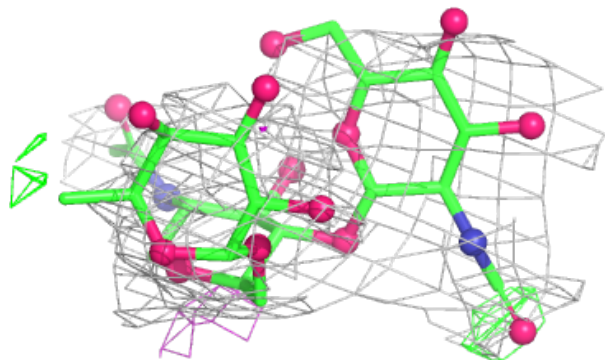
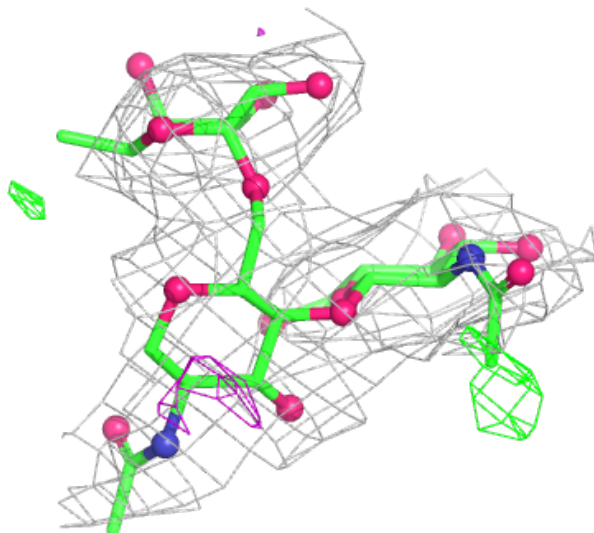
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

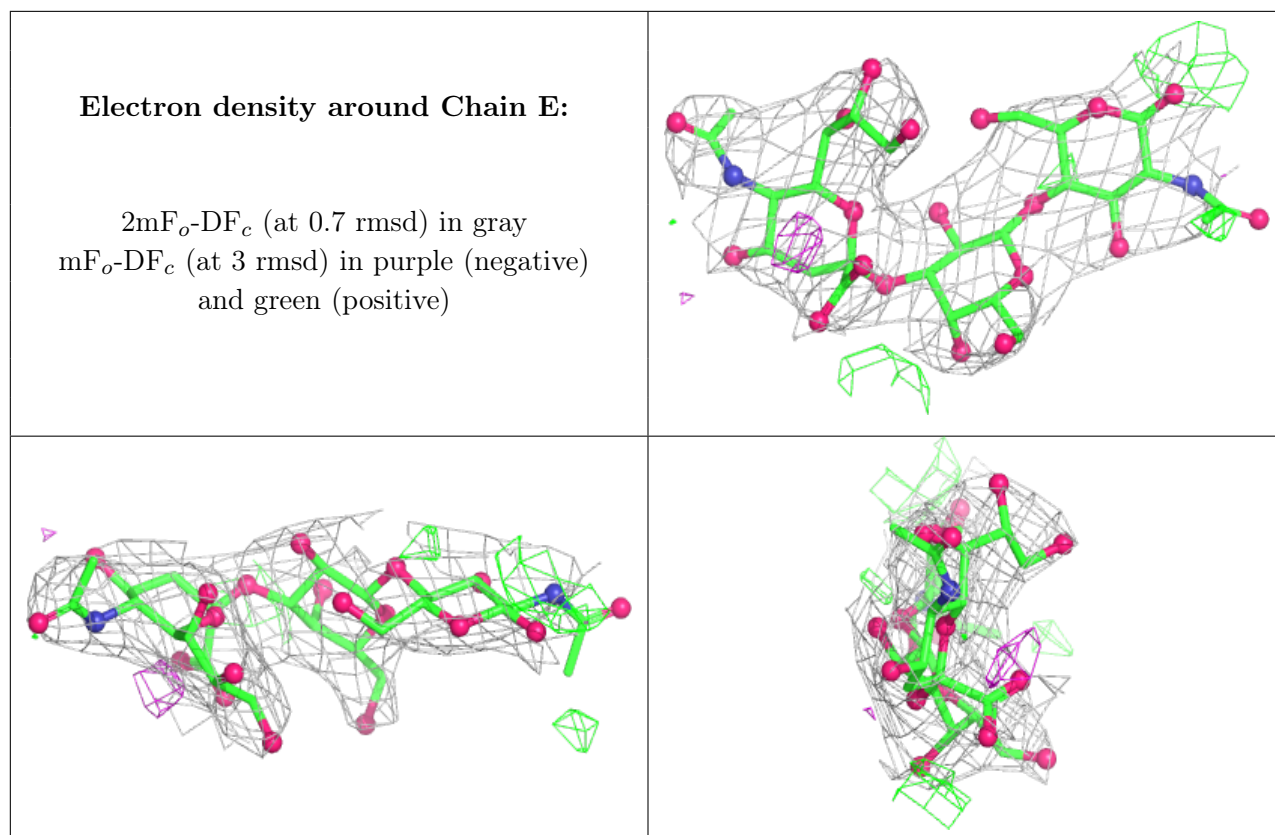




**Electron density around Chain D:**

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





## 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.

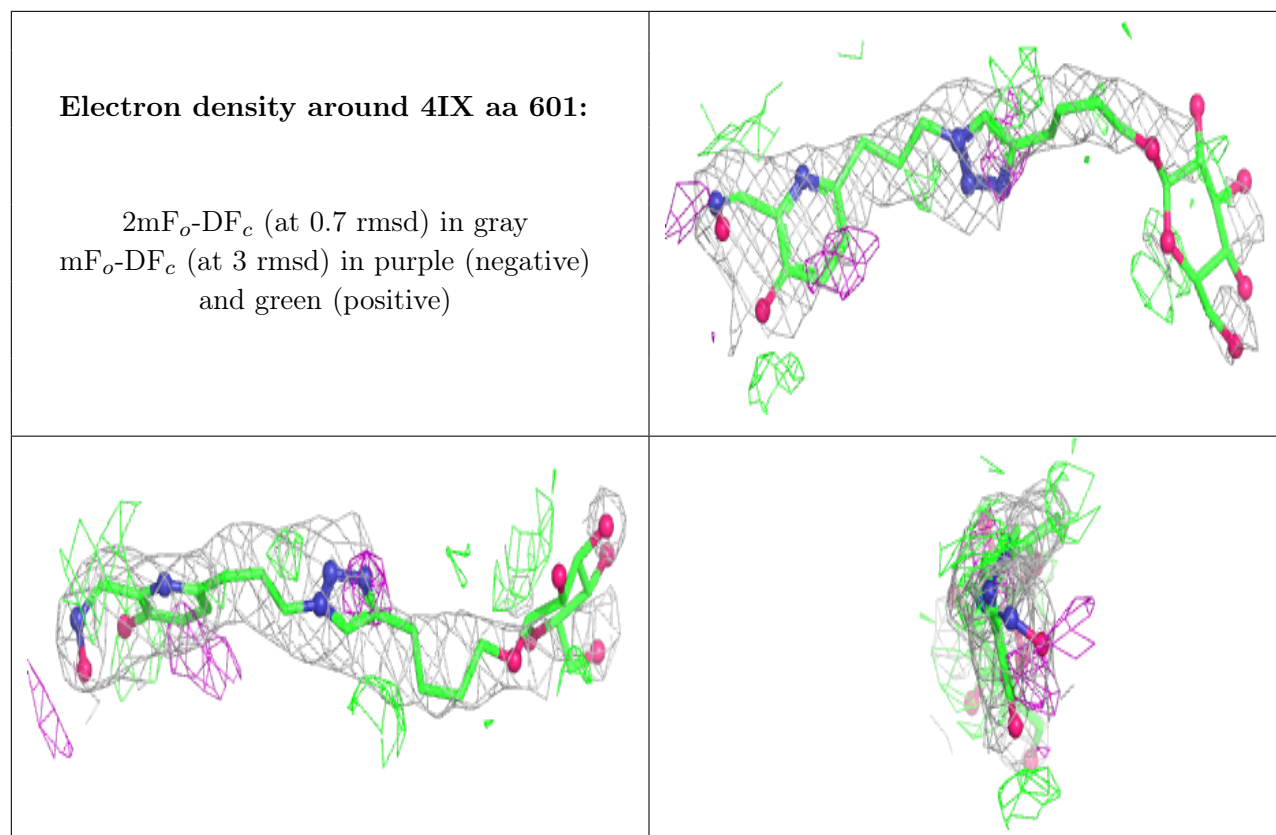
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	CL	B	611	1/1	0.41	0.14	111,111,111,111	0
8	CL	A	612	1/1	0.42	0.26	165,165,165,165	0
8	CL	A	609	1/1	0.42	0.16	107,107,107,107	0
8	CL	aa	605	1/1	0.43	0.18	118,118,118,118	0
8	CL	aa	607	1/1	0.63	0.14	117,117,117,117	0
8	CL	B	615	1/1	0.64	0.11	108,108,108,108	0
7	SO4	A	602	5/5	0.66	0.26	110,111,116,123	5
8	CL	bb	304	1/1	0.71	0.12	102,102,102,102	0
9	MG	B	606	1/1	0.71	0.13	68,68,68,68	0
8	CL	B	612	1/1	0.73	0.21	98,98,98,98	0
8	CL	B	614	1/1	0.76	0.11	92,92,92,92	0
8	CL	A	610	1/1	0.77	0.21	95,95,95,95	0
7	SO4	aa	603	5/5	0.79	0.26	136,146,147,158	0
8	CL	bb	306	1/1	0.80	0.16	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	CL	B	609	1/1	0.81	0.23	99,99,99,99	0
6	4IX	aa	601	34/34	0.82	0.39	79,97,114,118	7
8	CL	aa	606	1/1	0.82	0.19	101,101,101,101	0
7	SO4	B	604	5/5	0.83	0.18	118,121,139,139	0
9	MG	bb	303	1/1	0.85	0.15	78,78,78,78	0
7	SO4	bb	301	5/5	0.85	0.11	136,139,141,149	0
7	SO4	bb	302	5/5	0.86	0.28	138,140,147,149	0
8	CL	A	613	1/1	0.87	0.25	84,84,84,84	0
8	CL	B	616	1/1	0.87	0.12	124,124,124,124	0
8	CL	B	607	1/1	0.89	0.22	114,114,114,114	0
8	CL	B	610	1/1	0.89	0.12	107,107,107,107	0
8	CL	B	608	1/1	0.89	0.15	106,106,106,106	0
8	CL	bb	305	1/1	0.90	0.18	85,85,85,85	0
8	CL	B	613	1/1	0.91	0.14	72,72,72,72	0
8	CL	A	611	1/1	0.91	0.18	98,98,98,98	0
7	SO4	A	601	5/5	0.91	0.14	88,90,100,102	0
7	SO4	A	605	5/5	0.93	0.21	86,87,98,104	5
7	SO4	aa	604	5/5	0.93	0.19	121,125,130,141	0
9	MG	A	607	1/1	0.93	0.40	75,75,75,75	0
7	SO4	A	604	5/5	0.93	0.09	126,130,141,145	0
9	MG	B	605	1/1	0.93	0.12	96,96,96,96	0
7	SO4	B	602	5/5	0.93	0.18	91,95,101,103	5
7	SO4	A	606	5/5	0.94	0.17	109,112,128,130	0
7	SO4	aa	602	5/5	0.94	0.11	98,100,111,113	0
7	SO4	B	603	5/5	0.95	0.18	94,94,105,109	0
8	CL	A	608	1/1	0.95	0.28	91,91,91,91	0
7	SO4	A	603	5/5	0.95	0.16	92,97,98,106	0
7	SO4	B	601	5/5	0.97	0.18	77,77,82,83	5

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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.