



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2022 – 03:14 pm GMT

PDB ID : 7QBR  
Title : Human butyrylcholinesterase in complex with (Z)-N-tert-butyl-1-(8-(3-(4-(prop-2-yn-1-yl)piperazin-1-yl)propoxy)quinolin-2-yl)methanimine oxide  
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Deposited on : 2021-11-19  
Resolution : 2.13 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.

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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.31.3  
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) : 2.31.3

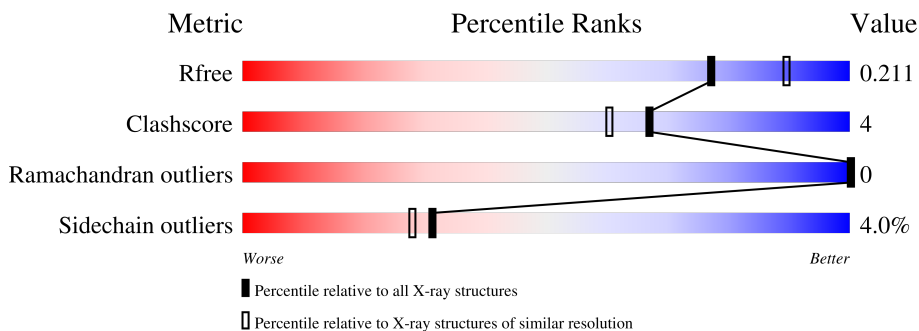
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.13 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	529	89% (green), 10% (yellow), 1% (orange), 0% (red)
2	B	3	67% (green), 33% (yellow)
2	D	3	67% (green), 33% (yellow)
2	E	3	100% (green)
3	C	2	50% (green), 50% (yellow)

## 2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 4709 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.

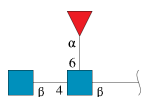
- Molecule 1 is a protein called Cholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	527	4224	2726	710	773	15	0	3	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	engineered mutation	UNP P06276
A	455	GLN	ASN	engineered mutation	UNP P06276
A	481	GLN	ASN	engineered mutation	UNP P06276
A	486	GLN	ASN	engineered mutation	UNP P06276

- Molecule 2 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			
2	B	3	38	22	2	14	0	0	0
2	D	3	38	22	2	14	0	0	0
2	E	3	38	22	2	14	0	0	0

- Molecule 3 is an oligosaccharide called 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	2	24	14	1	9	0	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



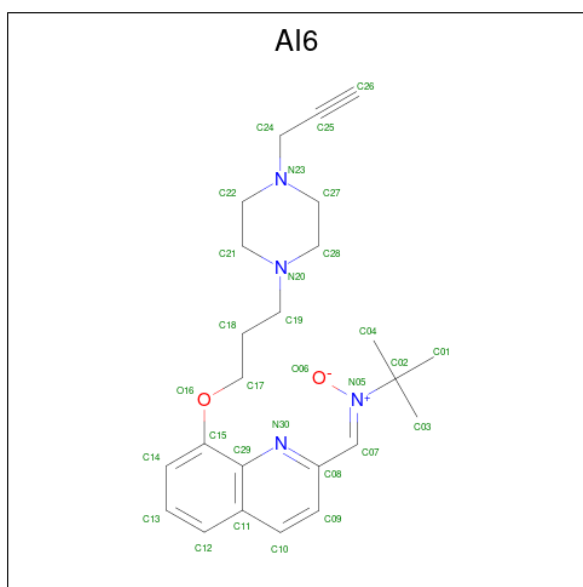
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
4	A	1	6	3	3	0	0
4	A	1	6	3	3	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



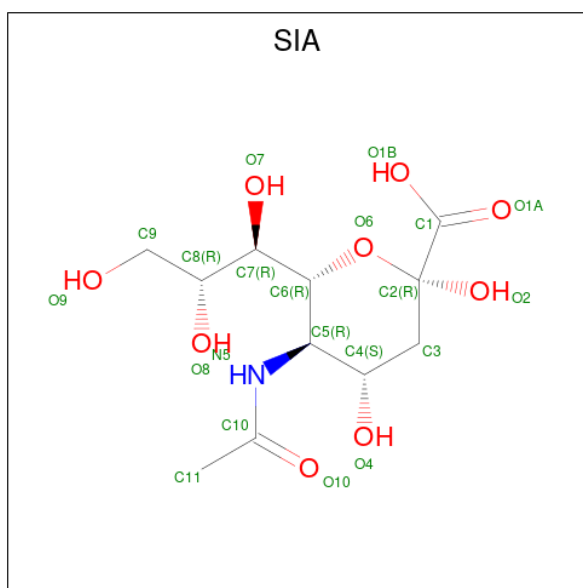
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is N-tert-butyl-1-[8-[3-(4-prop-2-ynylpiperazin-1-yl)propoxy]quinolin-2-yl]methanimine oxide (three-letter code: AI6) (formula: C<sub>24</sub>H<sub>32</sub>N<sub>4</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



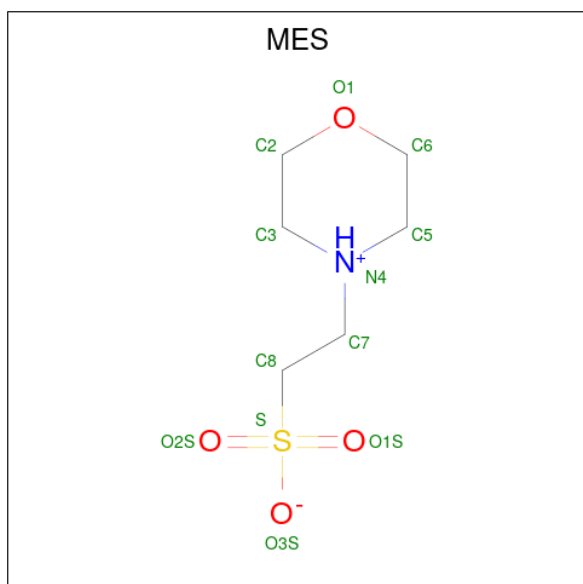
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			30	24	4	2		

- Molecule 7 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula:  $C_{11}H_{19}NO_9$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
7	A	1	21	11	1	9	0	0

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).

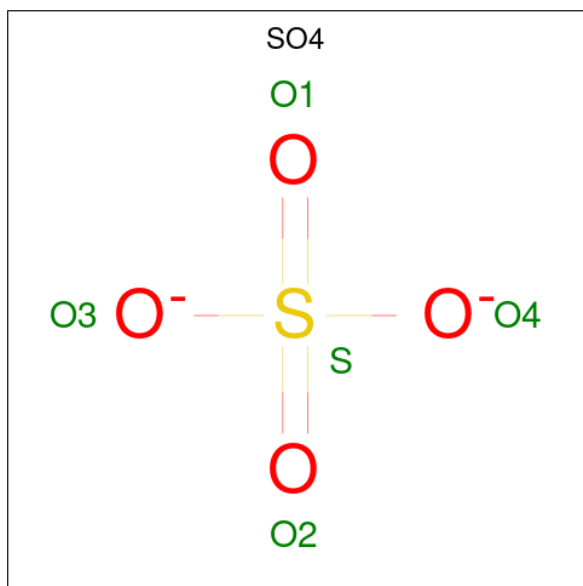


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
8	A	1	12	6	1	4	1	0	0

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	4	Total Cl 4 4	0	0

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total O S 5 4 1	0	0
10	A	1	Total O S 5 4 1	0	0
10	A	1	Total O S 5 4 1	0	0
10	A	1	Total O S 5 4 1	0	0


- Molecule 11 is water.

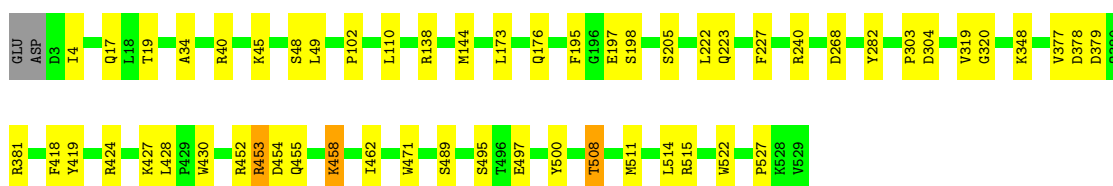
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	214	Total O 214 214	0	0

### 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. 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. 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: Cholinesterase

Chain A:  89% 10%



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

Chain B:  67% 33%



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

Chain E:  100%



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

Chain C:  50% 50%





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.22Å 156.22Å 128.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 2.13 49.70 – 2.13	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.70-2.13) 99.0 (49.70-2.13)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.01 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.180 , 0.214 0.178 , 0.211	Depositor DCC
$R_{free}$ test set	2223 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.5	Xtriage
Anisotropy	0.258	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>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4709	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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, MES, CL, AI6, FUC, GOL, SIA, 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	0.48	0/4347	0.61	0/5901

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4224	0	4122	34	0
2	B	38	0	34	0	0
2	D	38	0	34	0	0
2	E	38	0	34	0	0
3	C	24	0	22	0	0
4	A	18	0	24	1	0
5	A	28	0	26	0	0
6	A	30	0	0	0	0
7	A	21	0	18	0	0
8	A	12	0	12	3	0
9	A	4	0	0	1	0
10	A	20	0	0	0	0
11	A	214	0	0	7	0
All	All	4709	0	4326	34	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 (34) 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:138:ARG:NH2	11:A:701:HOH:O	1.98	0.96
1:A:102:PRO:O	11:A:701:HOH:O	1.83	0.95
1:A:452:ARG:NH1	11:A:703:HOH:O	2.17	0.76
1:A:515:ARG:NH1	8:A:606:MES:H71	2.15	0.60
1:A:453:ARG:N	1:A:453:ARG:HD2	2.18	0.59
1:A:454:ASP:OD2	11:A:702:HOH:O	2.16	0.58
1:A:514:LEU:HD12	8:A:606:MES:H52	1.84	0.58
1:A:515:ARG:HH12	8:A:606:MES:H71	1.69	0.58
1:A:522:TRP:O	1:A:527:PRO:HD3	2.05	0.56
1:A:227:PHE:CE1	1:A:303:PRO:HB2	2.41	0.56
1:A:497:GLU:HG3	11:A:758:HOH:O	2.09	0.52
1:A:4:ILE:HD11	1:A:17:GLN:HG2	1.94	0.49
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.47	0.49
1:A:320:GLY:HA3	1:A:419:TYR:CE2	2.49	0.48
1:A:427:LYS:HE3	1:A:455:GLN:OE1	2.15	0.47
1:A:319:VAL:O	1:A:418:PHE:HA	2.15	0.47
1:A:381:ARG:HB3	1:A:381:ARG:NH1	2.30	0.46
1:A:424:ARG:NH1	1:A:428:LEU:HD12	2.30	0.46
1:A:458:LYS:O	1:A:462:ILE:HG12	2.17	0.45
1:A:34:ALA:HB2	1:A:173:LEU:HD23	1.97	0.45
1:A:197:GLU:HA	1:A:223:GLN:O	2.17	0.44
1:A:508:THR:HG22	11:A:746:HOH:O	2.17	0.44
1:A:378:ASP:OD2	11:A:704:HOH:O	2.21	0.44
1:A:205:SER:HB3	1:A:222:LEU:HD21	2.00	0.44
1:A:320:GLY:HA3	1:A:419:TYR:CZ	2.53	0.43
1:A:49:LEU:HD23	1:A:49:LEU:HA	1.87	0.42
1:A:45:LYS:HE3	4:A:607:GOL:H2	2.01	0.42
1:A:427:LYS:HB3	1:A:427:LYS:HE2	1.81	0.42
1:A:304:ASP:OD2	1:A:304:ASP:N	2.51	0.42
1:A:428:LEU:HD13	1:A:430:TRP:H	1.84	0.42
1:A:240:ARG:HG2	1:A:240:ARG:HH11	1.86	0.41
1:A:40:ARG:HG2	9:A:610:CL:CL	2.58	0.41
1:A:227:PHE:CD1	1:A:227:PHE:C	2.94	0.40
1:A:240:ARG:HG2	1:A:240:ARG:NH1	2.37	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	A	528/529 (100%)	504 (96%)	24 (4%)	0	100   100

There are no Ramachandran outliers to report.

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

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	455/454 (100%)	436 (96%)	19 (4%)	30   26

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	48	SER
1	A	110[A]	LEU
1	A	110[B]	LEU
1	A	144	MET
1	A	176	GLN
1	A	195	PHE
1	A	198	SER
1	A	268	ASP
1	A	282	TYR
1	A	348	LYS
1	A	377	VAL
1	A	379	ASP

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Mol	Chain	Res	Type
1	A	453	ARG
1	A	458	LYS
1	A	471	TRP
1	A	489	SER
1	A	495	SER
1	A	508	THR

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

### 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](#)

11 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	NAG	B	1	1,2	14,14,15	0.44	0	17,19,21	0.65	0
2	NAG	B	2	2	14,14,15	0.27	0	17,19,21	0.53	0
2	FUC	B	3	2	10,10,11	1.63	2 (20%)	14,14,16	1.37	3 (21%)
3	NAG	C	1	3,1	14,14,15	0.37	0	17,19,21	0.45	0
3	FUC	C	2	3	10,10,11	1.51	3 (30%)	14,14,16	1.55	2 (14%)
2	NAG	D	1	1,2	14,14,15	0.53	0	17,19,21	0.59	0
2	NAG	D	2	2	14,14,15	0.45	0	17,19,21	0.55	0
2	FUC	D	3	2	10,10,11	2.03	2 (20%)	14,14,16	1.66	4 (28%)
2	NAG	E	1	1,2	14,14,15	0.30	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	E	2	2	14,14,15	0.37	0	17,19,21	0.55	0
2	FUC	E	3	2	10,10,11	0.99	0	14,14,16	0.86	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	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	FUC	B	3	2	-	-	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	FUC	C	2	3	-	-	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	FUC	D	3	2	-	-	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	FUC	E	3	2	-	-	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	FUC	C1-C2	4.45	1.62	1.52
2	B	3	FUC	O5-C5	3.11	1.50	1.43
2	D	3	FUC	C2-C3	3.00	1.56	1.52
3	C	2	FUC	C2-C3	2.95	1.56	1.52
3	C	2	FUC	C1-C2	2.68	1.58	1.52
3	C	2	FUC	C4-C3	2.15	1.57	1.52
2	B	3	FUC	C1-C2	2.12	1.57	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	FUC	C1-C2-C3	3.84	114.39	109.67
2	D	3	FUC	C1-C2-C3	3.12	113.50	109.67
2	D	3	FUC	O5-C5-C4	2.91	114.73	109.52
2	D	3	FUC	C1-O5-C5	2.76	119.03	112.78
2	D	3	FUC	O2-C2-C1	2.40	114.06	109.15
2	B	3	FUC	C1-C2-C3	2.35	112.56	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	FUC	O5-C5-C4	2.33	113.70	109.52
3	C	2	FUC	C2-C3-C4	2.23	114.75	110.89
2	B	3	FUC	C1-O5-C5	2.17	117.69	112.78

There are no chirality outliers.

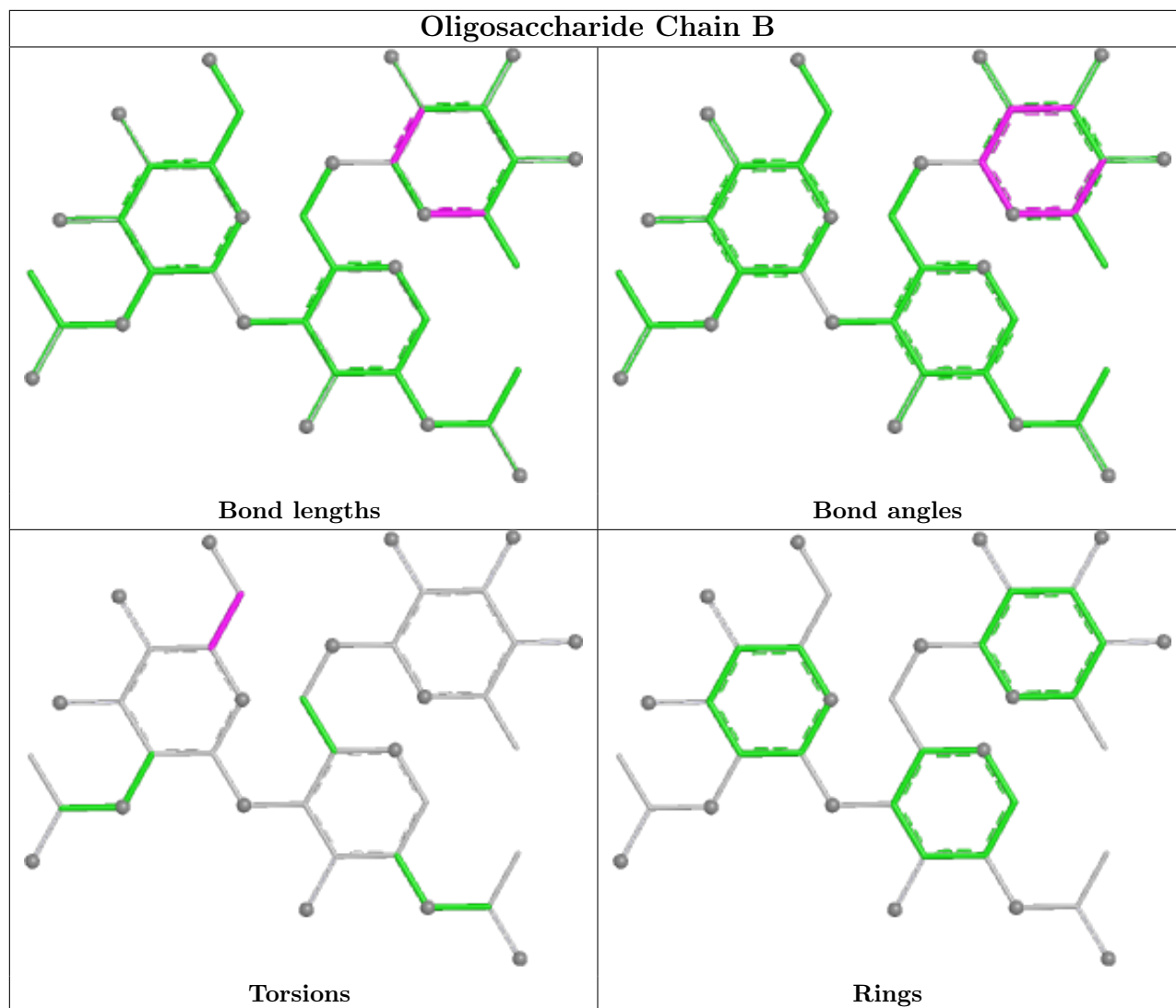
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6

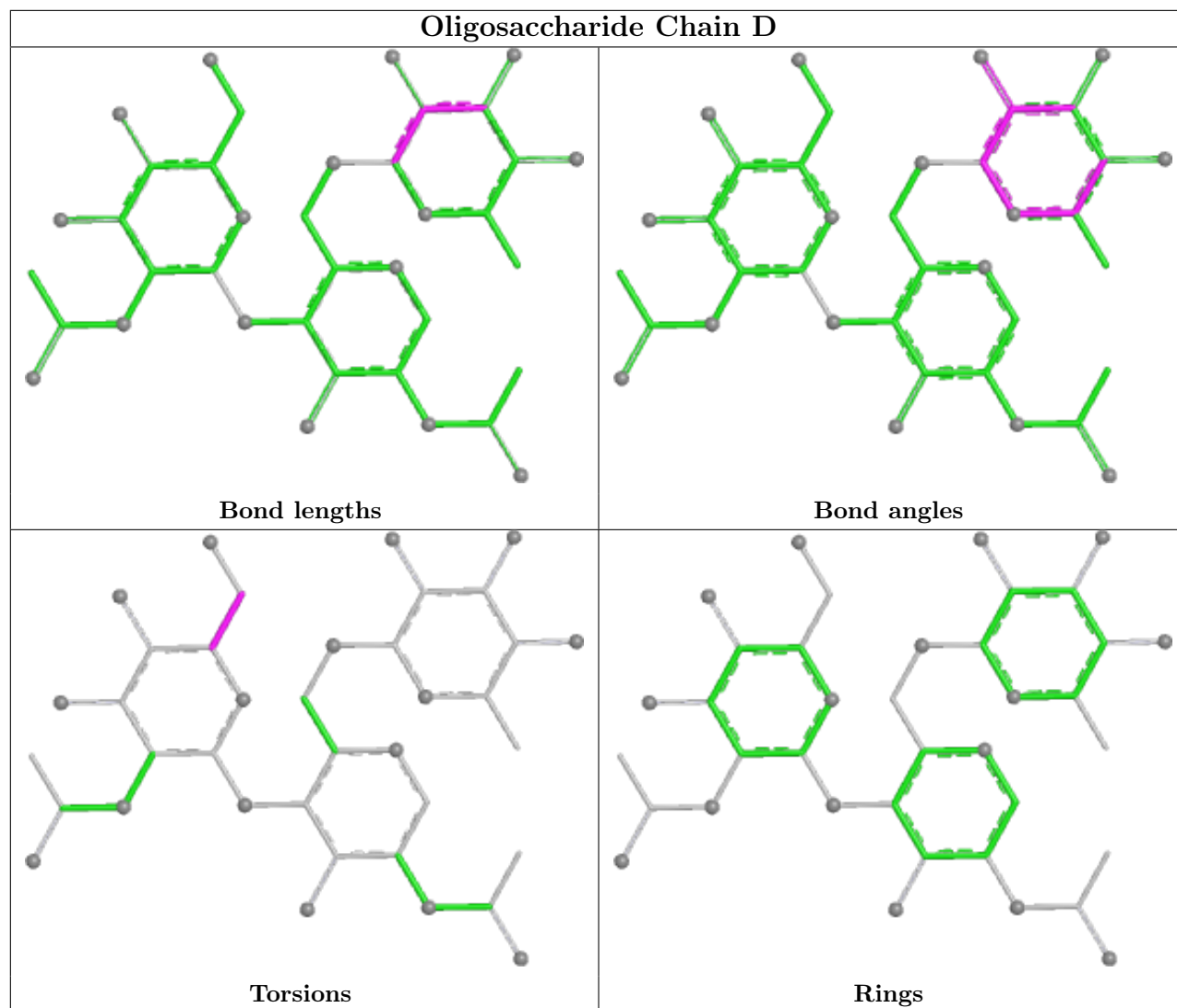
There are no ring outliers.

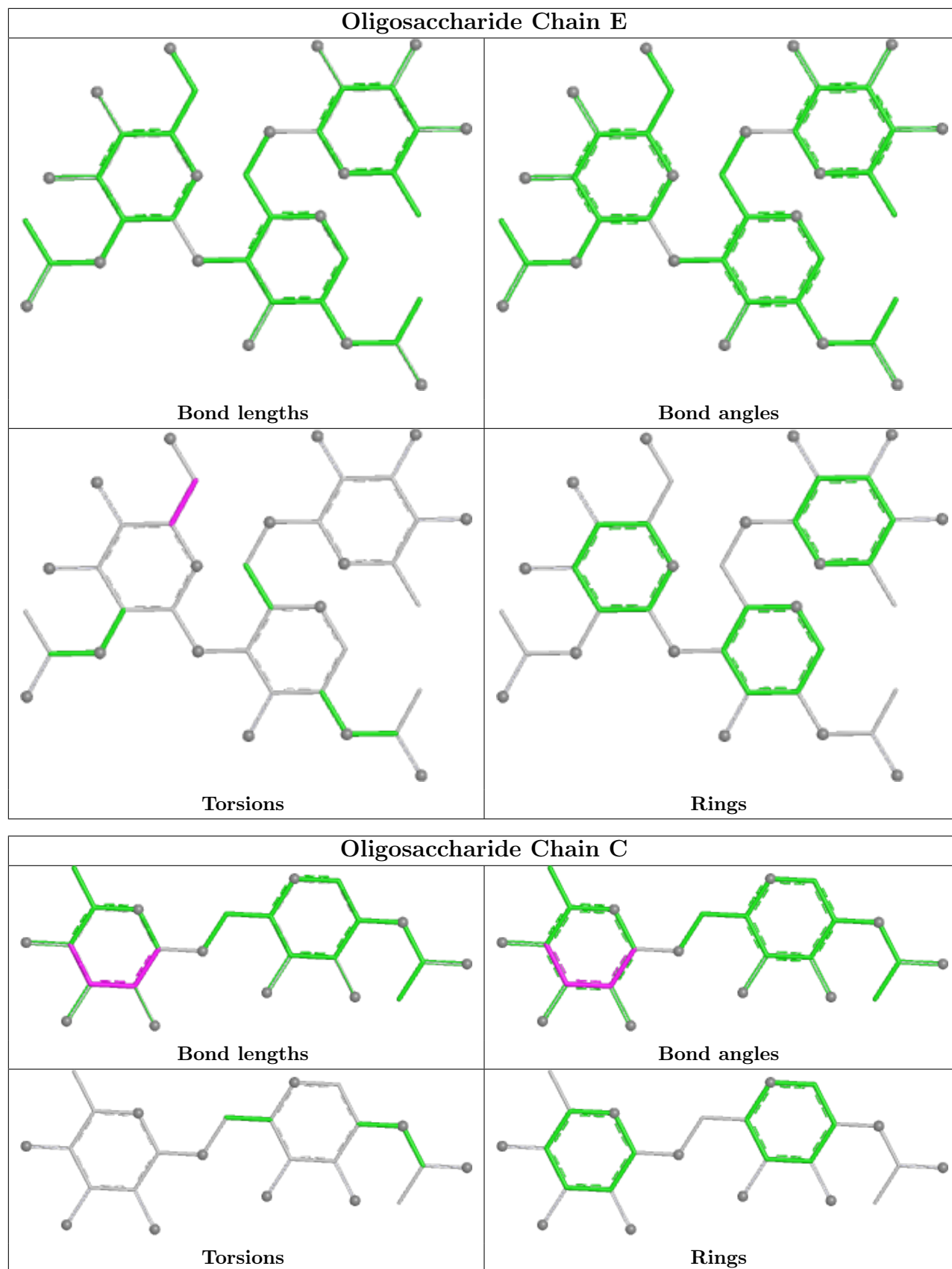
No monomer is involved in short contacts.

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

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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
10	SO4	A	616	-	4,4,4	0.15	0	6,6,6	0.13	0
4	GOL	A	608	-	5,5,5	0.83	0	5,5,5	1.09	0
4	GOL	A	601	-	5,5,5	1.18	0	5,5,5	0.85	0
10	SO4	A	614	-	4,4,4	0.17	0	6,6,6	0.35	0
10	SO4	A	615	-	4,4,4	0.18	0	6,6,6	0.10	0
5	NAG	A	602	1	14,14,15	0.38	0	17,19,21	0.43	0
6	AI6	A	604	-	31,32,32	3.91	13 (41%)	42,44,44	1.88	12 (28%)
7	SIA	A	605	-	21,21,21	1.81	5 (23%)	25,31,31	2.11	5 (20%)
4	GOL	A	607	-	5,5,5	0.94	0	5,5,5	0.97	0
8	MES	A	606	-	12,12,12	2.08	1 (8%)	14,16,16	2.04	4 (28%)
5	NAG	A	603	1	14,14,15	0.57	0	17,19,21	0.76	1 (5%)
10	SO4	A	613	-	4,4,4	0.20	0	6,6,6	0.22	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	GOL	A	608	-	-	2/4/4/4	-
4	GOL	A	601	-	-	0/4/4/4	-
5	NAG	A	602	1	-	2/6/23/26	0/1/1/1
6	AI6	A	604	-	-	10/18/30/30	0/3/3/3
7	SIA	A	605	-	-	10/20/38/38	0/1/1/1
4	GOL	A	607	-	-	0/4/4/4	-
8	MES	A	606	-	-	2/6/14/14	0/1/1/1
5	NAG	A	603	1	-	1/6/23/26	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	604	AI6	C24-N23	-16.78	1.28	1.46
6	A	604	AI6	C19-N20	-8.11	1.28	1.47
8	A	606	MES	C8-S	-6.87	1.67	1.77
7	A	605	SIA	O6-C2	4.79	1.48	1.43
6	A	604	AI6	C24-C25	4.77	1.53	1.47
6	A	604	AI6	C08-C07	4.58	1.57	1.47
7	A	605	SIA	C2-C1	3.48	1.59	1.53
6	A	604	AI6	C22-N23	-3.20	1.38	1.46
6	A	604	AI6	C28-N20	-3.01	1.38	1.46
6	A	604	AI6	C27-N23	-2.99	1.38	1.46
6	A	604	AI6	C21-N20	-2.97	1.38	1.46
6	A	604	AI6	C11-C29	-2.89	1.38	1.42
7	A	605	SIA	C3-C2	2.66	1.55	1.51
6	A	604	AI6	C08-N30	2.44	1.35	1.33
7	A	605	SIA	C7-C6	2.35	1.55	1.53
7	A	605	SIA	C6-C5	2.33	1.56	1.53
6	A	604	AI6	C01-C02	2.17	1.57	1.52
6	A	604	AI6	C10-C09	2.14	1.41	1.36
6	A	604	AI6	O16-C15	2.01	1.42	1.36

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	605	SIA	O1A-C1-C2	-7.59	112.10	123.59
6	A	604	AI6	C08-N30-C29	4.90	121.82	118.11
6	A	604	AI6	O16-C15-C29	4.67	120.90	115.16
8	A	606	MES	C5-N4-C3	4.61	119.20	108.83
8	A	606	MES	O2S-S-C8	3.69	111.36	106.92
6	A	604	AI6	C03-C02-N05	3.54	116.33	108.09
7	A	605	SIA	O6-C6-C7	-3.35	102.13	107.29
7	A	605	SIA	C6-C5-N5	3.18	116.19	110.91
6	A	604	AI6	C09-C08-N30	-3.14	118.76	122.79
6	A	604	AI6	C07-C08-N30	2.92	124.21	115.29
7	A	605	SIA	C5-N5-C10	2.74	129.84	123.18
5	A	603	NAG	C1-O5-C5	2.68	115.82	112.19
6	A	604	AI6	C24-N23-C22	-2.61	108.68	111.71
8	A	606	MES	O1S-S-C8	2.61	110.05	106.92
6	A	604	AI6	C09-C10-C11	-2.51	116.94	120.82
6	A	604	AI6	C28-N20-C21	2.50	114.45	108.83
6	A	604	AI6	O16-C15-C14	-2.50	118.96	124.46
6	A	604	AI6	C02-N05-C07	2.42	124.71	122.50
6	A	604	AI6	C24-N23-C27	2.41	114.52	111.71
8	A	606	MES	C7-N4-C3	2.31	117.15	111.23

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	604	AI6	C10-C09-C08	2.21	121.76	119.38
7	A	605	SIA	O2-C2-C1	-2.16	106.36	110.76

There are no chirality outliers.

All (27) torsion outliers are listed below:

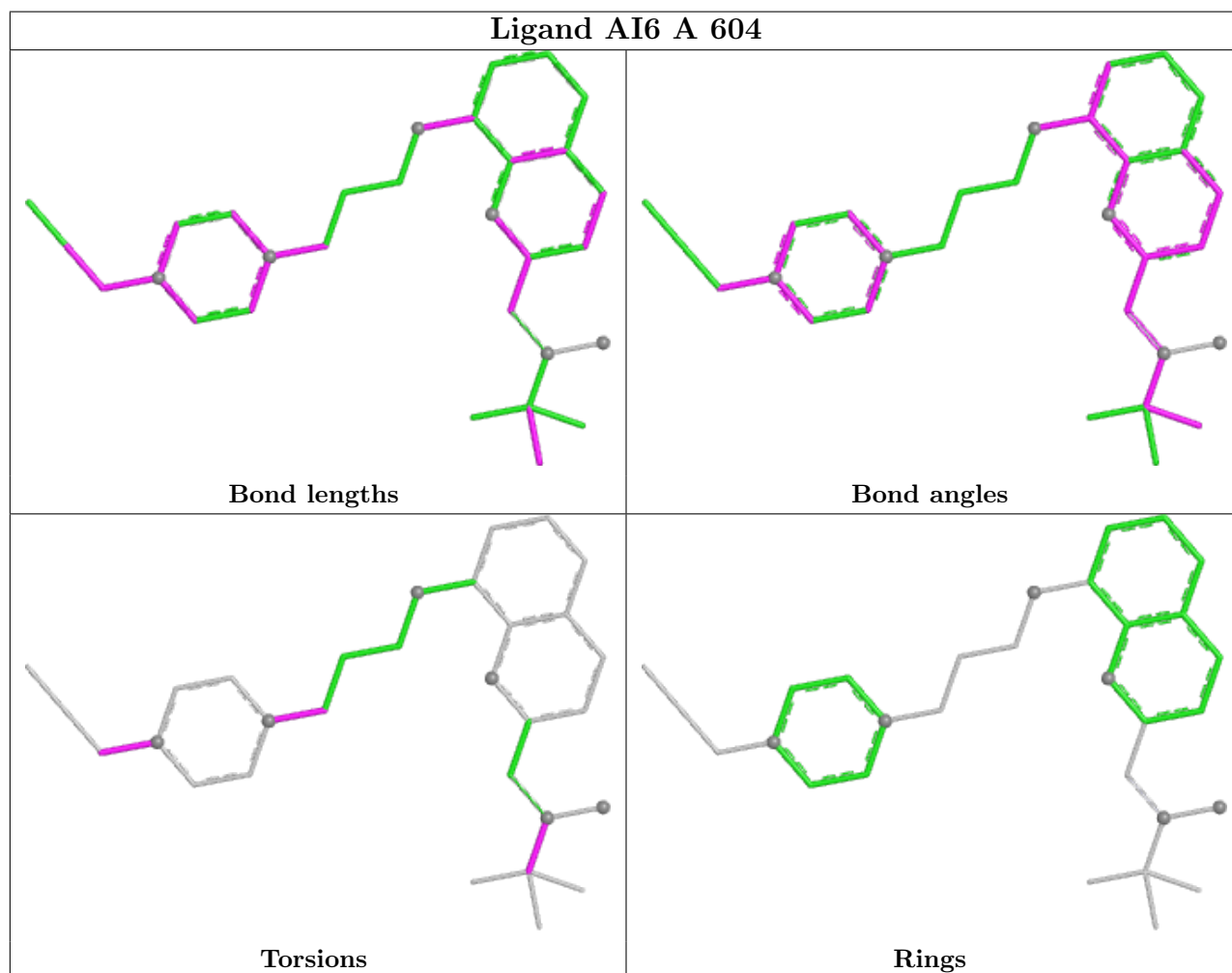
Mol	Chain	Res	Type	Atoms
4	A	608	GOL	C1-C2-C3-O3
6	A	604	AI6	C25-C24-N23-C22
6	A	604	AI6	C25-C24-N23-C27
7	A	605	SIA	O1B-C1-C2-O6
7	A	605	SIA	O6-C6-C7-O7
6	A	604	AI6	C18-C19-N20-C21
6	A	604	AI6	C01-C02-N05-C07
6	A	604	AI6	C01-C02-N05-O06
6	A	604	AI6	C03-C02-N05-C07
6	A	604	AI6	C03-C02-N05-O06
6	A	604	AI6	C04-C02-N05-C07
6	A	604	AI6	C04-C02-N05-O06
5	A	603	NAG	O5-C5-C6-O6
7	A	605	SIA	C4-C5-N5-C10
5	A	602	NAG	C4-C5-C6-O6
4	A	608	GOL	O2-C2-C3-O3
6	A	604	AI6	C18-C19-N20-C28
5	A	602	NAG	O5-C5-C6-O6
7	A	605	SIA	C5-C6-C7-O7
7	A	605	SIA	O6-C6-C7-C8
7	A	605	SIA	C6-C7-C8-O8
7	A	605	SIA	O1A-C1-C2-C3
7	A	605	SIA	C6-C5-N5-C10
7	A	605	SIA	O1A-C1-C2-O6
7	A	605	SIA	O1A-C1-C2-O2
8	A	606	MES	N4-C7-C8-S
8	A	606	MES	C8-C7-N4-C5

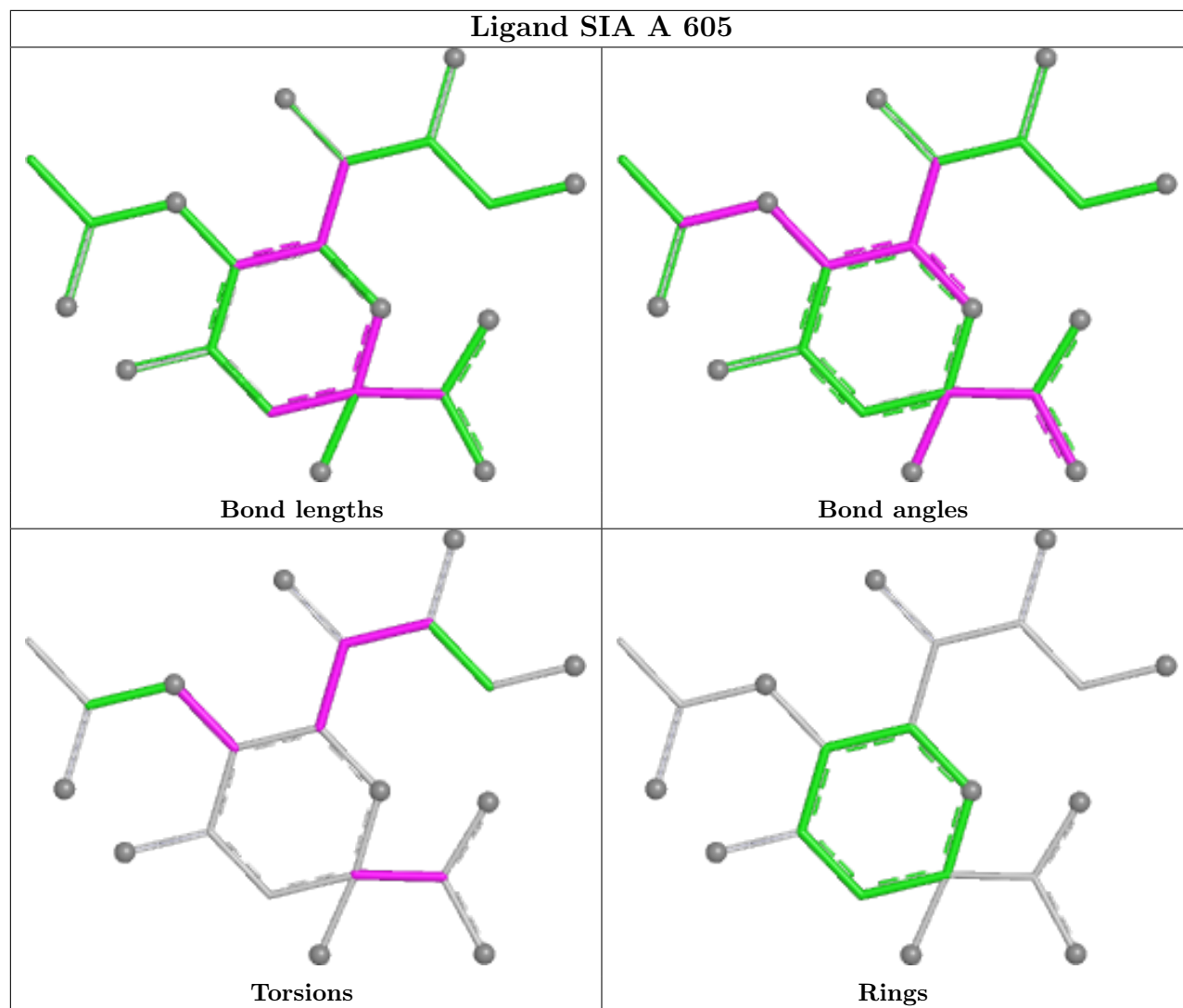
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	607	GOL	1	0
8	A	606	MES	3	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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

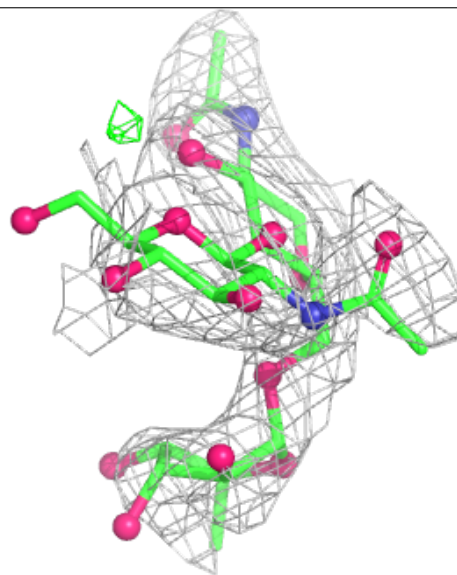
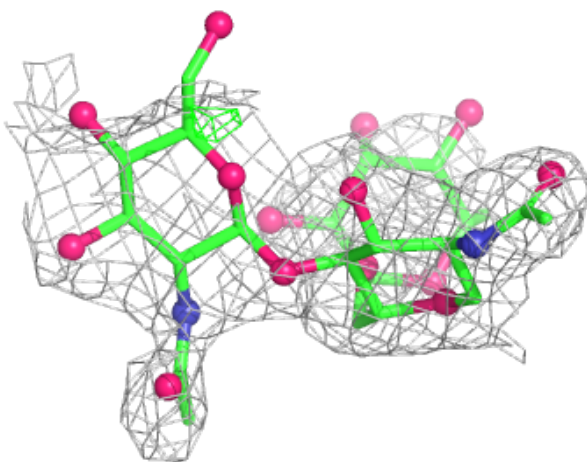
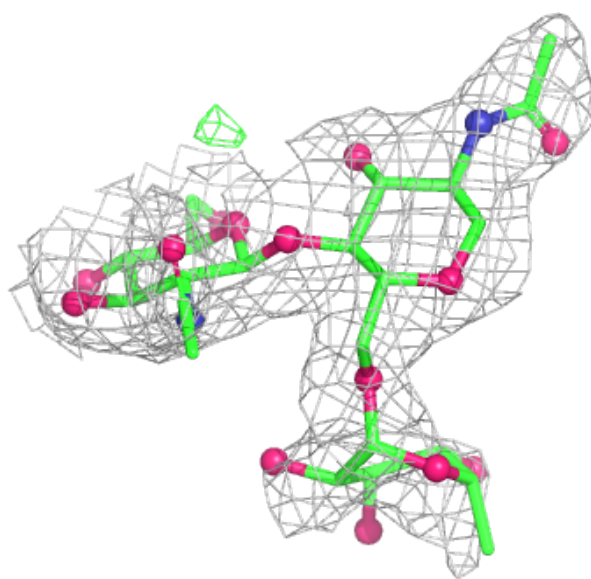
Unable to reproduce the depositors R factor - this section is therefore empty.

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.



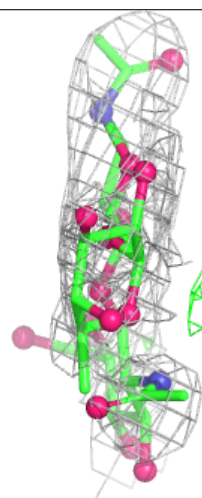
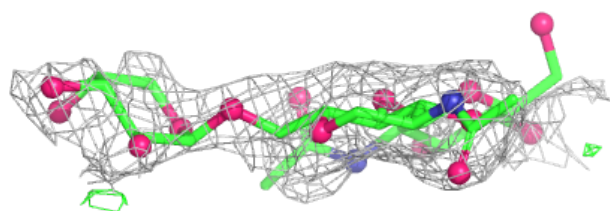
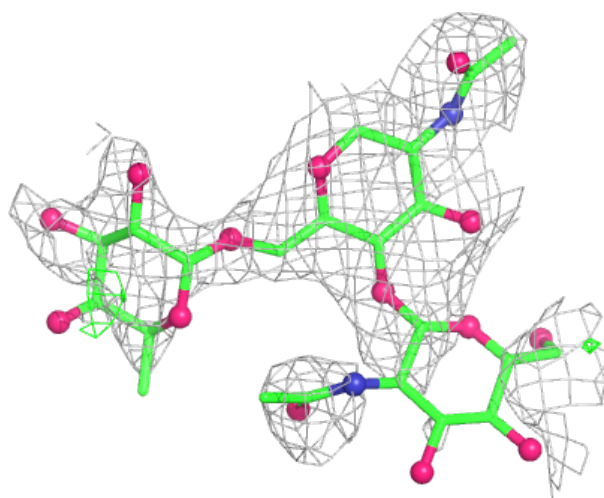
**Electron density around Chain B:**

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



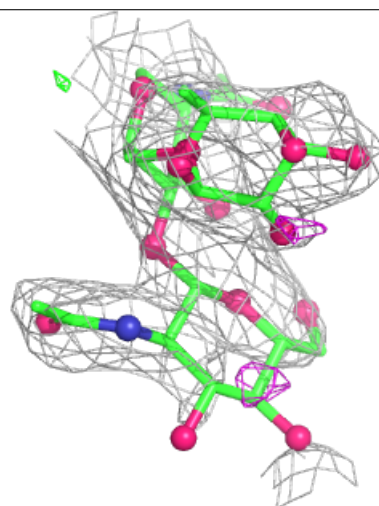
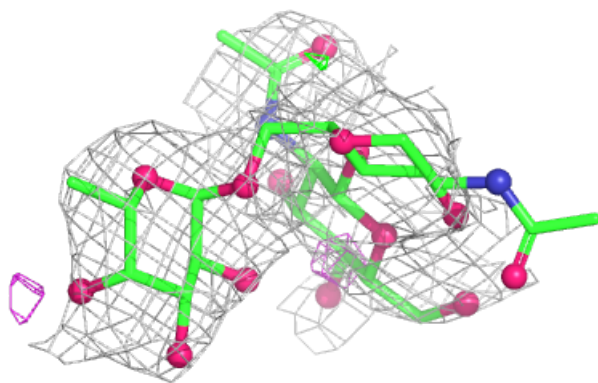
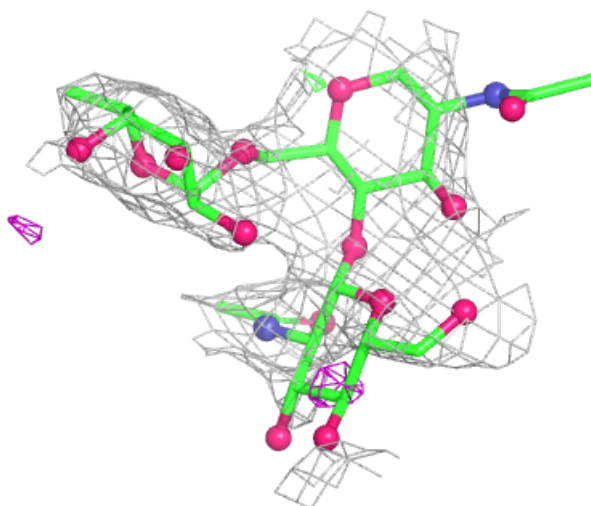
**Electron density around Chain D:**

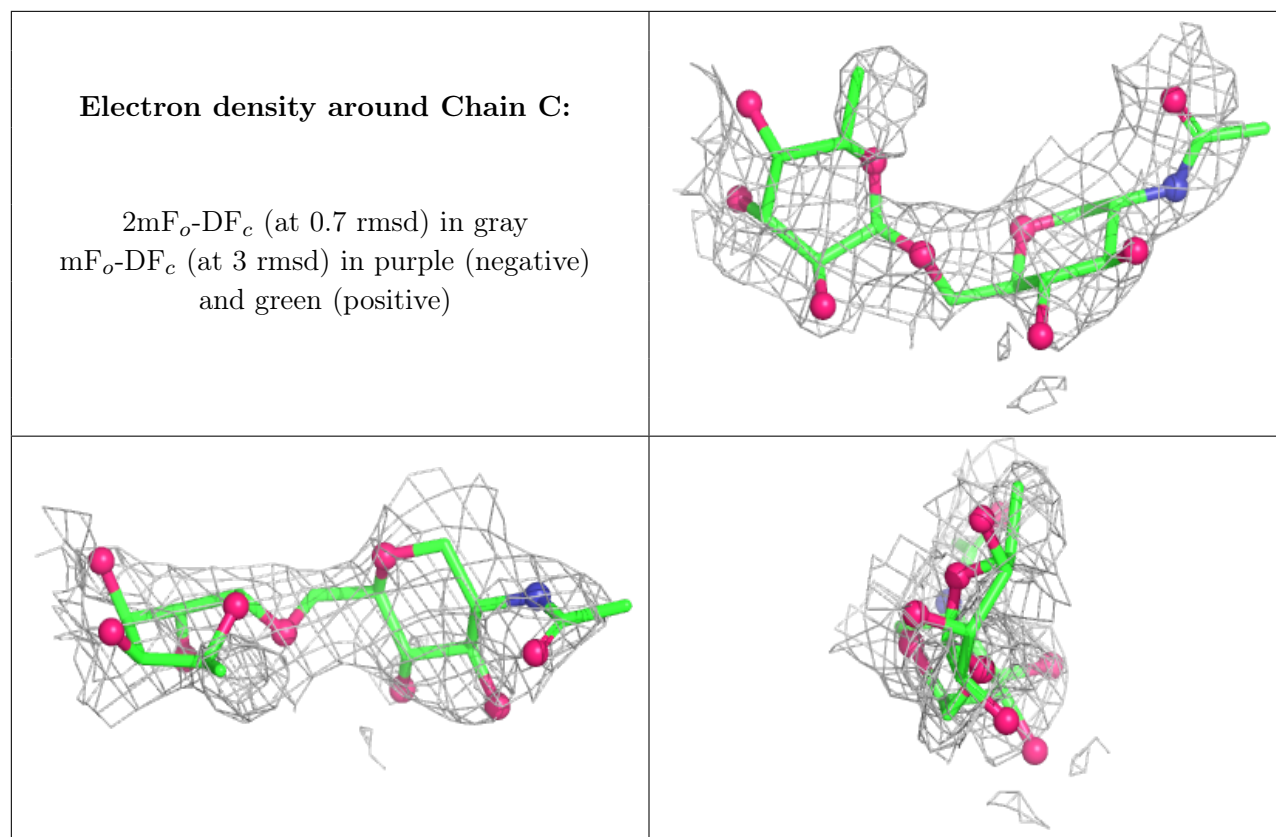
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain E:**

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





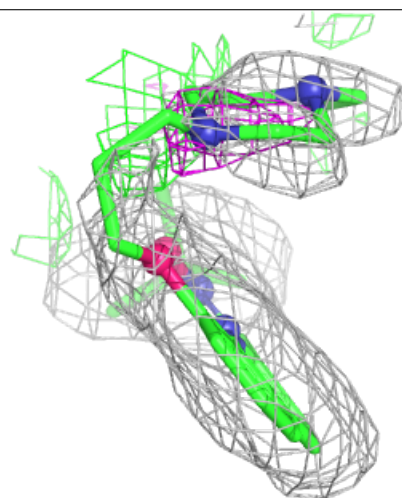
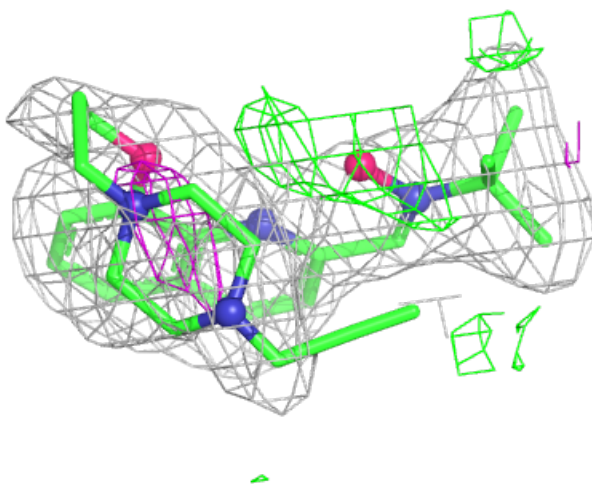
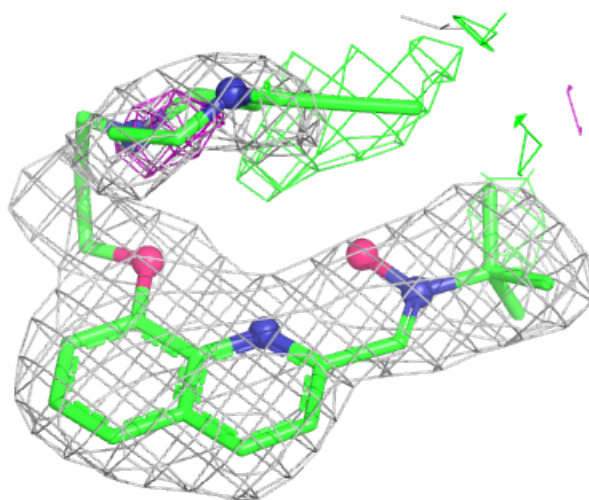
## 6.4 Ligands [i](#)

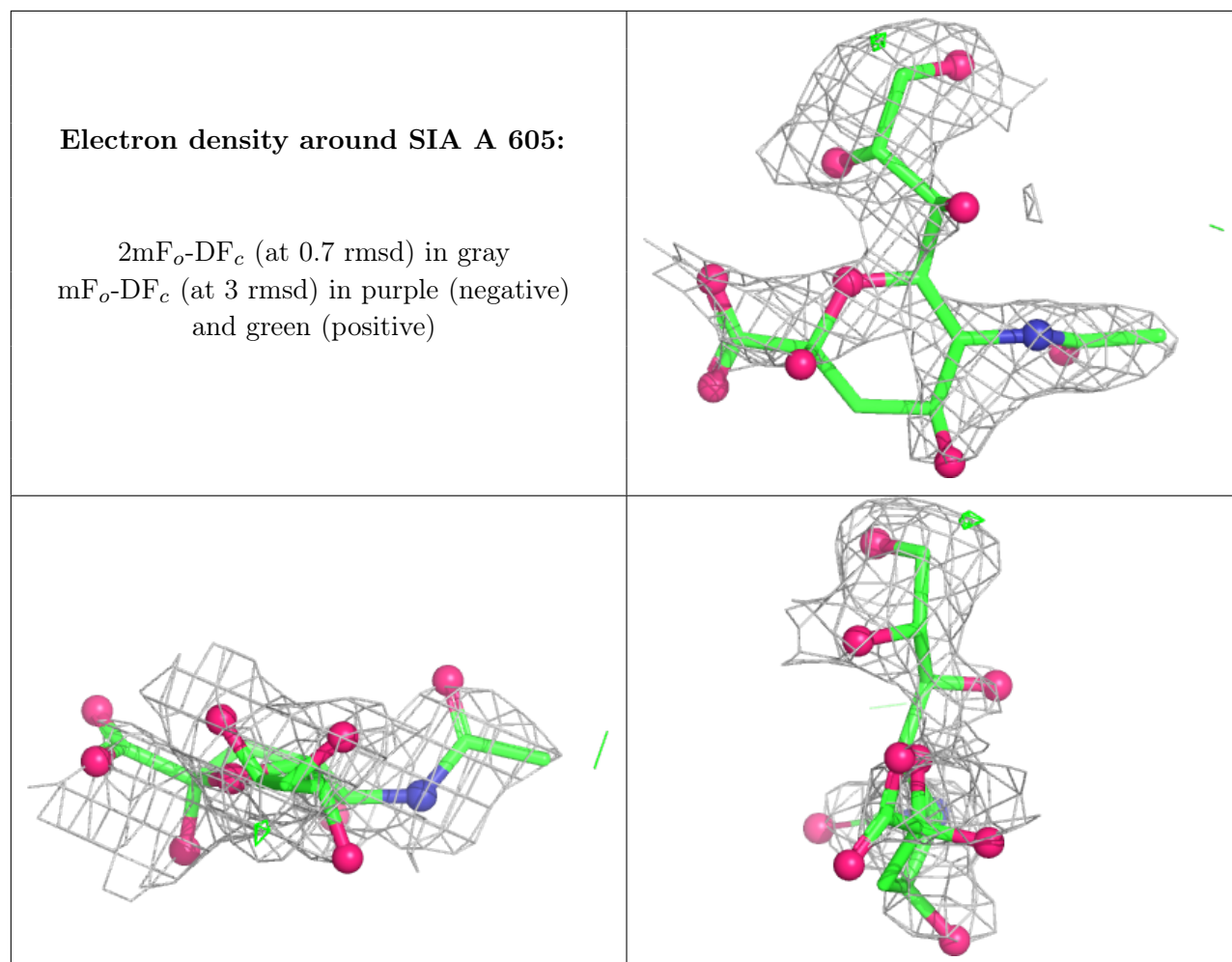
Unable to reproduce the depositor's R factor - this section is therefore empty.

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 AI6 A 604:**

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





## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.