W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 20, 2024 – 02:48 pm GMT

PDB ID	:	6ZR7
Title	:	X-ray structure of human Dscam Ig7-Ig9
Authors	:	Kozak, S.; Bento, I.; Meijers, R.
Deposited on	:	2020-07-11
Resolution	:	1.85 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

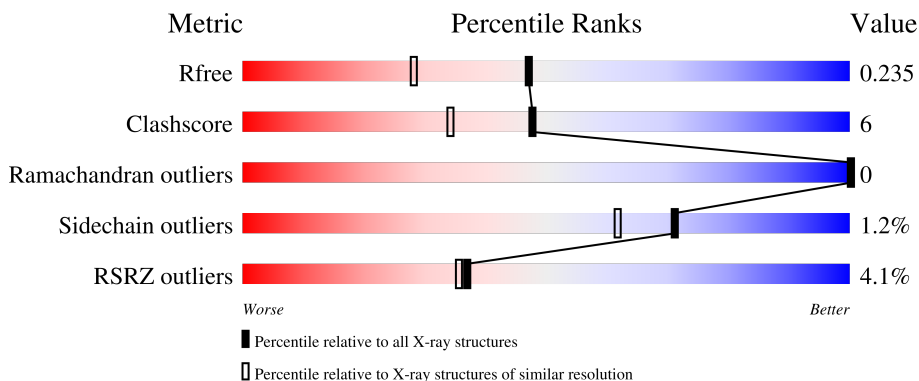|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.85 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	Percentile Ranks	Value
Rfree		0.235
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		1.2%
RSRZ outliers		4.1%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 >=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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	308	4% / 81% / 14% / 5%
2	A	3	67% / 33%
3	B	2	100%
3	C	2	100%

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 2563 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.
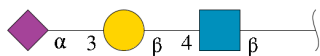
- Molecule 1 is a protein called Down syndrome cell adhesion molecule.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	292	2281	1454	386	430	11	0	2	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	593	GLY	-	expression tag	UNP O60469
AAA	594	THR	-	expression tag	UNP O60469
AAA	885	GLU	-	expression tag	UNP O60469
AAA	886	LEU	-	expression tag	UNP O60469
AAA	887	GLU	-	expression tag	UNP O60469
AAA	888	ASN	-	expression tag	UNP O60469
AAA	889	LEU	-	expression tag	UNP O60469
AAA	890	TYR	-	expression tag	UNP O60469
AAA	891	PHE	-	expression tag	UNP O60469
AAA	892	GLN	-	expression tag	UNP O60469
AAA	893	GLY	-	expression tag	UNP O60469
AAA	894	SER	-	expression tag	UNP O60469
AAA	895	HIS	-	expression tag	UNP O60469
AAA	896	HIS	-	expression tag	UNP O60469
AAA	897	HIS	-	expression tag	UNP O60469
AAA	898	HIS	-	expression tag	UNP O60469
AAA	899	HIS	-	expression tag	UNP O60469
AAA	900	HIS	-	expression tag	UNP O60469

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto pyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
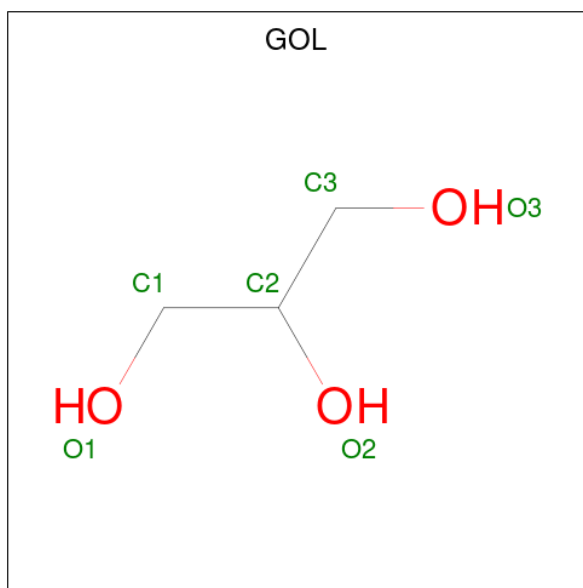
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	3	Total 45	C 25	N 2	O 18	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	2	Total 25	C 14	N 1	O 10	0	0	0
3	C	2	Total 25	C 14	N 1	O 10	0	0	0

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

GOL

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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	1	Total 1	Ca 1	0	0

- Molecule 6 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		
6	AAA	1	14	8	1	5	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	AAA	166	166	166	0	0

# 3   Residue-property plots ⓘ

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.
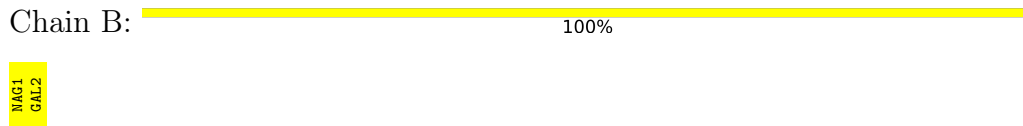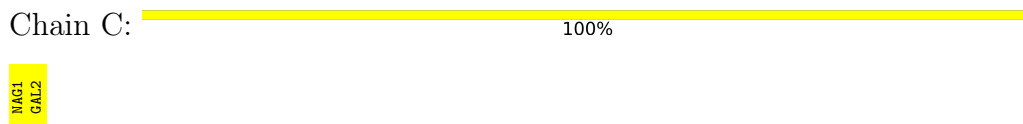
• Molecule 1: Down syndrome cell adhesion molecule
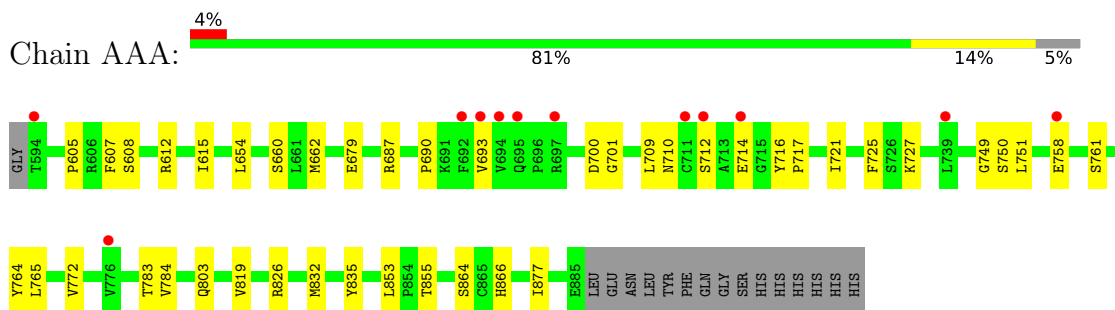
• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose
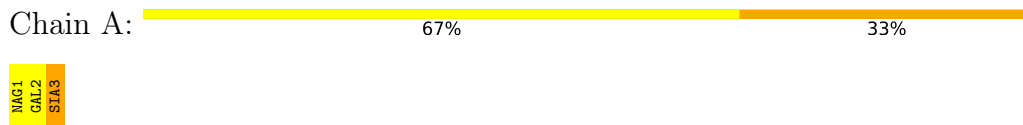
• Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

• Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	78.60Å 71.42Å 92.17Å 90.00° 113.06° 90.00°	Depositor
Resolution (Å)	84.81 – 1.85 84.81 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.8 (84.81-1.85) 98.8 (84.81-1.85)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.195 , 0.228 0.201 , 0.235	Depositor DCC
R_{free} test set	2001 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	44.0	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.2	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2563	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, CA, GOL, NAG, SIA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	AAA	0.83	1/2334 (0.0%)	0.96	2/3176 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	679	GLU	CD-OE1	5.14	1.31	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	612	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	AAA	612	ARG	NE-CZ-NH2	-6.58	117.01	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	2281	0	2289	25	0
2	A	45	0	37	3	0
3	B	25	0	22	0	0
3	C	25	0	22	0	0
4	AAA	6	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AAA	1	0	0	0	0
6	AAA	14	0	13	0	0
7	AAA	166	0	0	1	0
All	All	2563	0	2389	29	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.

The worst 5 of 29 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3:SIA:C7	2:A:3:SIA:C8	1.74	1.57
1:AAA:826:ARG:NH1	1:AAA:832:MET:SD	2.60	0.74
1:AAA:758:GLU:HA	1:AAA:784[A]:VAL:HG11	1.76	0.66
2:A:3:SIA:C7	2:A:3:SIA:C9	2.78	0.59
2:A:3:SIA:C8	2:A:3:SIA:C6	2.75	0.57

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	292/308 (95%)	282 (97%)	10 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	259/271 (96%)	256 (99%)	3 (1%)	71	62

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	608	SER
1	AAA	693	VAL
1	AAA	712	SER

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

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5   Carbohydrates ⓘ

7 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	A	1	2,1	14,14,15	0.82	0	17,19,21	1.35	2 (11%)
2	GAL	A	2	2	11,11,12	3.90	6 (54%)	15,15,17	2.00	5 (33%)
2	SIA	A	3	2	20,20,21	4.60	13 (65%)	24,28,31	1.54	4 (16%)
3	NAG	B	1	3,1	14,14,15	0.56	0	17,19,21	2.39	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	GAL	B	2	3	11,11,12	2.02	2 (18%)	15,15,17	2.13	3 (20%)
3	NAG	C	1	3,1	14,14,15	0.67	0	17,19,21	1.77	6 (35%)
3	GAL	C	2	3	11,11,12	1.85	4 (36%)	15,15,17	1.95	6 (40%)

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	A	1	2,1	-	0/6/23/26	0/1/1/1
2	GAL	A	2	2	-	2/2/19/22	0/1/1/1
2	SIA	A	3	2	-	9/18/34/38	0/1/1/1
3	NAG	B	1	3,1	-	2/6/23/26	0/1/1/1
3	GAL	B	2	3	-	1/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	2/6/23/26	0/1/1/1
3	GAL	C	2	3	-	0/2/19/22	0/1/1/1

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3	SIA	C2-C1	11.98	1.63	1.52
2	A	3	SIA	C8-C7	11.32	1.74	1.53
2	A	2	GAL	O5-C1	-10.03	1.27	1.43
2	A	3	SIA	C4-C5	6.56	1.58	1.53
2	A	3	SIA	C6-C5	4.67	1.60	1.53

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1	NAG	C1-O5-C5	8.91	124.27	112.19
3	B	2	GAL	O2-C2-C3	-5.45	99.22	110.14
2	A	2	GAL	O3-C3-C2	-4.30	101.76	109.99
2	A	1	NAG	O5-C5-C4	-3.87	101.41	110.83
3	C	2	GAL	O2-C2-C3	-3.86	102.41	110.14

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3	SIA	O8-C8-C9-O9
2	A	2	GAL	O5-C5-C6-O6
3	B	1	NAG	O5-C5-C6-O6
2	A	3	SIA	C6-C7-C8-C9
3	B	1	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3	SIA	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 oligosaccharide.

Oligosaccharide Chain A

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain B

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings
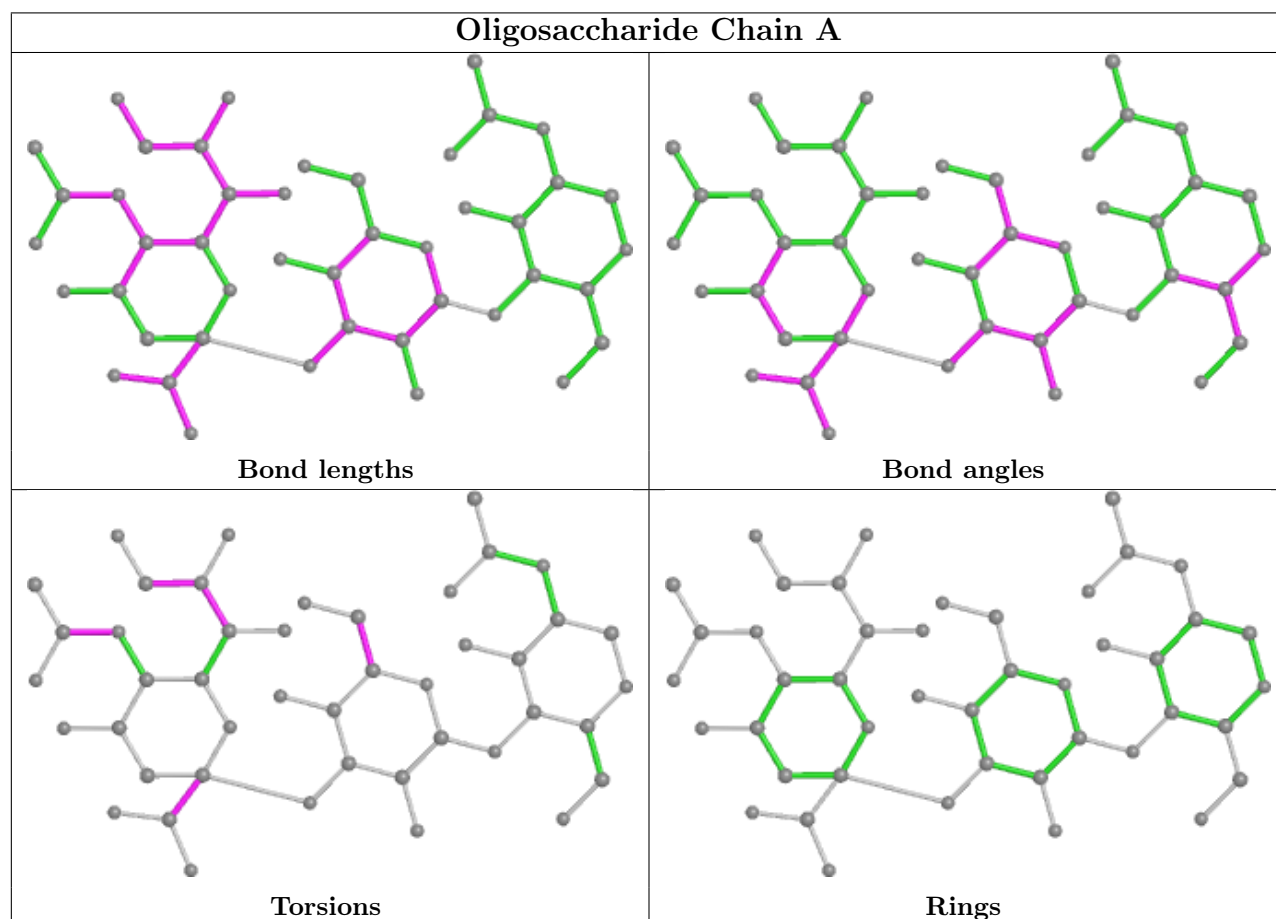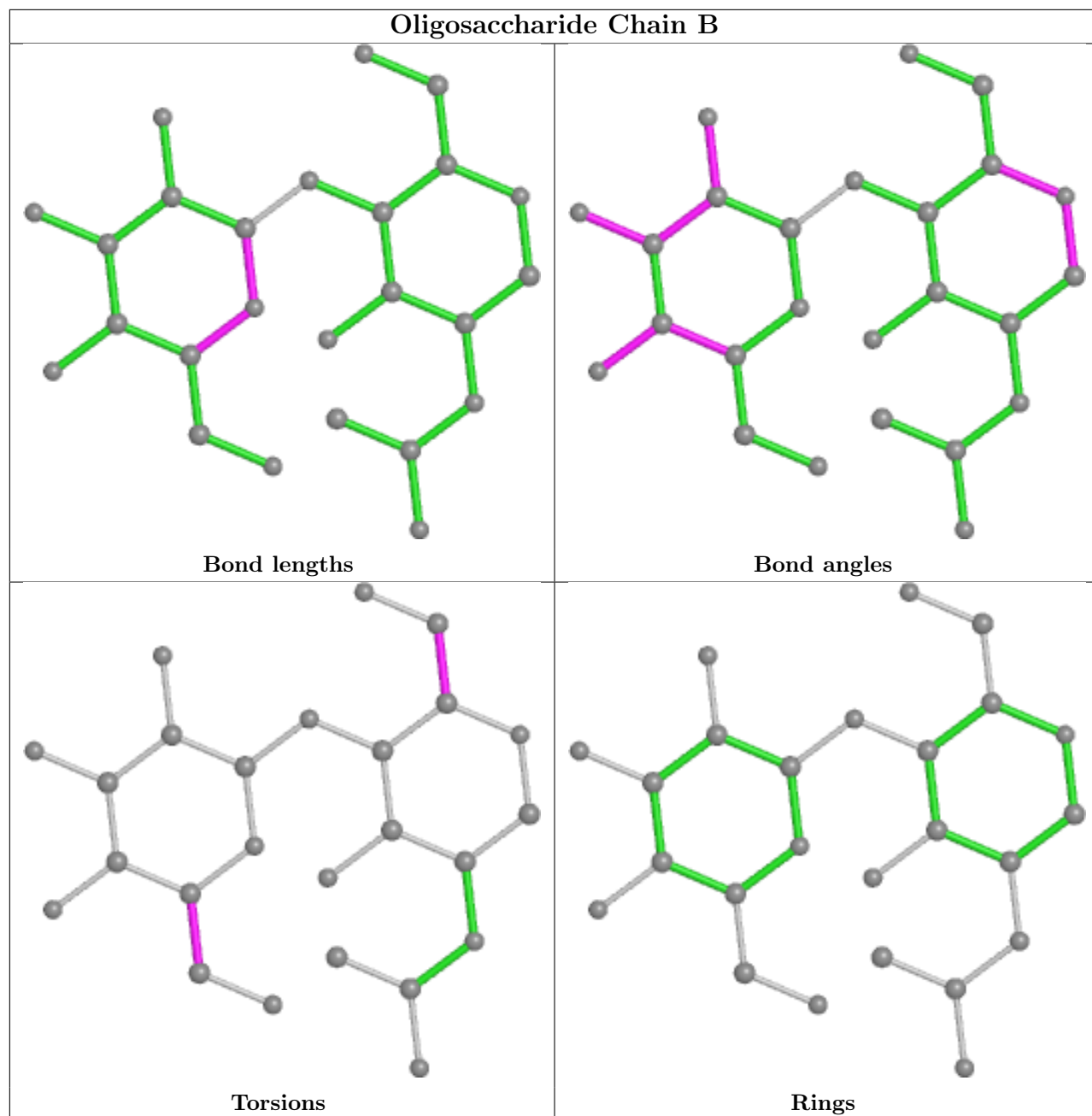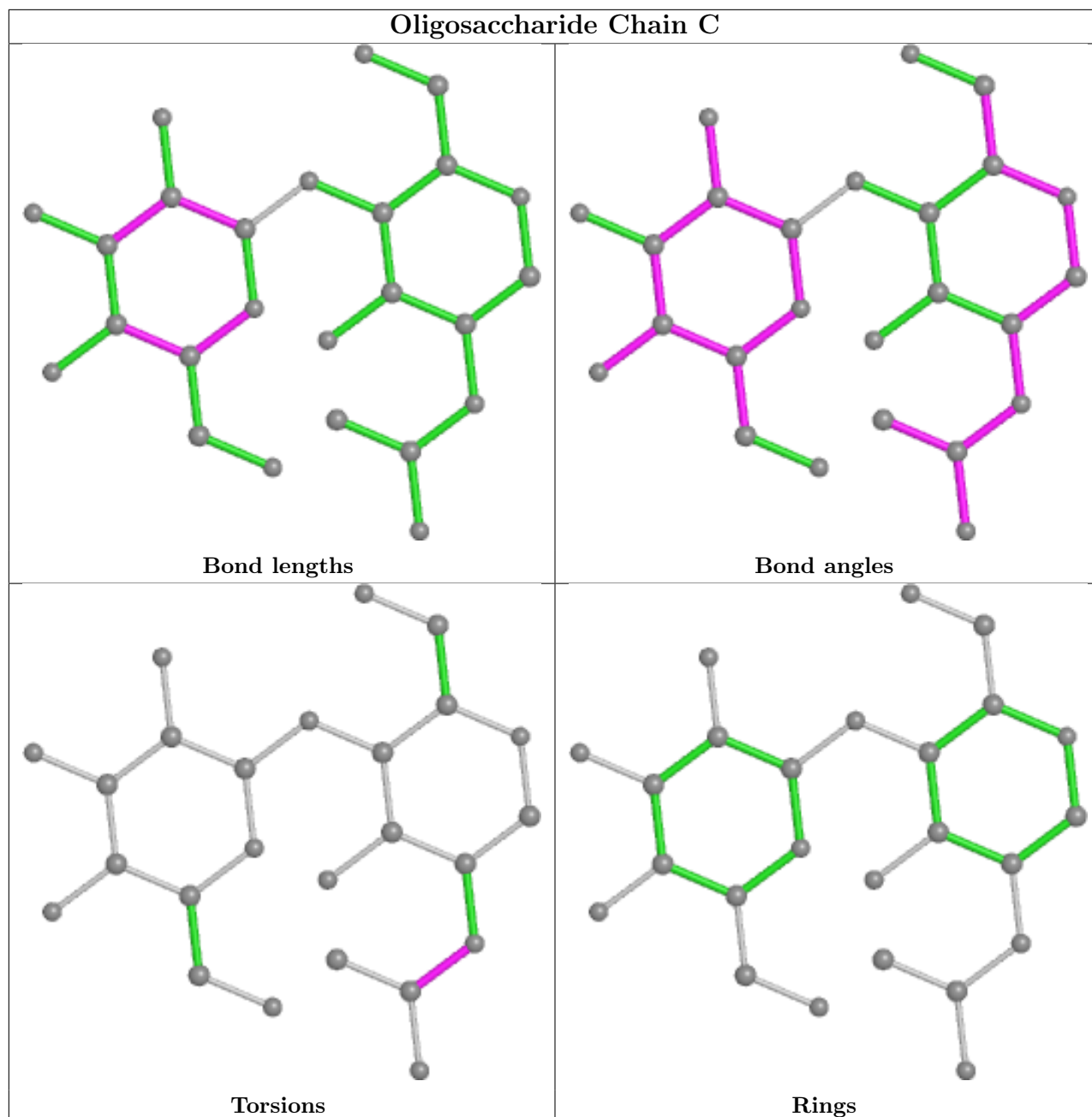
5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	GOL	AAA	1001	5	5,5,5	0.28	0	5,5,5	0.63	0
6	NAG	AAA	1003	1	14,14,15	0.52	0	17,19,21	2.37	8 (47%)

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	AAA	1001	5	-	2/4/4/4	-
6	NAG	AAA	1003	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	AAA	1003	NAG	C4-C3-C2	-4.67	104.17	111.02
6	AAA	1003	NAG	O5-C5-C6	4.62	114.44	107.20
6	AAA	1003	NAG	C3-C4-C5	-3.66	103.71	110.24
6	AAA	1003	NAG	C1-C2-N2	2.45	114.67	110.49
6	AAA	1003	NAG	O3-C3-C4	2.43	115.97	110.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	AAA	1003	NAG	C8-C7-N2-C2
6	AAA	1003	NAG	O7-C7-N2-C2
4	AAA	1001	GOL	C1-C2-C3-O3
4	AAA	1001	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AAA	1001	GOL	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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(Å²)	Q<0.9
1	AAA	292/308 (94%)	0.23	12 (4%)	37	35	35, 55, 102, 140	1 (0%)

The worst 5 of 12 RSRZ outliers are listed below:

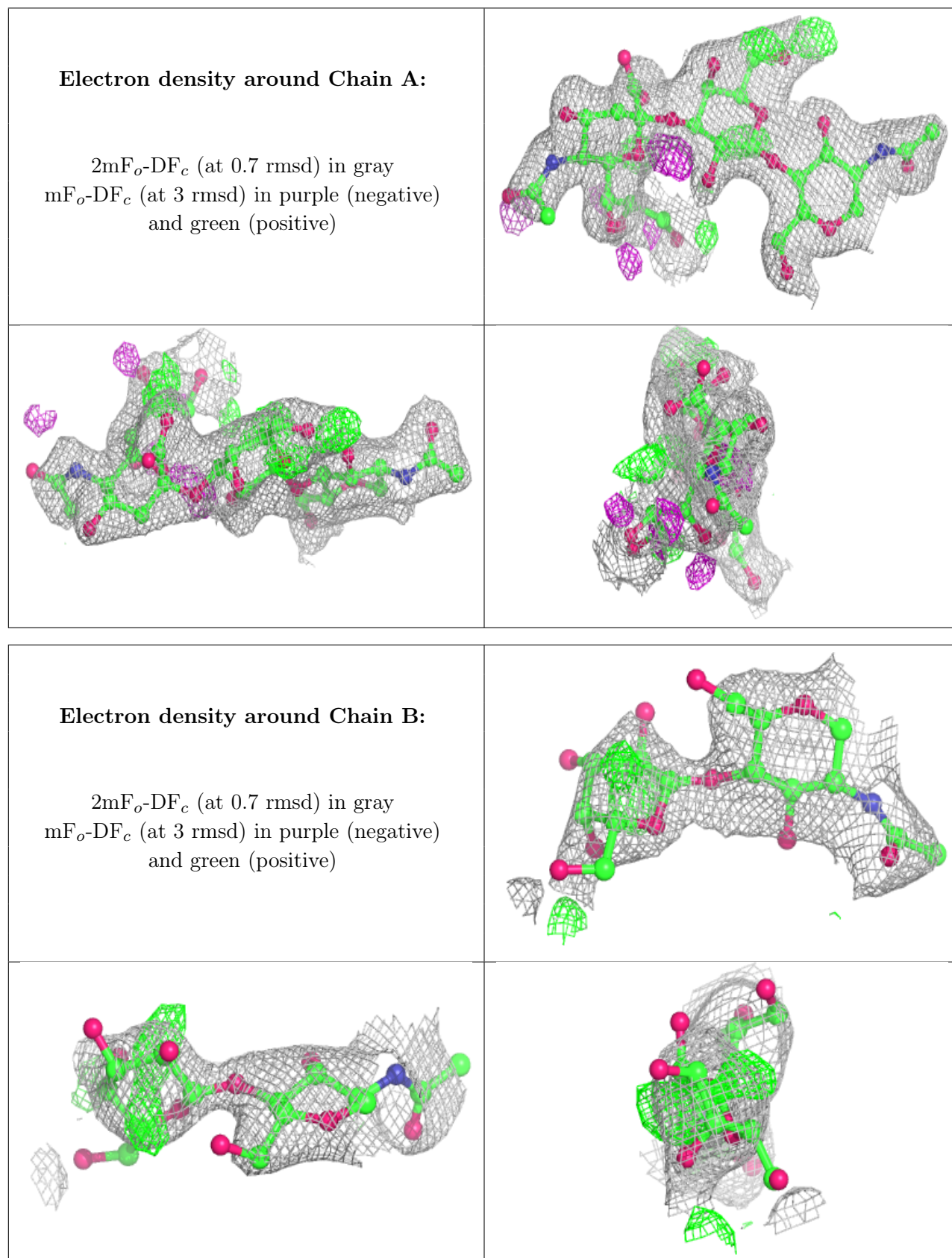| Mol	Chain	Res	Type	RSRZ
1	AAA	693	VAL	12.6
1	AAA	694	VAL	6.8
1	AAA	714	GLU	3.1
1	AAA	739	LEU	2.9
1	AAA	697	ARG	2.9

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

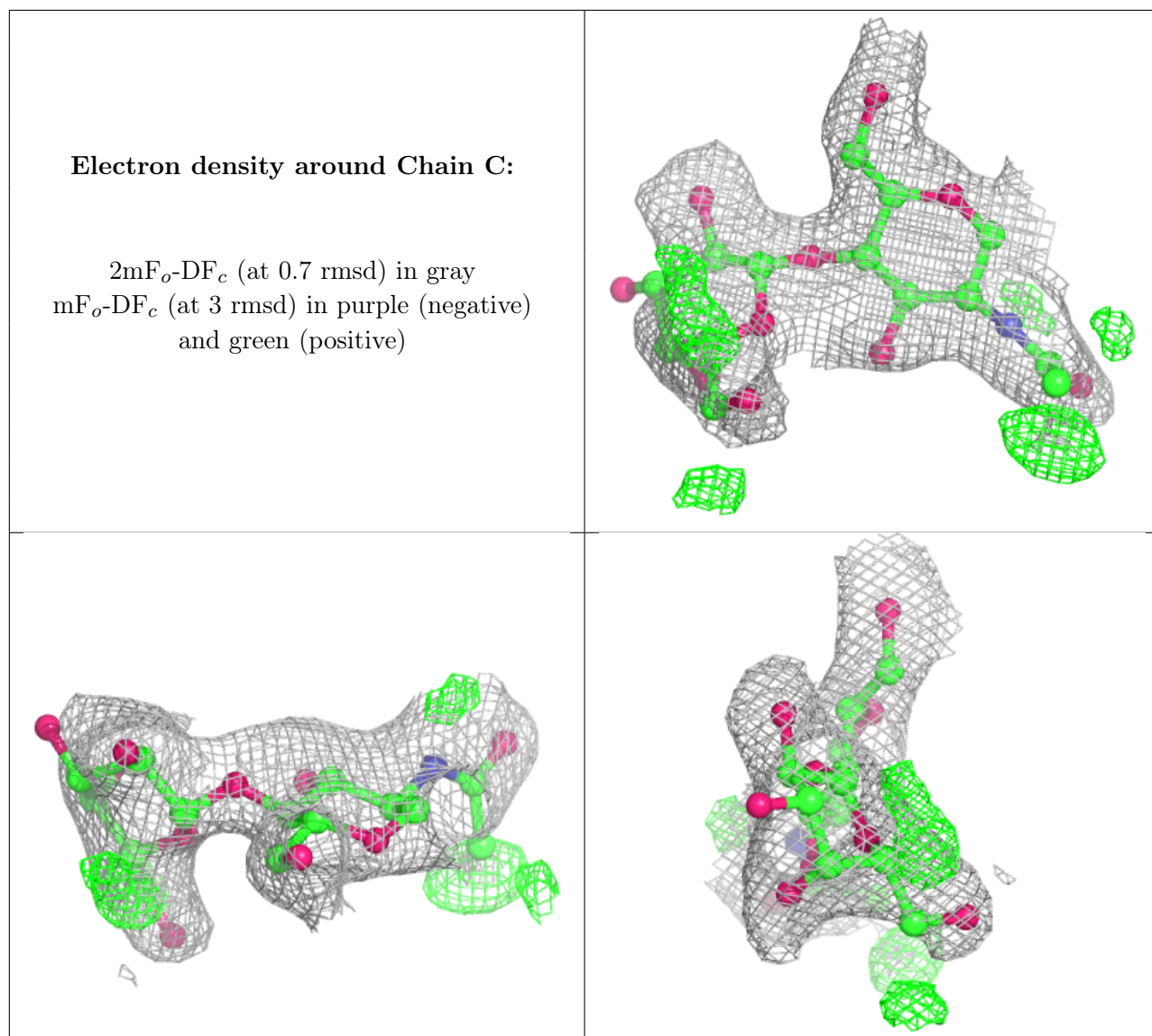There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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, 95th 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(Å²)	Q<0.9
3	GAL	B	2	11/12	0.74	0.21	74,84,88,93	11
3	GAL	C	2	11/12	0.76	0.15	62,72,78,84	11
3	NAG	C	1	14/15	0.86	0.10	72,80,87,91	0
2	GAL	A	2	11/12	0.89	0.10	49,60,68,69	0
2	SIA	A	3	20/21	0.92	0.18	46,70,93,97	0
3	NAG	B	1	14/15	0.94	0.12	98,103,111,113	0
2	NAG	A	1	14/15	0.98	0.11	31,38,44,45	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 A:

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 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 C:

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

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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^2)	Q<0.9
6	NAG	AAA	1003	14/15	0.84	0.12	79,89,93,97	14
4	GOL	AAA	1001	6/6	0.96	0.08	39,54,72,87	0
5	CA	AAA	1002	1/1	0.99	0.15	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.