



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2022 – 03:37 pm GMT

PDB ID : 7QHD  
Title : Human Butyrylcholinesterase in complex with (S)-1-(4-((2-(1H-indol-3-yl)ethyl)carbamoyl)benzyl)-N-(3-((1,2,3,4-tetrahydroacridin-9-yl)amino)propyl)piperidine-3-carboxamide  
Authors : Brazzolotto, X.; Jing, L.; Zhan, P.; Liu, X.; Nachon, F.  
Deposited on : 2021-12-12  
Resolution : 2.04 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>.

---

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

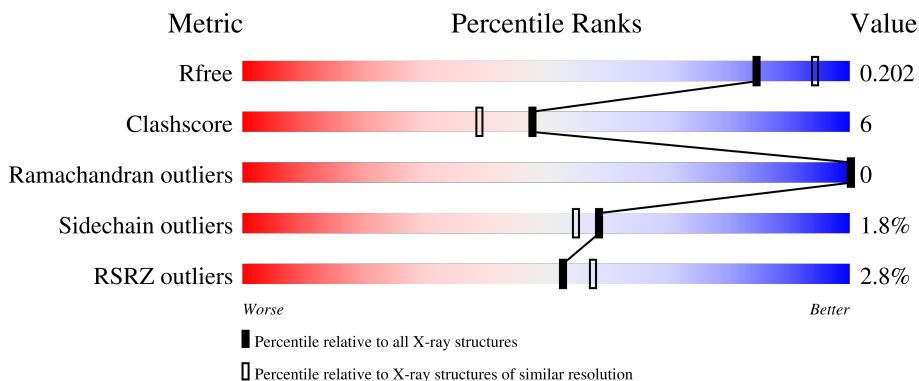
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.04 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	529	 3% 87% 12%
2	B	2	 50% 50%
3	C	3	 67% 33%
3	D	3	 67% 33%

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 4807 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	4234	2733	711	774	16	0	5	0

There are 4 discrepancies between the modelled and reference sequences:

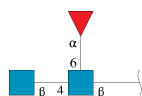
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	engineered mutation	UNP P06276
A	455	GLN	ASN	engineered mutation	UNP P06276
A	481	GLN	ASN	engineered mutation	UNP P06276
A	486	GLN	ASN	engineered mutation	UNP P06276

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



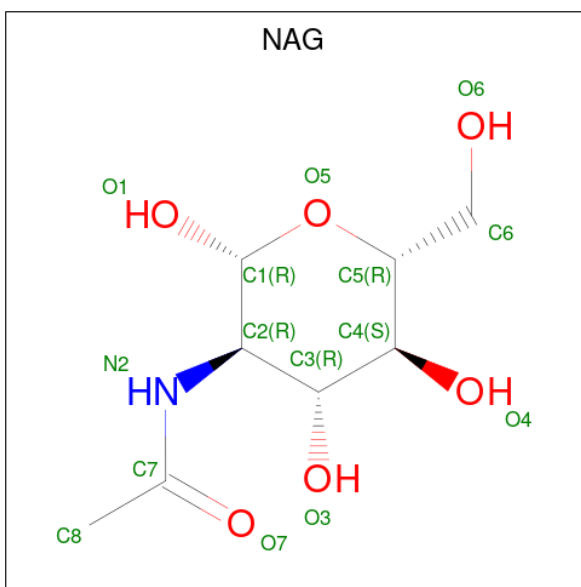
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	24	14	1	9	0	0	0

- Molecule 3 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			
3	C	3	38	22	2	14	0	0	0
3	D	3	38	22	2	14	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 5 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		
5	A	1	12	6	1	4	1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



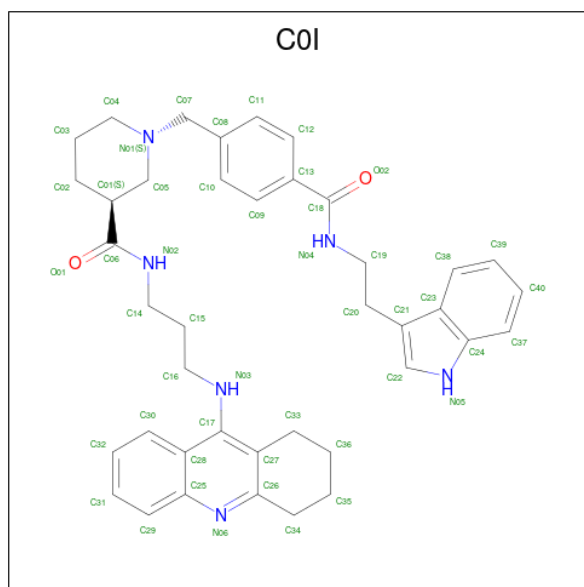
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	6	3	3	0	0
6	A	1	6	3	3	0	0
6	A	1	6	3	3	0	0

*Continued on next page...*

Continued from previous page...

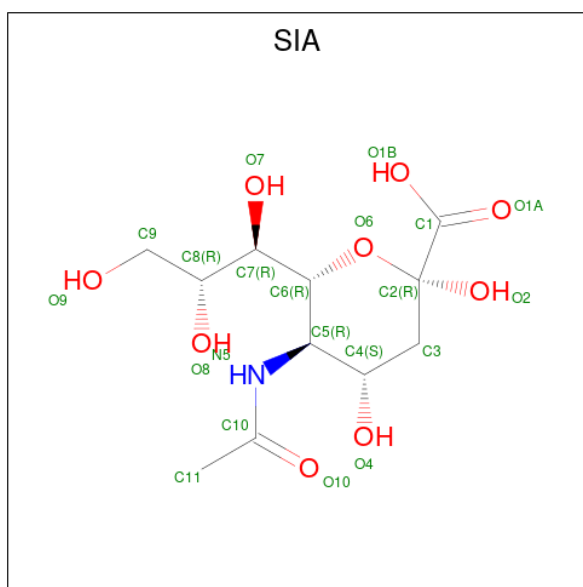
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is (3 {S})-1-[[4-[2-(1 {H}-indol-3-yl)ethylcarbamoyl]phenyl]methyl]- {N}-[3-(1,2,3,4-tetrahydroacridin-9-ylamino)propyl]piperidine-3-carboxamide (three-letter code: C0I) (formula: C<sub>40</sub>H<sub>46</sub>N<sub>6</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			48	40	6	2		

- Molecule 8 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: C<sub>11</sub>H<sub>19</sub>NO<sub>9</sub>).



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

- Molecule 9 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	7	Total	Cl	0	0
			7	7		

- Molecule 11 is water.

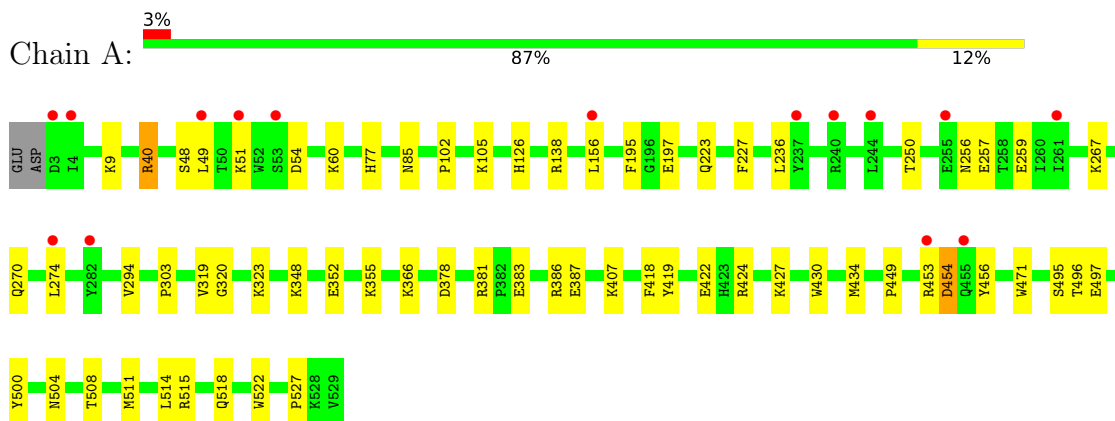
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	293	Total	O	0	0
			293	293		



### 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.

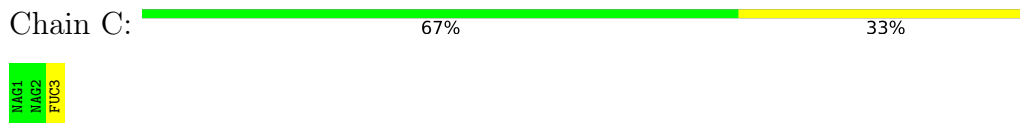
- Molecule 1: Cholinesterase



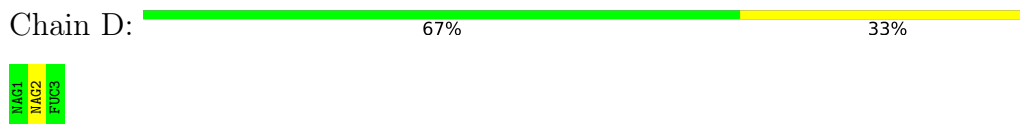
- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.52Å 154.52Å 127.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.26 – 2.04 77.26 – 2.04	Depositor EDS
% Data completeness (in resolution range)	98.2 (77.26-2.04) 98.2 (77.26-2.04)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 2.03Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.171 , 0.204 0.167 , 0.202	Depositor DCC
$R_{free}$ test set	2422 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.9	Xtrriage
Anisotropy	0.392	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	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4807	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: NAG, MES, C0I, GOL, CL, FUC, SIA, SO4

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	0.41	0/4367	0.59	0/5927

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	4234	0	4134	53	0
2	B	24	0	22	0	0
3	C	38	0	34	0	0
3	D	38	0	34	1	0
4	A	42	0	39	0	0
5	A	12	0	12	5	0
6	A	30	0	40	5	0
7	A	48	0	0	0	0
8	A	21	0	18	1	0
9	A	20	0	0	0	0
10	A	7	0	0	1	0
11	A	293	0	0	13	0
All	All	4807	0	4333	54	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 6.

All (54) 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:427:LYS:HB2	6:A:610:GOL:H12	1.58	0.83
1:A:497:GLU:OE1	11:A:701:HOH:O	1.96	0.81
1:A:430:TRP:HB3	1:A:434:MET:HE2	1.64	0.80
1:A:386:ARG:HH12	6:A:609:GOL:H2	1.48	0.78
1:A:270:GLN:O	1:A:274:LEU:HG	1.89	0.73
1:A:454:ASP:OD1	11:A:702:HOH:O	2.05	0.72
1:A:508:THR:HG22	11:A:736:HOH:O	1.91	0.69
1:A:77:HIS:ND1	11:A:705:HOH:O	2.26	0.67
1:A:515:ARG:H	5:A:604:MES:H52	1.64	0.62
1:A:48:SER:OG	11:A:703:HOH:O	2.16	0.61
1:A:85:ASN:HD22	6:A:608:GOL:H2	1.66	0.61
1:A:407:LYS:NZ	11:A:708:HOH:O	2.35	0.60
1:A:102:PRO:O	1:A:138:ARG:NH2	2.40	0.55
1:A:378:ASP:HB3	1:A:381:ARG:HE	1.71	0.54
1:A:500:TYR:CZ	1:A:511[B]:MET:HB2	2.43	0.54
1:A:51:LYS:HD3	1:A:51:LYS:H	1.75	0.52
1:A:496:THR:HG23	1:A:497:GLU:H	1.74	0.52
1:A:40:ARG:NH1	11:A:712:HOH:O	2.40	0.51
1:A:250:THR:HB	1:A:267:LYS:HD2	1.92	0.51
1:A:60:LYS:NZ	8:A:607:SIA:O1B	2.35	0.51
1:A:236:LEU:HD22	11:A:715:HOH:O	2.11	0.50
1:A:378:ASP:HB3	1:A:381:ARG:NE	2.26	0.50
1:A:522:TRP:O	1:A:527:PRO:HD3	2.11	0.50
1:A:51:LYS:HD3	1:A:51:LYS:N	2.27	0.50
1:A:54:ASP:OD1	1:A:54:ASP:N	2.37	0.49
1:A:227:PHE:CE1	1:A:303:PRO:HB2	2.48	0.48
1:A:352:GLU:HG3	11:A:940:HOH:O	2.13	0.48
1:A:319:VAL:O	1:A:418:PHE:HA	2.14	0.47
1:A:256:ASN:HB3	1:A:259:GLU:HB2	1.96	0.47
11:A:990:HOH:O	3:D:2:NAG:H61	2.15	0.47
1:A:156:LEU:HD13	1:A:257:GLU:HB3	1.96	0.47
1:A:320:GLY:HA3	1:A:419:TYR:CE2	2.50	0.47
1:A:500:TYR:CZ	1:A:511[A]:MET:HB2	2.50	0.46
1:A:514:LEU:HD12	5:A:604:MES:H52	1.97	0.46
1:A:323:LYS:HE2	11:A:710:HOH:O	2.16	0.46
1:A:515:ARG:NH1	5:A:604:MES:H71	2.32	0.45
1:A:236:LEU:HD21	1:A:294:VAL:HB	1.99	0.44

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:GLN:HE22	5:A:604:MES:H22	1.83	0.44
1:A:383:GLU:O	1:A:387:GLU:HG3	2.17	0.44
1:A:355:LYS:HG2	1:A:366:LYS:HE3	2.00	0.43
1:A:227:PHE:CD1	1:A:227:PHE:C	2.92	0.43
1:A:496:THR:HG22	11:A:967:HOH:O	2.17	0.43
1:A:197:GLU:HA	1:A:223:GLN:O	2.18	0.42
1:A:40:ARG:HG3	10:A:617:CL:CL	2.57	0.42
1:A:449:PRO:HA	1:A:456:TYR:CD2	2.54	0.42
1:A:430:TRP:CE3	1:A:434:MET:HE1	2.54	0.42
1:A:386:ARG:HH12	6:A:609:GOL:C2	2.26	0.41
1:A:515:ARG:HH12	5:A:604:MES:H71	1.85	0.41
1:A:422:GLU:HG3	1:A:504:ASN:HB3	2.01	0.41
1:A:453:ARG:HA	1:A:453:ARG:HD3	1.97	0.41
1:A:49:LEU:HD12	1:A:49:LEU:HA	1.92	0.40
1:A:126:HIS:HE1	11:A:702:HOH:O	2.04	0.40
1:A:386:ARG:NH1	6:A:609:GOL:H2	2.25	0.40
1:A:424:ARG:NH2	1:A:430:TRP:O	2.53	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	530/529 (100%)	512 (97%)	18 (3%)	0	<b>100</b> <b>100</b>

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	457/454 (101%)	449 (98%)	8 (2%)	59 55

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

Mol	Chain	Res	Type
1	A	9	LYS
1	A	40	ARG
1	A	105	LYS
1	A	195	PHE
1	A	348	LYS
1	A	454	ASP
1	A	471	TRP
1	A	495	SER

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](#)

8 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	2,1	14,14,15	0.34	0	17,19,21	0.40	0
2	FUC	B	2	2	10,10,11	0.94	0	14,14,16	1.31	2 (14%)
3	NAG	C	1	3,1	14,14,15	0.26	0	17,19,21	0.46	0
3	NAG	C	2	3	14,14,15	0.32	0	17,19,21	0.35	0
3	FUC	C	3	3	10,10,11	1.41	1 (10%)	14,14,16	1.20	1 (7%)
3	NAG	D	1	3,1	14,14,15	0.47	0	17,19,21	0.50	0
3	NAG	D	2	3	14,14,15	0.35	0	17,19,21	0.47	0
3	FUC	D	3	3	10,10,11	0.85	0	14,14,16	0.94	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	2,1	-	0/6/23/26	0/1/1/1
2	FUC	B	2	2	-	-	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	FUC	C	3	3	-	-	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	FUC	D	3	3	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	FUC	C1-C2	2.40	1.57	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	FUC	O5-C5-C4	2.95	114.81	109.52
3	C	3	FUC	C1-C2-C3	2.91	113.24	109.67
2	B	2	FUC	C1-O5-C5	2.56	118.58	112.78

There are no chirality outliers.

All (4) torsion outliers are listed below:

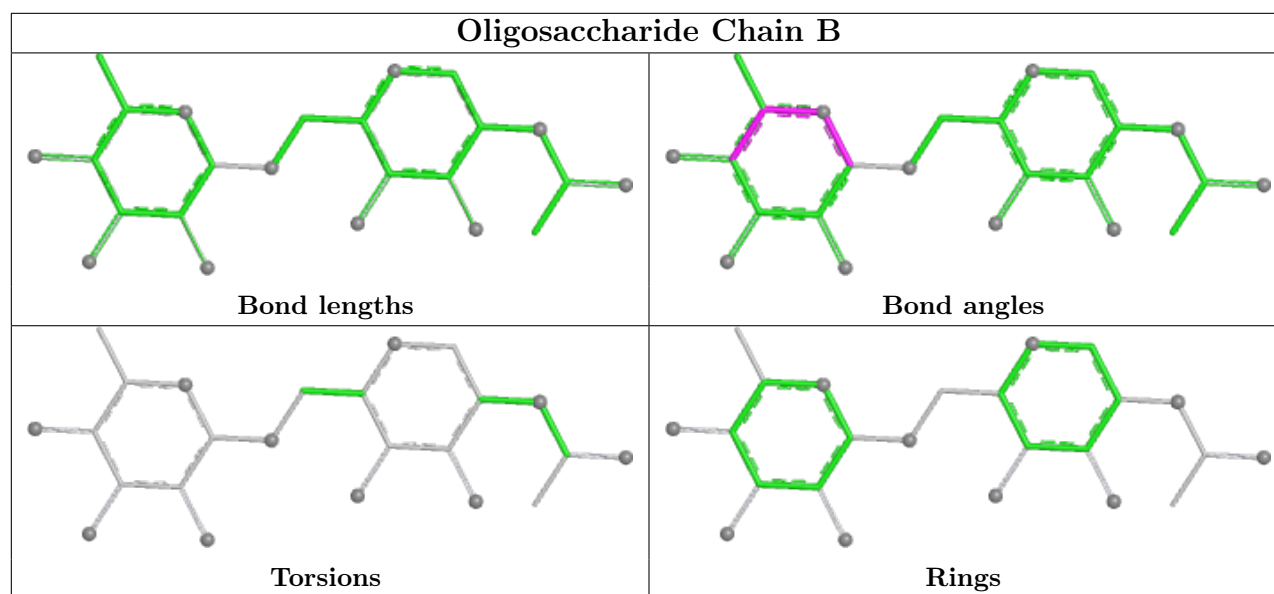
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6

There are no ring outliers.

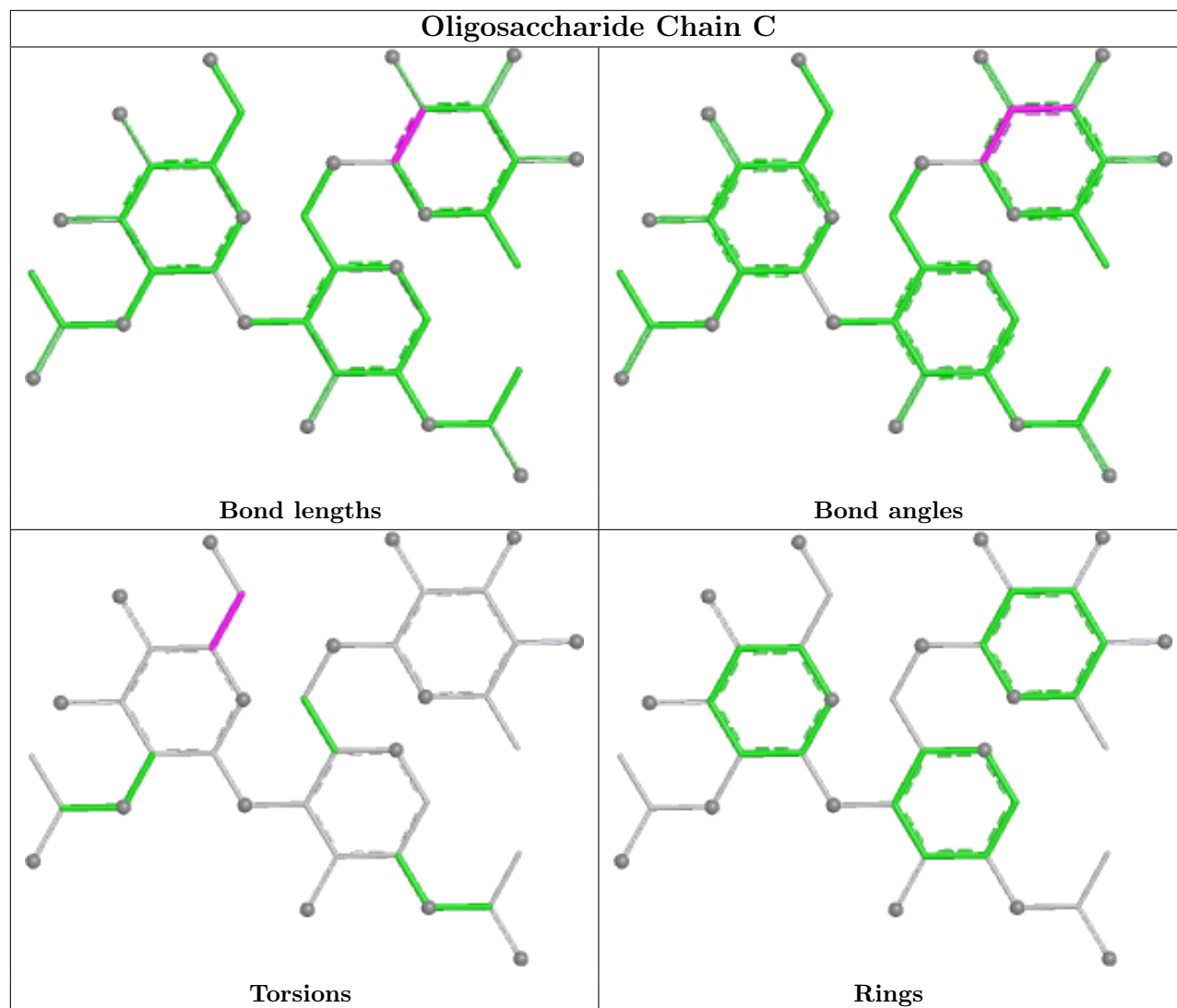
1 monomer is involved in 1 short contact:

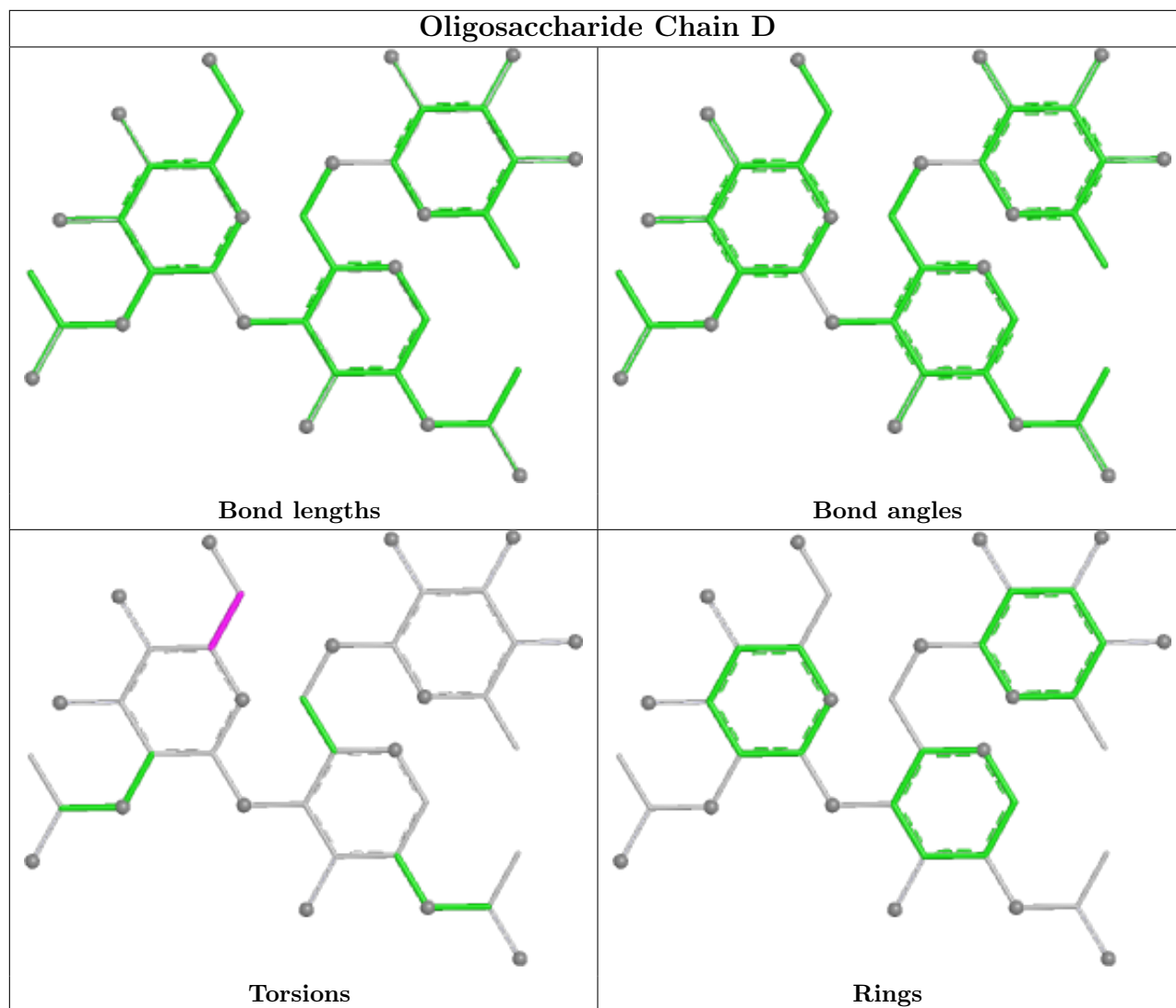
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	NAG	1	0

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 22 ligands modelled in this entry, 7 are monoatomic - leaving 15 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	$\# Z  > 2$
4	NAG	A	603	1	14,14,15	0.33	0	17,19,21	0.44	0
6	GOL	A	605	-	5,5,5	0.93	0	5,5,5	0.89	0
6	GOL	A	609	-	5,5,5	0.87	0	5,5,5	1.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GOL	A	611	-	5,5,5	0.84	0	5,5,5	1.21	0
9	SO4	A	613	-	4,4,4	0.14	0	6,6,6	0.04	0
7	C0I	A	606	-	53,54,54	1.79	13 (24%)	66,74,74	1.79	13 (19%)
9	SO4	A	614	-	4,4,4	0.13	0	6,6,6	0.13	0
5	MES	A	604	-	12,12,12	1.93	1 (8%)	14,16,16	2.34	6 (42%)
4	NAG	A	601	1	14,14,15	0.23	0	17,19,21	0.60	0
6	GOL	A	610	-	5,5,5	0.52	0	5,5,5	0.90	0
6	GOL	A	608	-	5,5,5	0.81	0	5,5,5	1.05	0
9	SO4	A	615	-	4,4,4	0.27	0	6,6,6	0.16	0
8	SIA	A	607	-	21,21,21	1.63	4 (19%)	25,31,31	1.26	1 (4%)
9	SO4	A	612	-	4,4,4	0.13	0	6,6,6	0.19	0
4	NAG	A	602	1	14,14,15	0.47	0	17,19,21	0.56	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	NAG	A	603	1	-	2/6/23/26	0/1/1/1
6	GOL	A	605	-	-	3/4/4/4	-
6	GOL	A	609	-	-	4/4/4/4	-
6	GOL	A	611	-	-	2/4/4/4	-
7	C0I	A	606	-	-	6/26/43/43	0/7/7/7
5	MES	A	604	-	-	2/6/14/14	0/1/1/1
4	NAG	A	601	1	-	3/6/23/26	0/1/1/1
6	GOL	A	610	-	-	2/4/4/4	-
6	GOL	A	608	-	-	2/4/4/4	-
8	SIA	A	607	-	-	6/20/38/38	0/1/1/1
4	NAG	A	602	1	-	0/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	604	MES	C8-S	-6.33	1.68	1.77
8	A	607	SIA	O6-C2	4.56	1.47	1.43
7	A	606	C0I	C28-C25	-4.09	1.35	1.42
7	A	606	C0I	C26-N06	4.04	1.37	1.32
7	A	606	C0I	C34-C26	3.75	1.56	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	607	SIA	C2-C1	3.75	1.59	1.53
7	A	606	C0I	C18-N04	3.42	1.41	1.33
7	A	606	C0I	C17-C28	3.21	1.48	1.43
7	A	606	C0I	C05-C01	2.92	1.57	1.53
7	A	606	C0I	C29-C25	2.80	1.46	1.41
7	A	606	C0I	C40-C39	2.57	1.44	1.38
7	A	606	C0I	C25-N06	2.56	1.41	1.37
7	A	606	C0I	C17-C27	2.40	1.43	1.38
8	A	607	SIA	C3-C2	2.31	1.54	1.51
7	A	606	C0I	C37-C24	-2.29	1.37	1.41
8	A	607	SIA	C7-C6	2.26	1.55	1.53
7	A	606	C0I	C05-N01	2.08	1.50	1.46
7	A	606	C0I	C32-C31	2.06	1.43	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	606	C0I	C01-C06-N02	7.50	125.72	115.99
5	A	604	MES	O1S-S-C8	4.60	112.45	106.92
7	A	606	C0I	C19-N04-C18	4.08	131.40	122.08
7	A	606	C0I	C33-C27-C26	-3.78	117.55	121.08
8	A	607	SIA	O1A-C1-C2	-3.74	117.92	123.59
7	A	606	C0I	O01-C06-N02	-3.70	115.06	122.99
5	A	604	MES	C5-N4-C3	3.51	116.73	108.83
7	A	606	C0I	C08-C07-N01	-3.38	106.57	113.12
7	A	606	C0I	C13-C18-N04	3.18	123.91	117.09
7	A	606	C0I	C36-C33-C27	3.16	119.33	112.84
5	A	604	MES	C7-N4-C5	2.91	118.68	111.23
5	A	604	MES	O2S-S-C8	2.91	110.42	106.92
7	A	606	C0I	O02-C18-N04	-2.91	116.81	122.61
5	A	604	MES	C7-N4-C3	2.88	118.61	111.23
7	A	606	C0I	C07-N01-C04	-2.80	104.83	111.06
7	A	606	C0I	C20-C21-C22	-2.24	122.47	127.19
7	A	606	C0I	O01-C06-C01	-2.23	119.22	122.12
7	A	606	C0I	C29-C25-N06	-2.17	115.38	118.69
7	A	606	C0I	C38-C23-C24	-2.11	115.36	118.17
5	A	604	MES	O3S-S-C8	2.10	109.17	105.77

There are no chirality outliers.

All (32) torsion outliers are listed below:

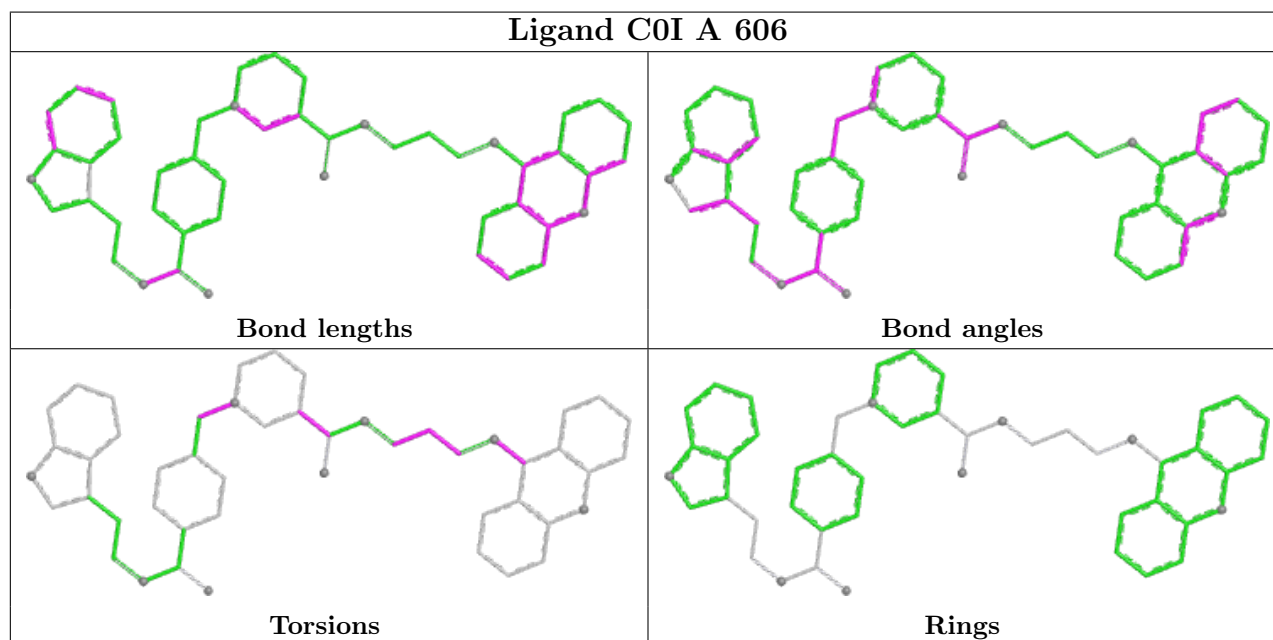
Mol	Chain	Res	Type	Atoms
5	A	604	MES	C8-C7-N4-C3
6	A	605	GOL	O1-C1-C2-C3
6	A	611	GOL	O1-C1-C2-C3
8	A	607	SIA	O1A-C1-C2-C3
8	A	607	SIA	O1A-C1-C2-O2
8	A	607	SIA	O1B-C1-C2-O6
7	A	606	C0I	N02-C14-C15-C16
7	A	606	C0I	C14-C15-C16-N03
4	A	601	NAG	O5-C5-C6-O6
7	A	606	C0I	C05-C01-C06-N02
4	A	601	NAG	C4-C5-C6-O6
8	A	607	SIA	C11-C10-N5-C5
8	A	607	SIA	O10-C10-N5-C5
6	A	609	GOL	O1-C1-C2-O2
6	A	608	GOL	C1-C2-C3-O3
6	A	609	GOL	O1-C1-C2-C3
6	A	609	GOL	C1-C2-C3-O3
6	A	610	GOL	O1-C1-C2-C3
6	A	605	GOL	O1-C1-C2-O2
6	A	609	GOL	O2-C2-C3-O3
6	A	611	GOL	O1-C1-C2-O2
7	A	606	C0I	C05-C01-C06-O01
4	A	603	NAG	C4-C5-C6-O6
5	A	604	MES	N4-C7-C8-S
4	A	603	NAG	O5-C5-C6-O6
6	A	605	GOL	O2-C2-C3-O3
6	A	608	GOL	O2-C2-C3-O3
8	A	607	SIA	O1A-C1-C2-O6
7	A	606	C0I	C08-C07-N01-C05
4	A	601	NAG	C3-C2-N2-C7
6	A	610	GOL	O1-C1-C2-O2
7	A	606	C0I	C28-C17-N03-C16

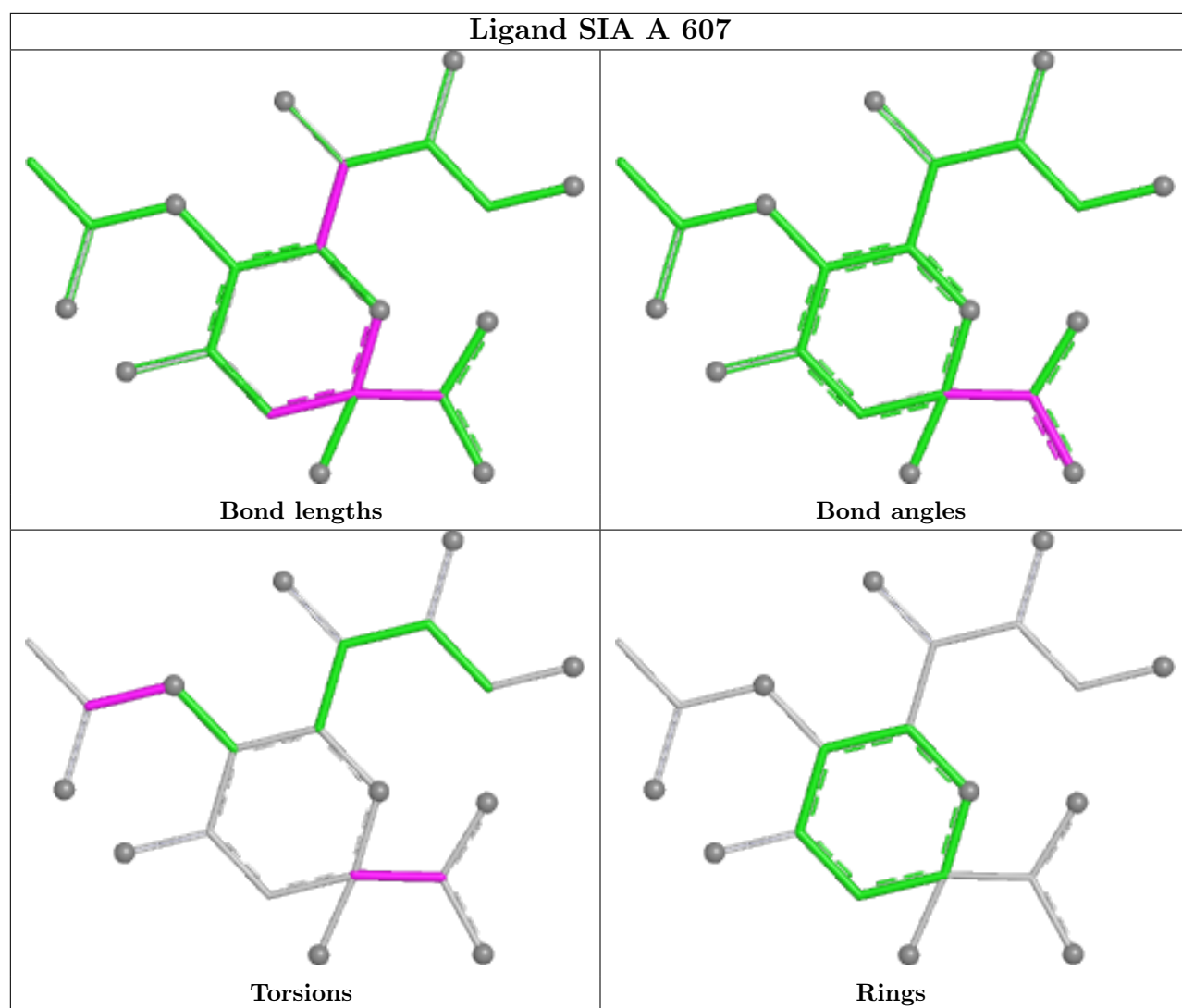
There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	609	GOL	3	0
5	A	604	MES	5	0
6	A	610	GOL	1	0
6	A	608	GOL	1	0
8	A	607	SIA	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	A	527/529 (99%)	0.26	15 (2%) 53 58	28, 40, 66, 97	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	TYR	5.6
1	A	237	TYR	5.4
1	A	51	LYS	3.6
1	A	3	ASP	3.6
1	A	255	GLU	3.5
1	A	49	LEU	3.5
1	A	4	ILE	3.1
1	A	240	ARG	2.9
1	A	274	LEU	2.8
1	A	453	ARG	2.7
1	A	455	GLN	2.6
1	A	261	ILE	2.6
1	A	244	LEU	2.4
1	A	156	LEU	2.1
1	A	53	SER	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.

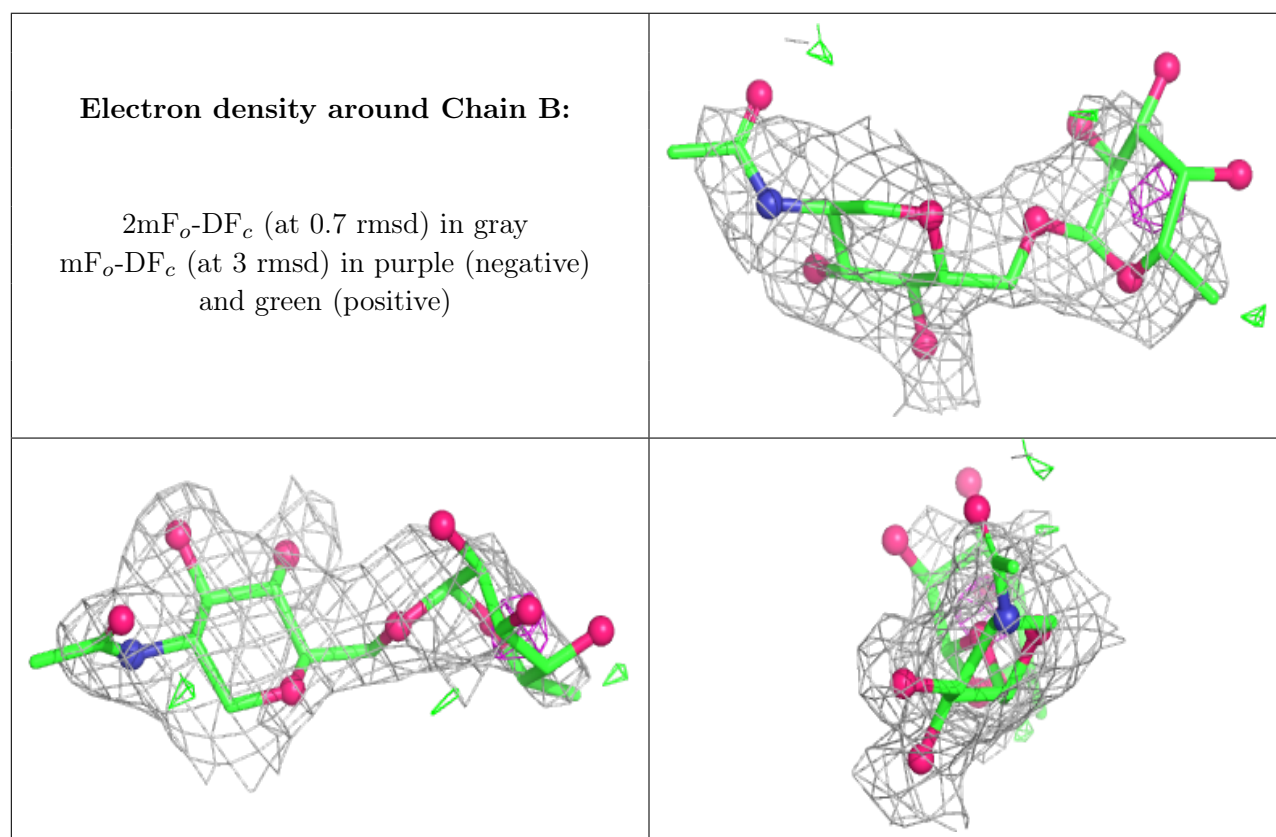
### 6.3 Carbohydrates [i](#)

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.



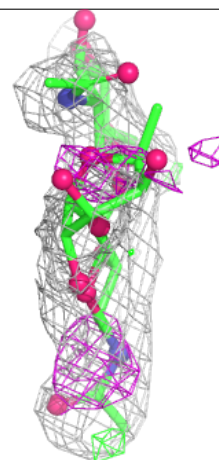
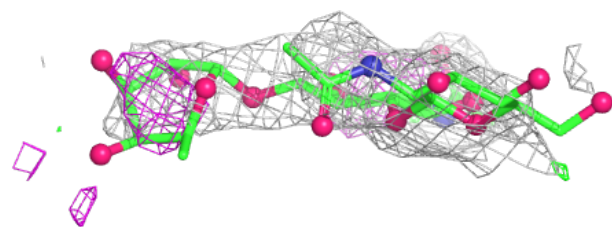
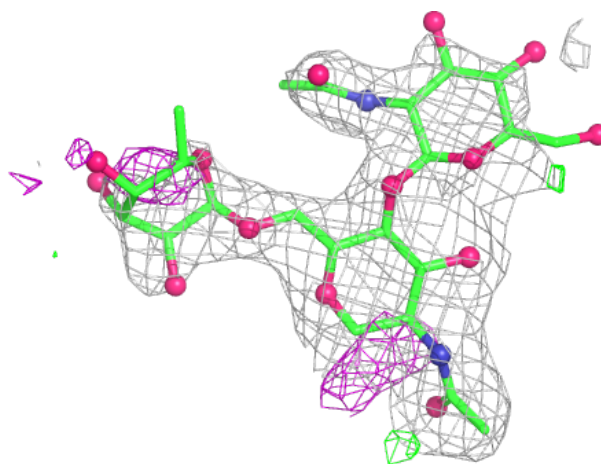
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	C	2	14/15	0.77	0.26	93,99,112,114	0
2	FUC	B	2	10/11	0.78	0.36	104,111,115,116	0
3	FUC	C	3	10/11	0.81	0.45	90,92,103,106	0
2	NAG	B	1	14/15	0.82	0.20	74,80,90,97	0
3	NAG	C	1	14/15	0.83	0.15	66,73,81,88	0
3	NAG	D	2	14/15	0.83	0.20	64,74,89,92	0
3	FUC	D	3	10/11	0.93	0.26	58,66,70,70	0
3	NAG	D	1	14/15	0.97	0.13	53,56,64,64	0

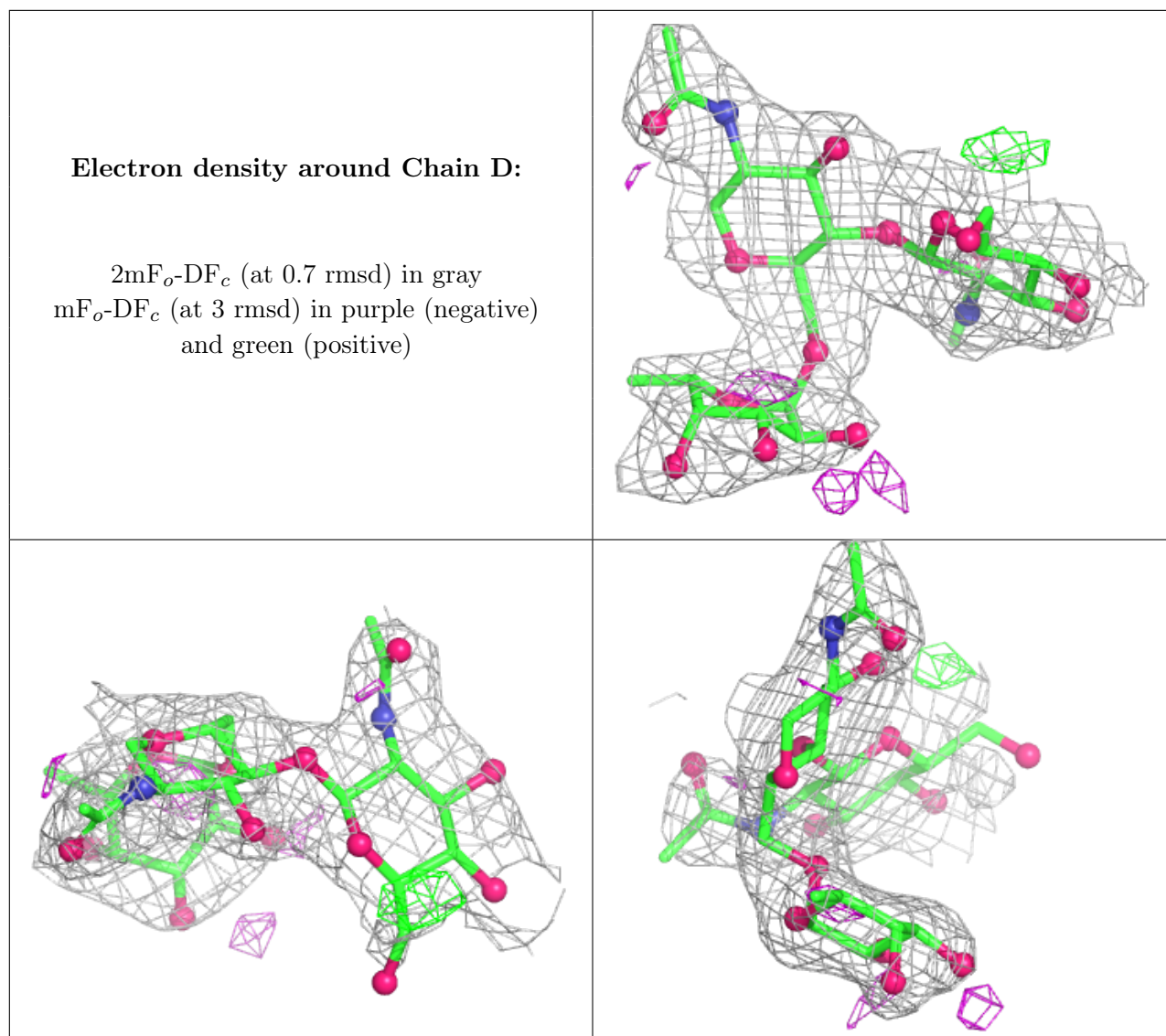
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around Chain C:**

$2mF_o-DF_c$  (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
10	CL	A	620	1/1	0.51	0.27	86,86,86,86	0
4	NAG	A	603	14/15	0.72	0.30	83,96,105,106	0
10	CL	A	621	1/1	0.73	0.16	82,82,82,82	0
5	MES	A	604	12/12	0.77	0.24	74,80,95,106	0
4	NAG	A	602	14/15	0.79	0.18	51,70,81,81	0
4	NAG	A	601	14/15	0.80	0.23	109,113,117,118	0
8	SIA	A	607	21/21	0.80	0.27	48,73,86,87	0

*Continued on next page...*

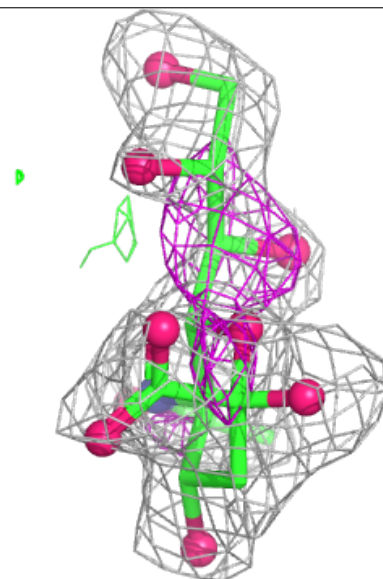
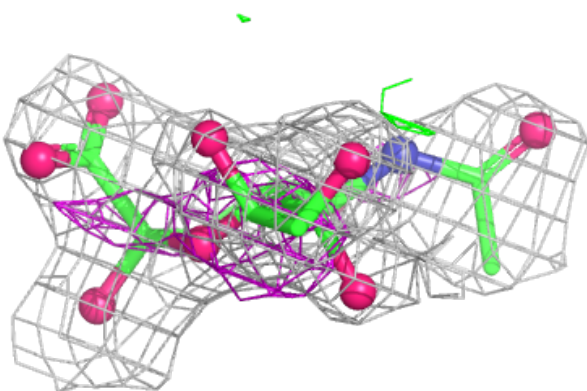
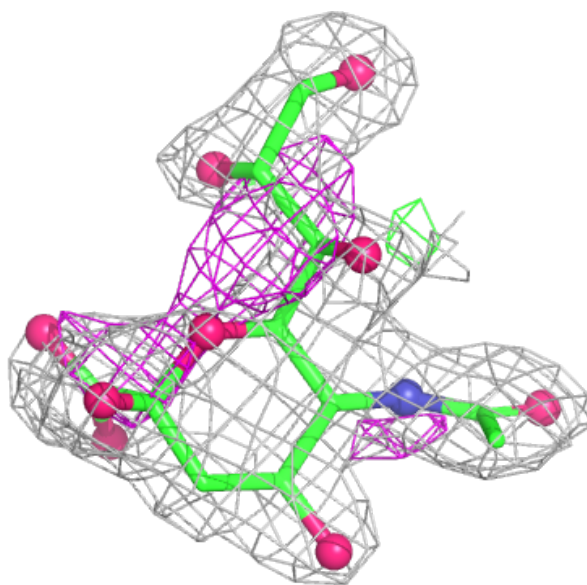
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GOL	A	608	6/6	0.85	0.17	75,77,80,82	0
6	GOL	A	610	6/6	0.88	0.27	40,45,55,62	0
10	CL	A	618	1/1	0.88	0.19	78,78,78,78	0
6	GOL	A	609	6/6	0.89	0.26	66,66,69,74	0
10	CL	A	616	1/1	0.93	0.07	85,85,85,85	0
9	SO4	A	614	5/5	0.93	0.13	59,67,72,73	0
6	GOL	A	605	6/6	0.94	0.11	42,46,50,54	0
9	SO4	A	613	5/5	0.95	0.15	83,84,87,94	0
10	CL	A	622	1/1	0.95	0.07	72,72,72,72	0
7	C0I	A	606	48/48	0.96	0.12	28,35,41,45	0
10	CL	A	617	1/1	0.96	0.04	77,77,77,77	0
6	GOL	A	611	6/6	0.96	0.15	39,46,50,62	0
9	SO4	A	612	5/5	0.97	0.16	42,47,56,64	0
9	SO4	A	615	5/5	0.97	0.11	45,56,60,60	0
10	CL	A	619	1/1	0.98	0.13	62,62,62,62	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.

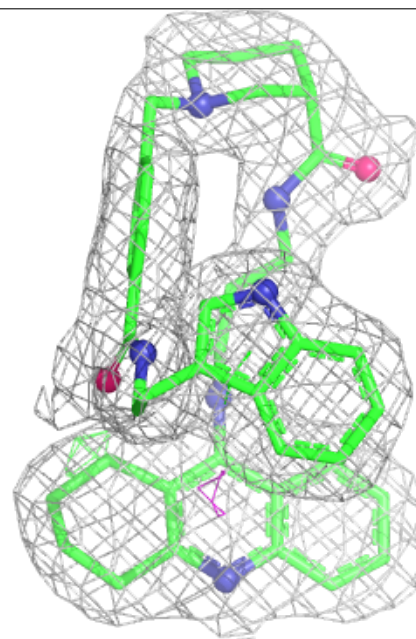
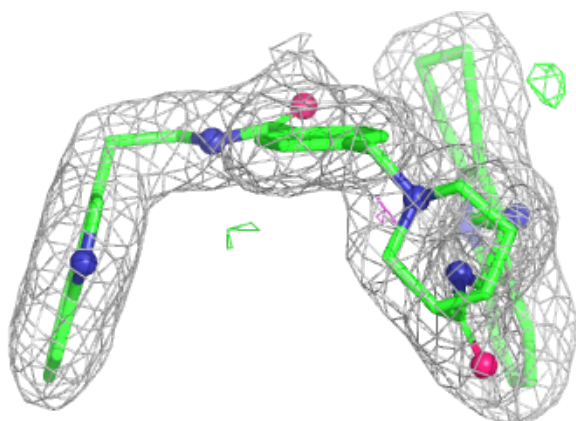
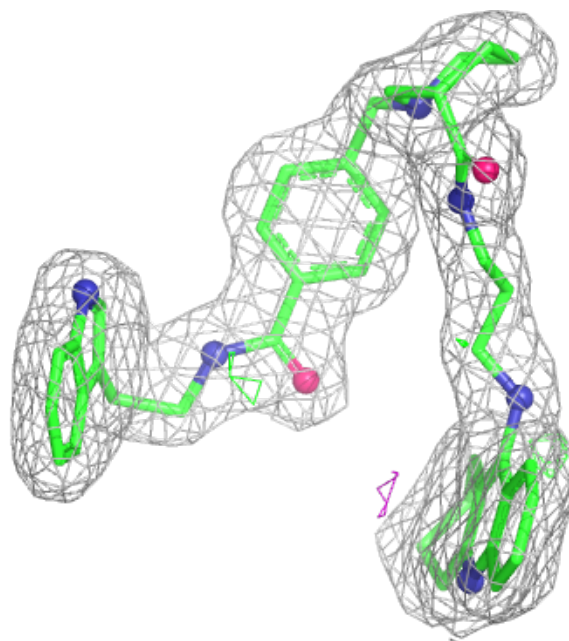
**Electron density around SIA A 607:**

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



**Electron density around COI A 606:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.