



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:48 PM UTC

PDB ID : 2C6F / pdb\_00002c6f  
Title : Structure of human somatic angiotensin-I converting enzyme N domain  
Authors : Corradi, H.R.; Schwager, S.L.U.; Nichinda, A.; Sturrock, E.D.; Acharya, K.R.  
Deposited on : 2005-11-09  
Resolution : 3.01 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.

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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

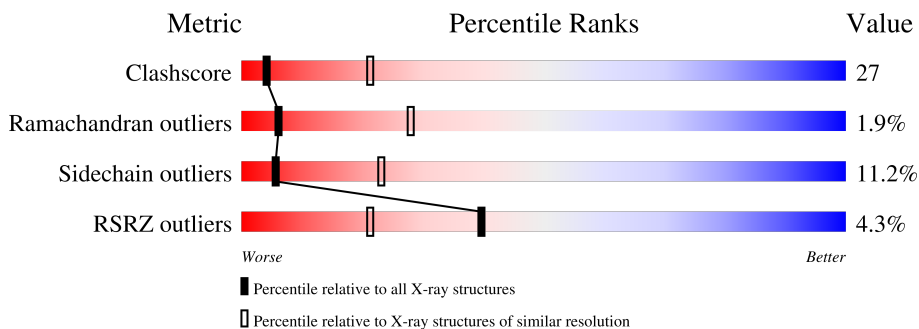
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.01 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))
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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	A	612	
1	B	612	
2	C	2	
2	D	2	
2	E	2	
2	F	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	707	-	X	-	-
6	GOL	B	706	-	X	-	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9970 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 ANGIOTENSIN-CONVERTING ENZYME, SOMATIC ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	612	4884	3145	840	880	19	6	0	0
1	B	611	4852	3124	830	879	19	14	0	0

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0
2	D	2	28	16	2	10	0	0	0
2	E	2	28	16	2	10	0	0	0
2	F	2	28	16	2	10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	1	1	1	0	0
4	B	1	1	1	0	0

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	B	1	Total	Cl	0	0
			1	1		

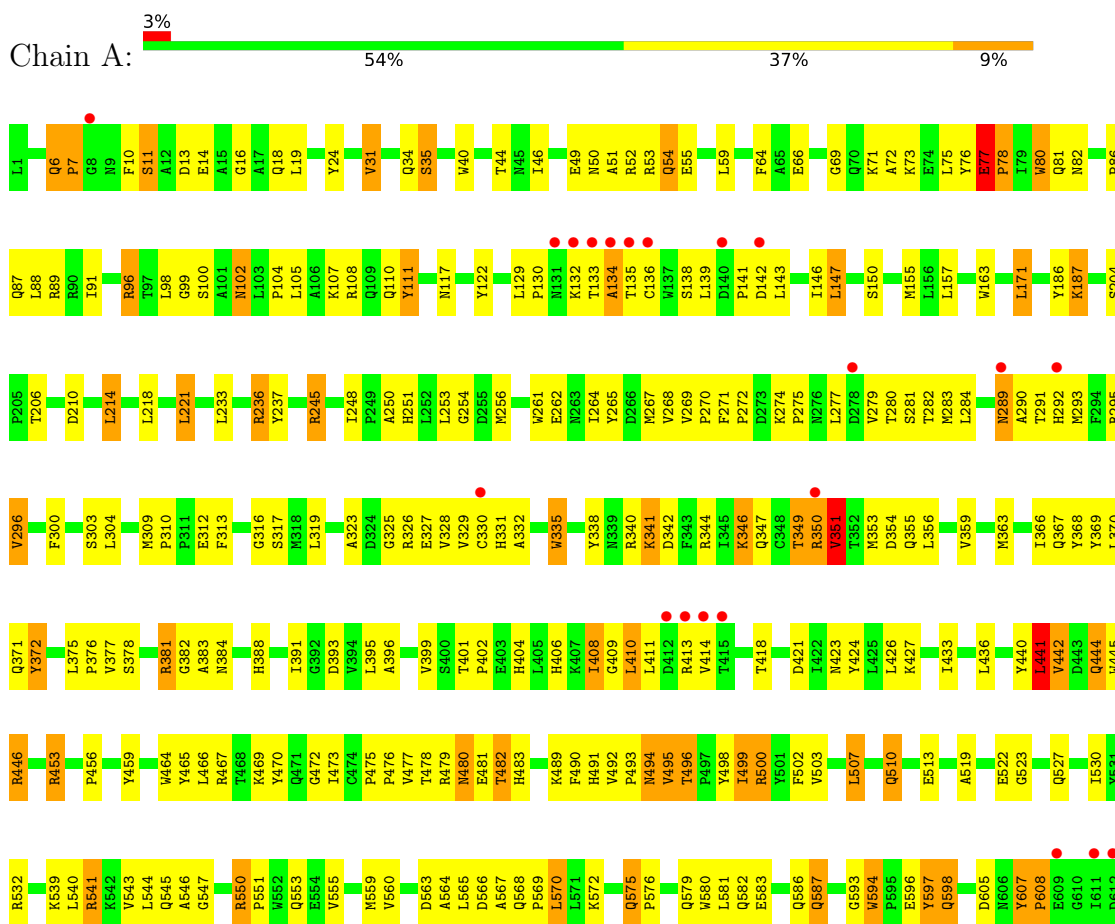
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	11	Total	O	0	0
			11	11		
8	B	13	Total	O	0	0
			13	13		

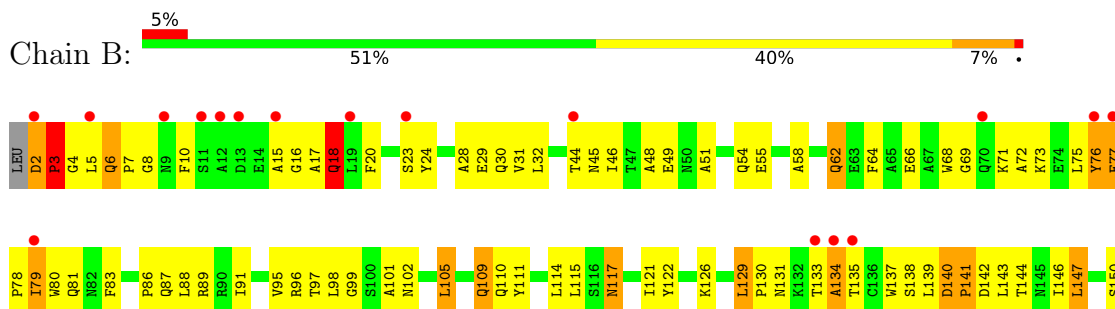
### 3 Residue-property plots [i](#)

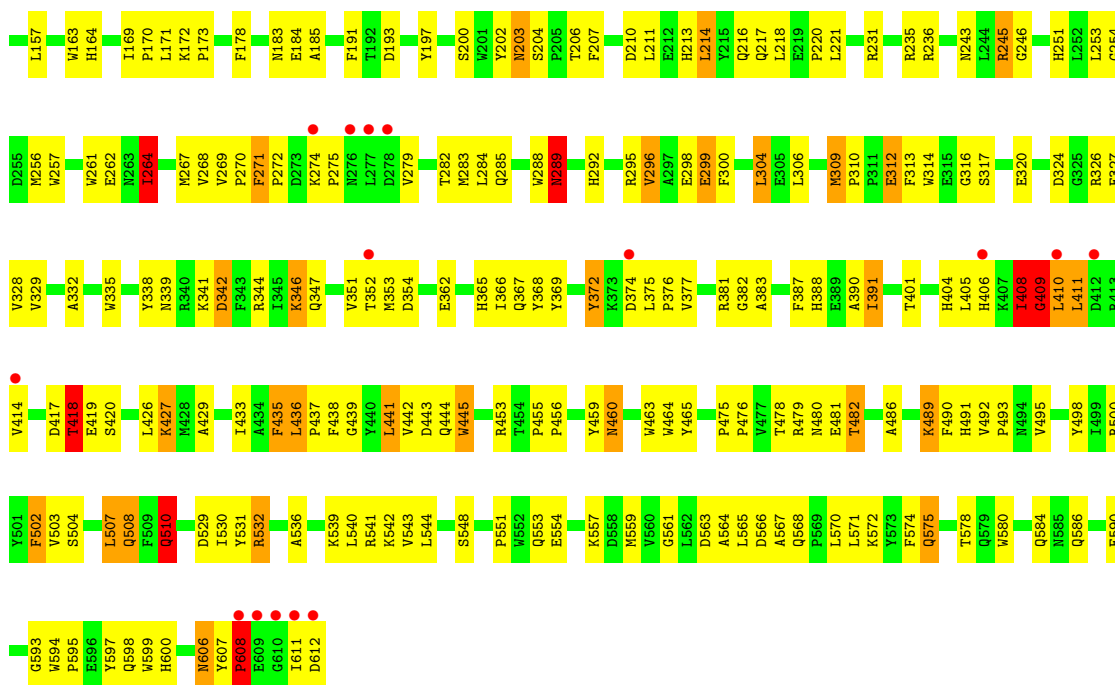
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ANGIOTENSIN-CONVERTING ENZYME, SOMATIC ISOFORM



#### • Molecule 1: ANGIOTENSIN-CONVERTING ENZYME, SOMATIC ISOFORM





- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 50% 50%

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 50% 50%

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 50% 50%

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 50% 50%

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.12Å 211.32Å 171.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.91 – 3.01 47.91 – 3.01	Depositor EDS
% Data completeness (in resolution range)	96.7 (47.91-3.01) 96.9 (47.91-3.01)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 3.01Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.224 , 0.273 0.219 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtrriage
Anisotropy	0.335	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	9970	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: CL, ZN, NAG, ACT, GOL

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	0.63	2/5042 (0.0%)	1.14	46/6885 (0.7%)
1	B	0.62	4/5010 (0.1%)	1.27	70/6845 (1.0%)
All	All	0.62	6/10052 (0.1%)	1.21	116/13730 (0.8%)

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	A	0	1
1	B	3	2
All	All	3	3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	ASN	CA-CB	-6.30	1.43	1.53
1	B	436	LEU	CA-CB	-5.73	1.48	1.54
1	B	575	GLN	CA-CB	-5.62	1.49	1.54
1	A	117	ASN	CB-CG	-5.43	1.38	1.52
1	B	264	ILE	CA-CB	-5.19	1.47	1.54

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	PRO	CA-N-CD	-23.00	79.80	112.00
1	B	608	PRO	CA-N-CD	-19.25	85.05	112.00
1	A	598	GLN	OE1-CD-NE2	-10.43	112.17	122.60
1	A	527	GLN	OE1-CD-NE2	-10.28	112.33	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	410	LEU	N-CA-C	-10.26	100.08	112.59

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	79	ILE	CA
1	B	410	LEU	CA
1	B	530	ILE	CB

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	607	TYR	Peptide
1	B	275	PRO	Peptide
1	B	409	GLY	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	A	4884	0	4582	266	1
1	B	4852	0	4514	256	0
2	C	28	0	25	1	1
2	D	28	0	25	6	0
2	E	28	0	25	3	0
2	F	28	0	25	2	0
3	A	42	0	36	4	0
3	B	28	0	23	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	8	0	6	0	0
5	B	4	0	3	0	0
6	A	6	0	6	1	0
6	B	6	0	6	1	0
7	A	1	0	0	1	0
7	B	1	0	0	0	0
8	A	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	13	0	0	0	0
All	All	9970	0	9276	526	1

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 27.

The worst 5 of 526 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:B:3:PRO:HD3	1:B:6:GLN:NE2	1.36	1.40
1:B:282:THR:HG21	1:B:410:LEU:CB	1.60	1.31
1:A:279:VAL:HG21	1:A:410:LEU:CD1	1.60	1.29
1:B:282:THR:CG2	1:B:410:LEU:CB	2.18	1.20
1:A:279:VAL:CG1	1:A:410:LEU:HD13	1.73	1.17

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:GLU:OE2	2:C:1:NAG:O7[3_554]	2.01	0.19

## 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	610/612 (100%)	537 (88%)	60 (10%)	13 (2%)	<b>5</b> 25
1	B	609/612 (100%)	526 (86%)	73 (12%)	10 (2%)	<b>7</b> 32
All	All	1219/1224 (100%)	1063 (87%)	133 (11%)	23 (2%)	<b>6</b> 28

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	608	PRO
1	B	3	PRO
1	B	608	PRO
1	A	7	PRO
1	A	250	ALA

### 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	496/526 (94%)	440 (89%)	56 (11%)	<b>5</b> <b>23</b>
1	B	489/526 (93%)	435 (89%)	54 (11%)	<b>6</b> <b>24</b>
All	All	985/1052 (94%)	875 (89%)	110 (11%)	<b>6</b> <b>23</b>

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	18	GLN
1	B	214	LEU
1	B	608	PRO
1	B	507	LEU
1	B	66	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	587	GLN
1	B	553	GLN
1	B	18	GLN
1	B	579	GLN
1	B	371	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](#)

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	C	1	1,2	14,14,15	0.57	0	17,19,21	0.76	1 (5%)
2	NAG	C	2	2	14,14,15	0.52	0	17,19,21	0.69	0
2	NAG	D	1	1,2	14,14,15	0.58	0	17,19,21	0.75	1 (5%)
2	NAG	D	2	2	14,14,15	0.51	0	17,19,21	0.68	0
2	NAG	E	1	1,2	14,14,15	0.57	0	17,19,21	0.75	1 (5%)
2	NAG	E	2	2	14,14,15	0.53	0	17,19,21	0.68	0
2	NAG	F	1	1,2	14,14,15	2.36	1 (7%)	17,19,21	1.06	1 (5%)
2	NAG	F	2	2	14,14,15	2.35	1 (7%)	17,19,21	1.06	1 (5%)

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	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	3/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	NAG	C8-C7	-8.77	1.32	1.50
2	F	2	NAG	C8-C7	-8.72	1.32	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C1-C2-N2	-3.44	105.01	110.43
2	F	2	NAG	C1-C2-N2	-3.42	105.04	110.43
2	C	1	NAG	C2-N2-C7	-2.17	120.00	122.90
2	D	1	NAG	C2-N2-C7	-2.14	120.04	122.90
2	E	1	NAG	C2-N2-C7	-2.13	120.05	122.90

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

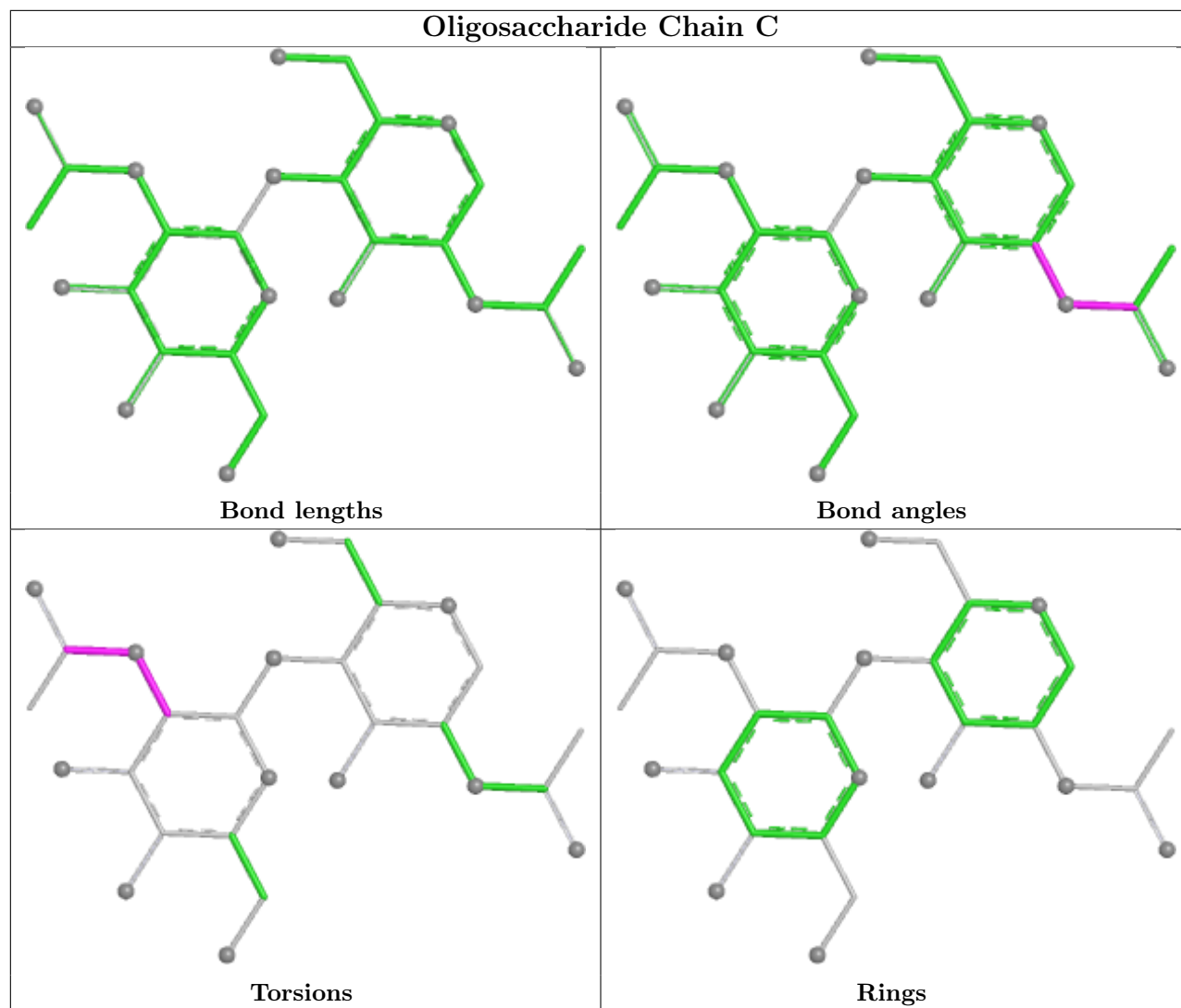
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C3-C2-N2-C7
2	D	2	NAG	C3-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2

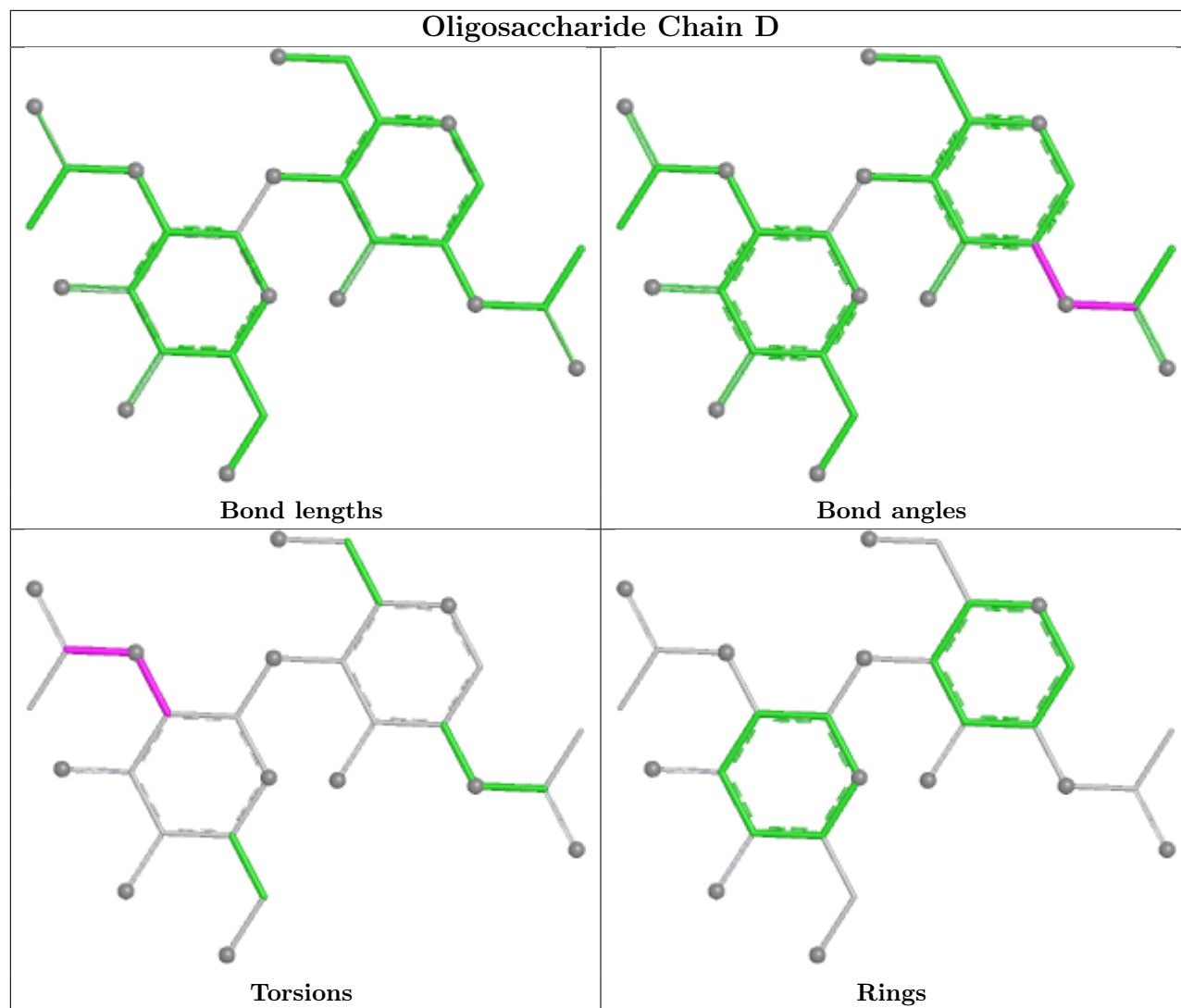
There are no ring outliers.

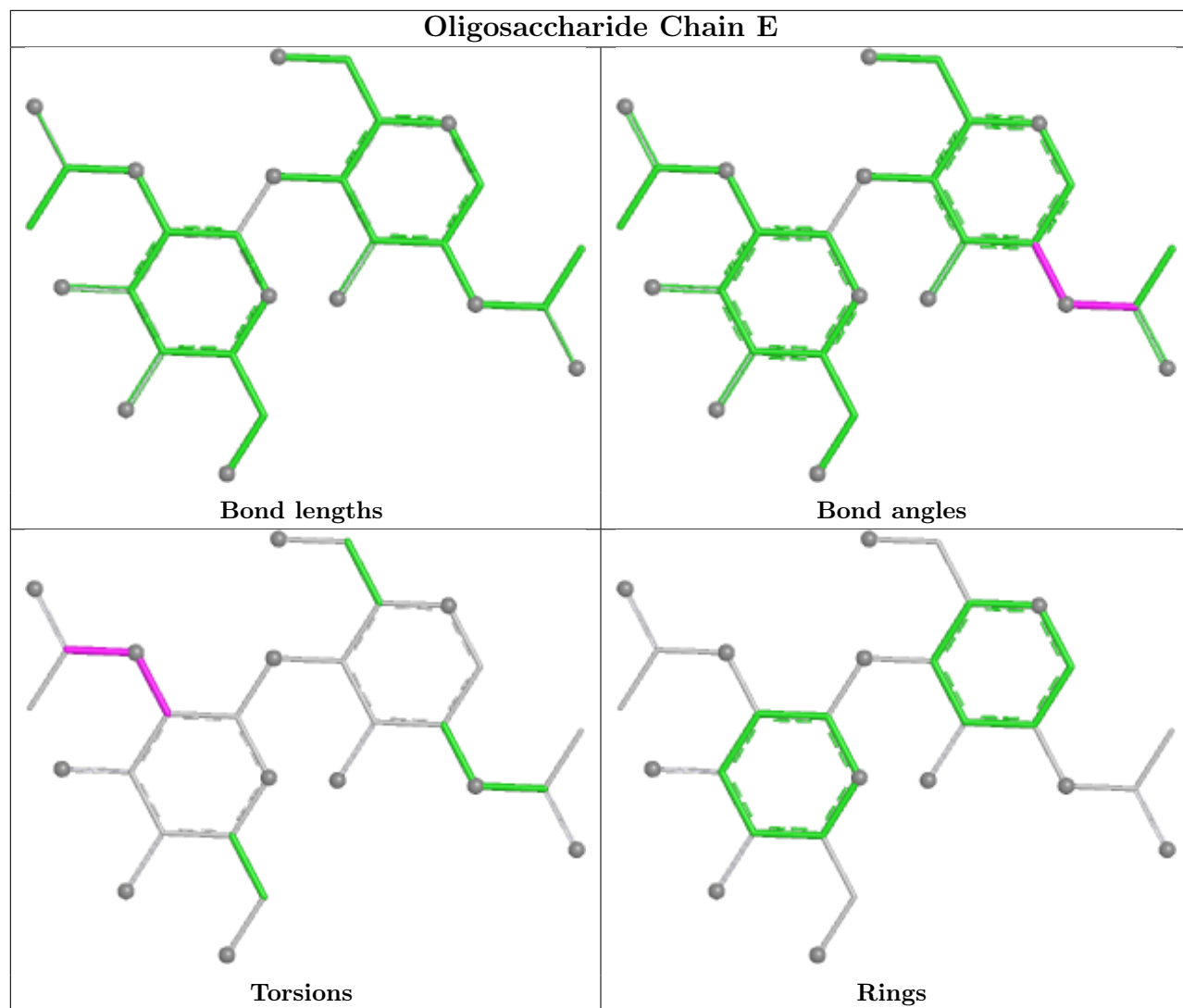
5 monomers are involved in 13 short contacts:

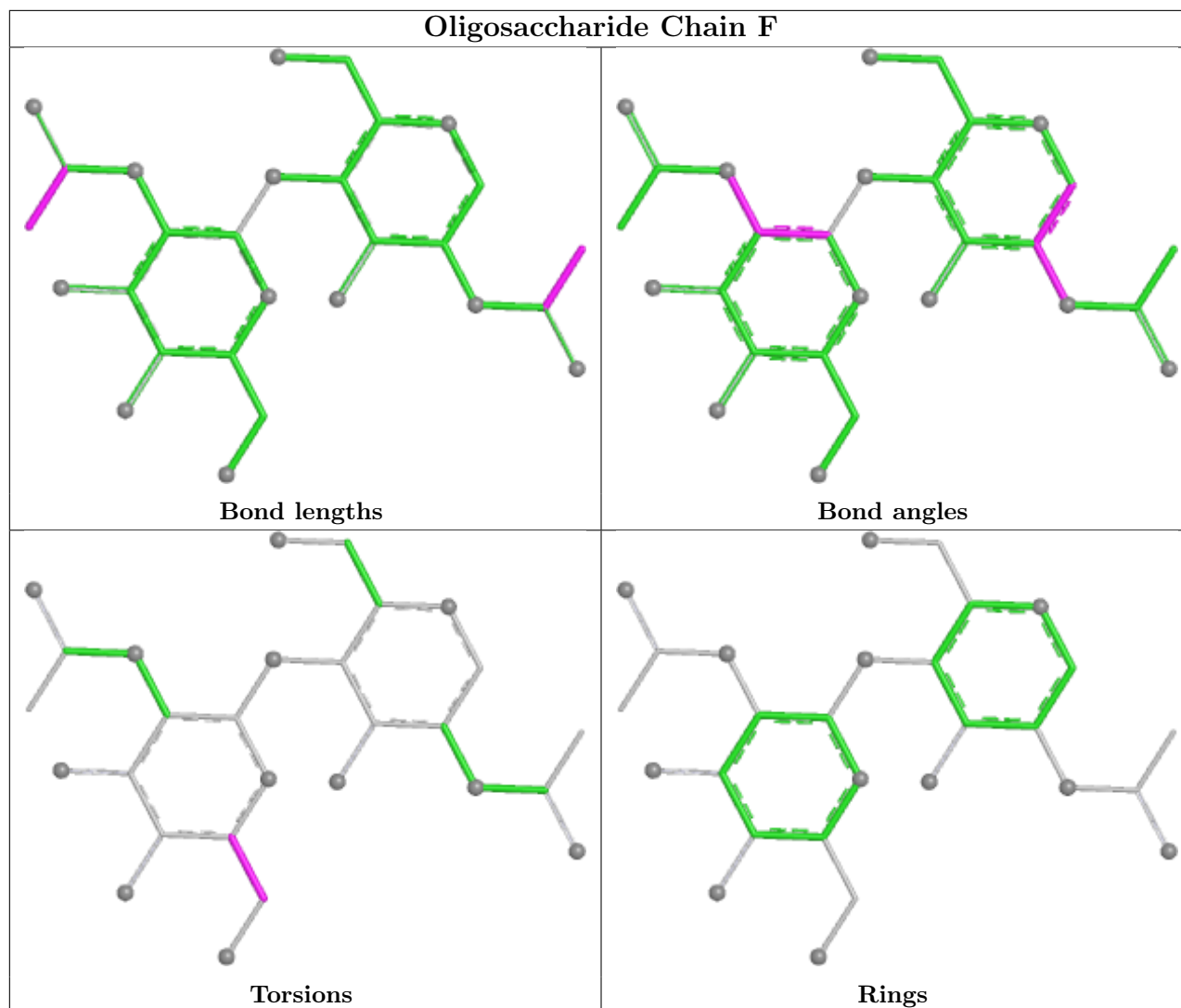
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	1	0
2	C	1	NAG	1	1
2	F	1	NAG	2	0
2	E	1	NAG	3	0
2	D	2	NAG	6	0

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 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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$
6	GOL	B	706	-	5,5,5	3.49	3 (60%)	5,5,5	2.22	4 (80%)
6	GOL	A	707	-	5,5,5	3.46	3 (60%)	5,5,5	2.04	4 (80%)
3	NAG	A	702	1	14,14,15	0.58	0	17,19,21	0.75	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ACT	B	705	-	3,3,3	1.36	1 (33%)	3,3,3	1.60	1 (33%)
3	NAG	A	703	1	14,14,15	0.57	0	17,19,21	0.75	1 (5%)
3	NAG	B	703	1	14,14,15	0.57	0	17,19,21	0.75	1 (5%)
3	NAG	B	702	1	14,14,15	3.79	2 (14%)	17,19,21	1.63	3 (17%)
5	ACT	A	705	-	3,3,3	1.24	0	3,3,3	1.50	1 (33%)
3	NAG	A	701	1	14,14,15	3.99	3 (21%)	17,19,21	1.93	4 (23%)
5	ACT	A	706	-	3,3,3	1.36	0	3,3,3	1.57	1 (33%)

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	GOL	B	706	-	-	1/4/4/4	-
6	GOL	A	707	-	-	1/4/4/4	-
3	NAG	A	702	1	-	0/6/23/26	0/1/1/1
3	NAG	A	703	1	-	0/6/23/26	0/1/1/1
3	NAG	B	703	1	-	0/6/23/26	0/1/1/1
3	NAG	B	702	1	-	5/6/23/26	0/1/1/1
3	NAG	A	701	1	-	5/6/23/26	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	NAG	C8-C7	-13.57	1.22	1.50
3	B	702	NAG	C8-C7	-13.53	1.22	1.50
6	B	706	GOL	C3-C2	-6.59	1.26	1.51
6	A	707	GOL	C3-C2	-6.53	1.26	1.51
3	A	701	NAG	O5-C5	4.55	1.52	1.43

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	NAG	C1-O5-C5	-4.45	106.22	112.19
3	A	701	NAG	C8-C7-N2	4.14	122.98	116.12
3	B	702	NAG	C8-C7-N2	4.12	122.96	116.12
3	B	702	NAG	C1-C2-N2	-3.45	104.99	110.43
3	A	701	NAG	C1-C2-N2	-3.43	105.03	110.43

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	702	NAG	C3-C2-N2-C7
3	A	701	NAG	O5-C5-C6-O6
3	A	701	NAG	C4-C5-C6-O6
3	B	702	NAG	O5-C5-C6-O6
3	A	701	NAG	C8-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	706	GOL	1	0
6	A	707	GOL	1	0
3	A	703	NAG	1	0
3	B	702	NAG	2	0
3	A	701	NAG	3	0

## 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	612/612 (100%)	0.16	21 (3%)	48 27	12, 35, 58, 82	3 (0%)
1	B	611/612 (99%)	0.28	32 (5%)	33 16	12, 38, 67, 84	6 (0%)
All	All	1223/1224 (99%)	0.22	53 (4%)	40 21	12, 37, 64, 84	9 (0%)

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	GLY	6.0
1	A	612	ASP	5.6
1	B	77	GLU	4.8
1	B	12	ALA	4.4
1	B	278	ASP	4.3

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

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

### 6.3 Carbohydrates [i](#)

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

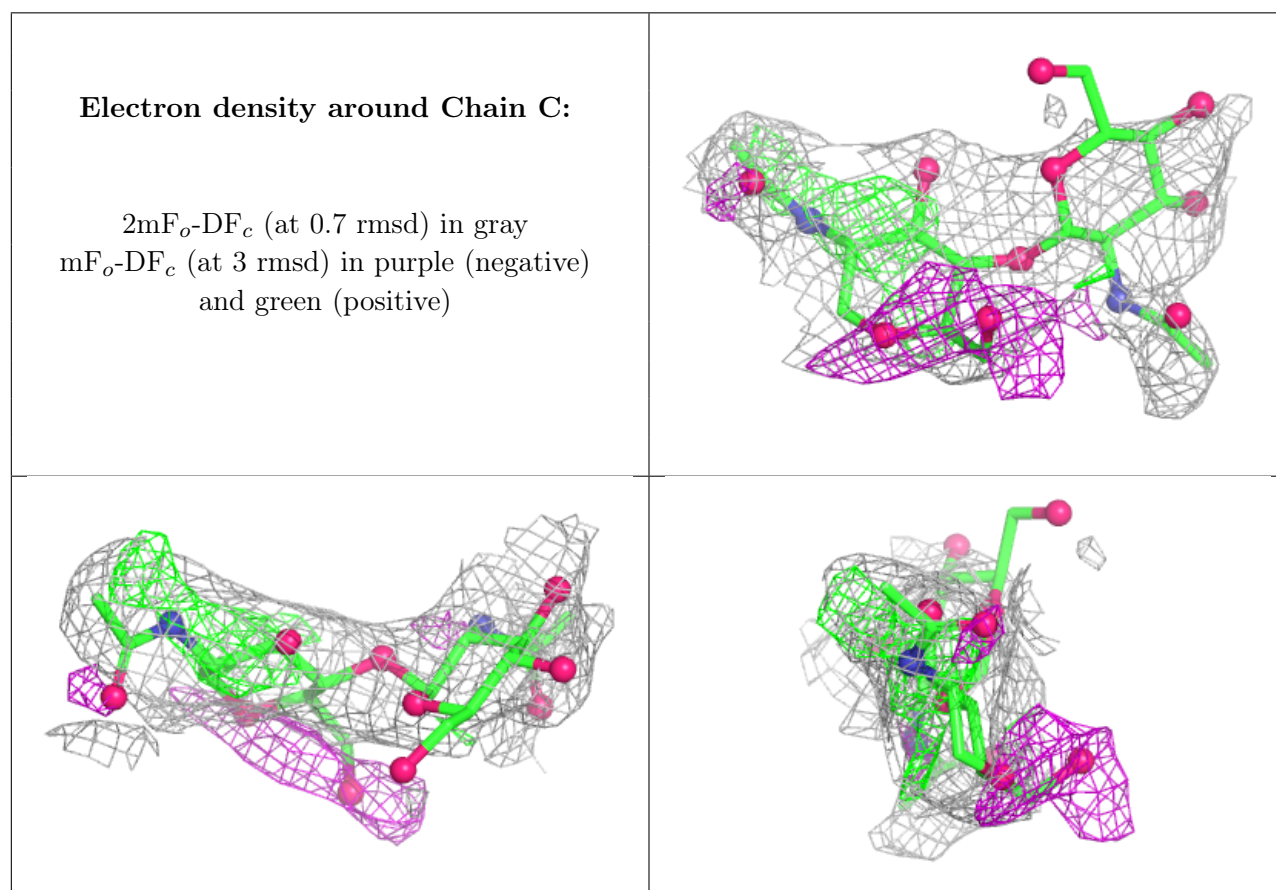
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	E	2	14/15	0.45	0.23	86,90,91,91	0
2	NAG	D	2	14/15	0.47	0.29	69,72,73,75	0
2	NAG	C	2	14/15	0.54	0.21	95,96,97,97	0
2	NAG	F	2	14/15	0.60	0.24	79,80,81,81	0
2	NAG	C	1	14/15	0.64	0.29	56,60,68,72	0

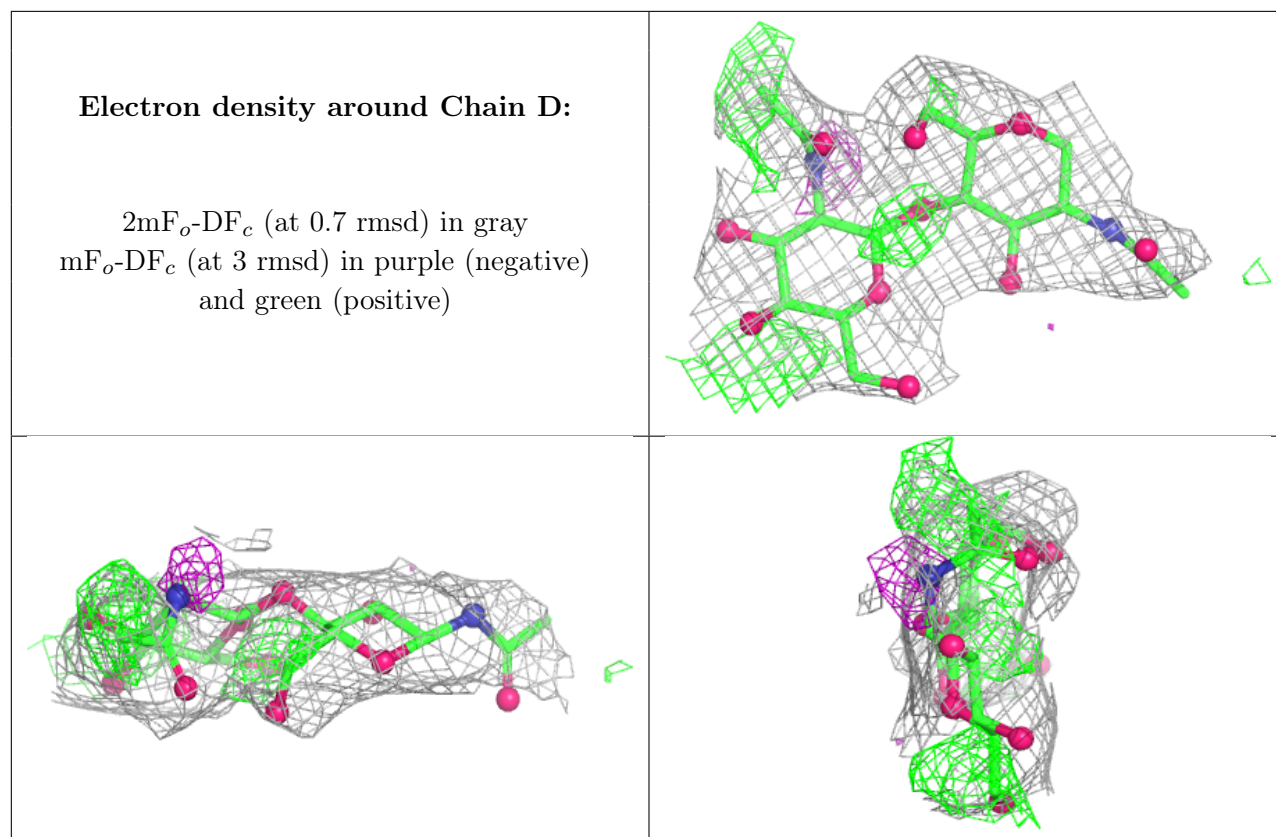
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	E	1	14/15	0.69	0.26	55,57,62,69	0
2	NAG	F	1	14/15	0.70	0.22	61,65,67,68	0
2	NAG	D	1	14/15	0.82	0.19	56,58,60,60	0

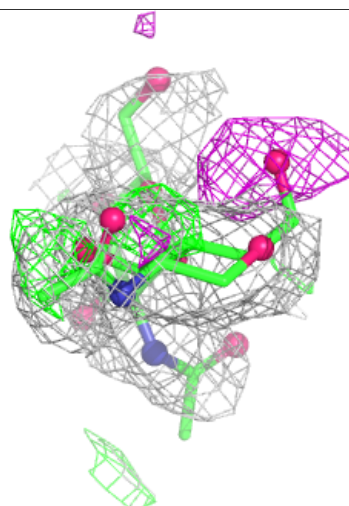
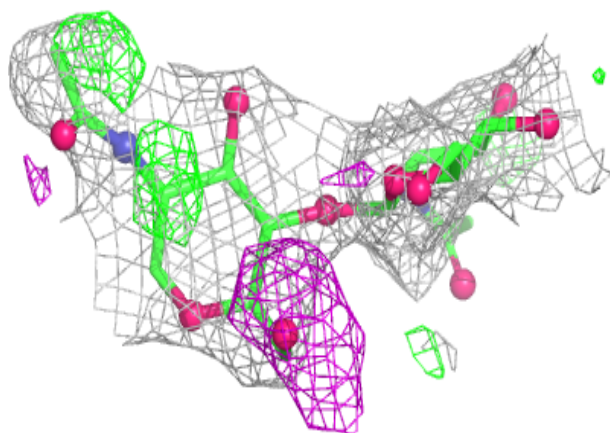
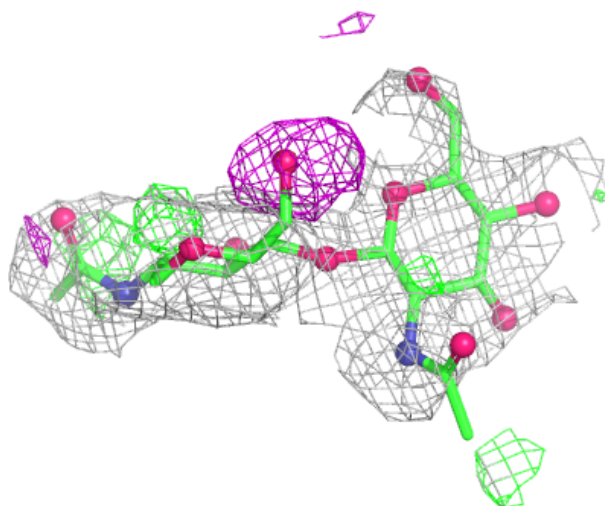
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

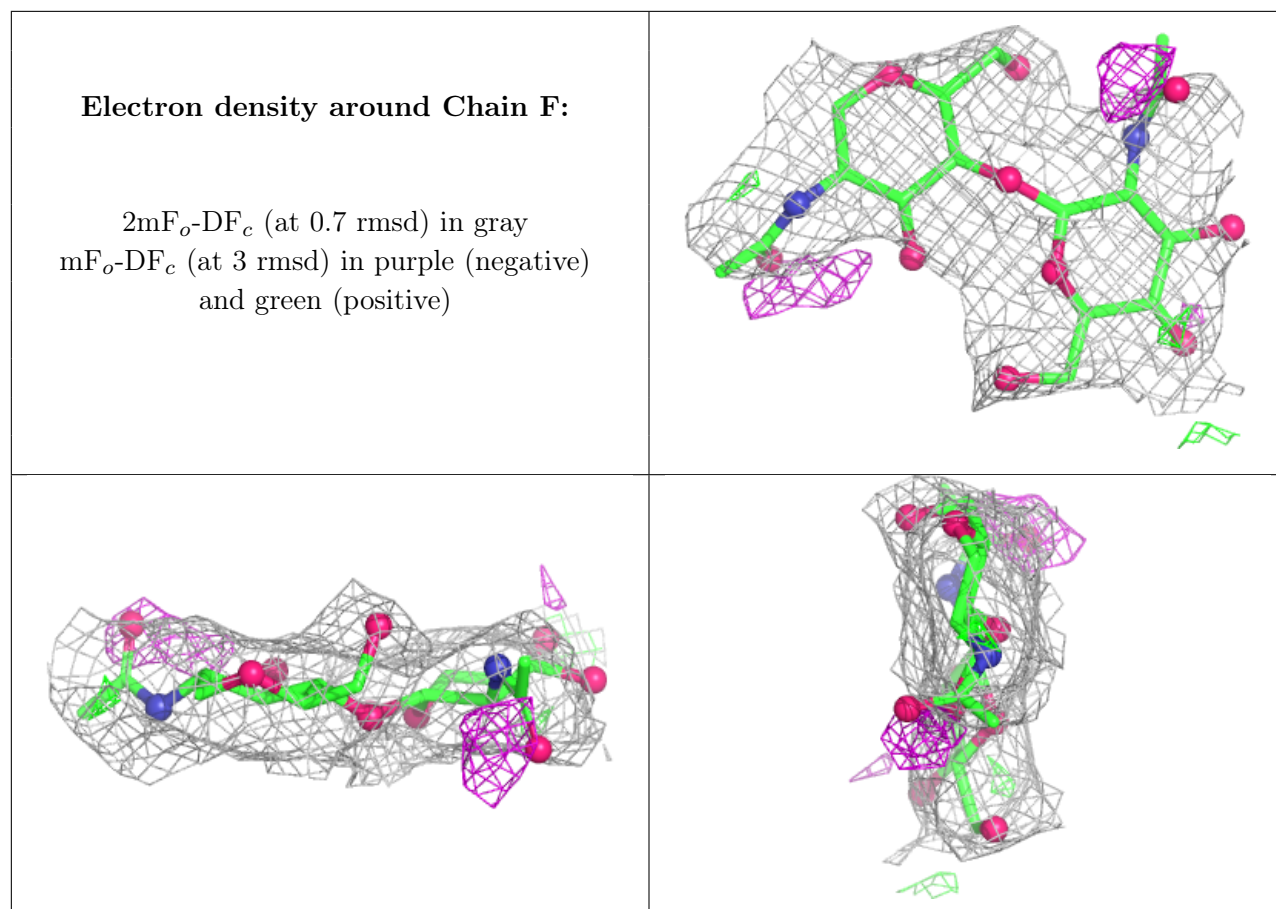




**Electron density around Chain E:**

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





## 6.4 Ligands [i](#)

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	NAG	A	703	14/15	0.40	0.29	116,117,118,119	0
3	NAG	B	702	14/15	0.52	0.27	83,86,86,87	0
3	NAG	A	701	14/15	0.55	0.20	66,68,70,71	0
5	ACT	A	705	4/4	0.64	0.30	49,51,52,53	0
3	NAG	B	703	14/15	0.77	0.21	76,78,80,83	0
3	NAG	A	702	14/15	0.77	0.20	75,76,79,79	0
5	ACT	A	706	4/4	0.81	0.20	32,33,34,35	0
5	ACT	B	705	4/4	0.84	0.23	52,52,53,53	0
6	GOL	A	707	6/6	0.91	0.16	29,31,32,33	0
6	GOL	B	706	6/6	0.91	0.18	31,34,35,39	0
7	CL	A	708	1/1	0.91	0.07	29,29,29,29	0
7	CL	B	701	1/1	0.95	0.06	37,37,37,37	0
4	ZN	B	704	1/1	0.99	0.05	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ZN	A	704	1/1	1.00	0.02	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.