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 (i)

Sep 24, 2023 – 09:42 AM EDT

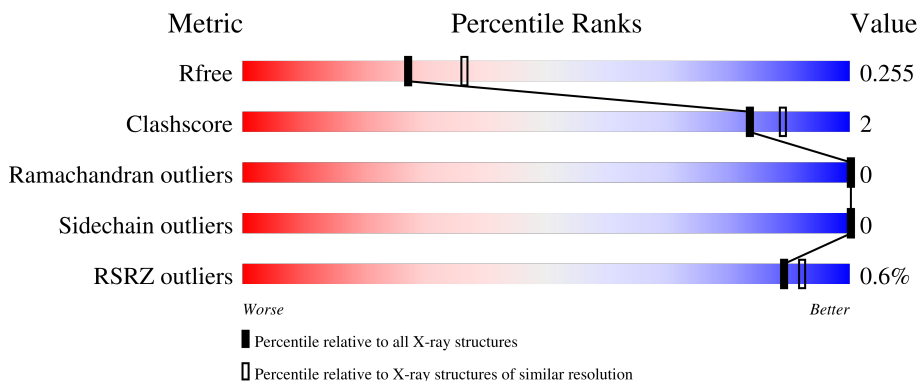|		
PDB ID	:	5TZ2
Title	:	Crystal structure of human CD47 ECD bound to Fab of C47B222
Authors	:	Cardoso, R.M.F.
Deposited on	:	2016-11-21
Resolution	:	2.30 Å(reported)

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 2.30 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		0.255
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		0
RSRZ outliers		0.6%

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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	H	229	87% 6% 7%
2	L	214	96%
3	C	129	78% 10% 12%
4	A	2	50% 50%
4	B	2	100%

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 4197 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 C47B222 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	213	Total	C	N	O	S	0	0	0
			1578	1011	255	306	6			

- Molecule 2 is a protein called C47B222 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	0	0
			1554	987	266	297	4			

- Molecule 3 is a protein called Leukocyte surface antigen CD47.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	114	Total	C	N	O	S	0	0	0
			856	545	134	173	4			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	15	GLY	CYS	engineered mutation	UNP Q08722
C	124	HIS	-	expression tag	UNP Q08722
C	125	HIS	-	expression tag	UNP Q08722
C	126	HIS	-	expression tag	UNP Q08722
C	127	HIS	-	expression tag	UNP Q08722
C	128	HIS	-	expression tag	UNP Q08722
C	129	HIS	-	expression tag	UNP Q08722

- Molecule 4 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
4	A	2	Total 28	C 16	N 2	O 10	0	0	0
4	B	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG

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

- Molecule 7 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	46	Total	O	0	0
			46	46		
7	L	39	Total	O	0	0
			39	39		
7	C	20	Total	O	0	0
			20	20		

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.
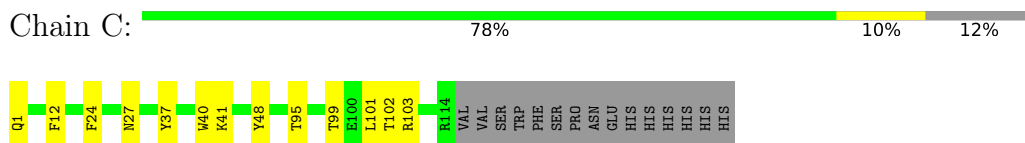
• Molecule 1: C47B222 Fab Heavy Chain
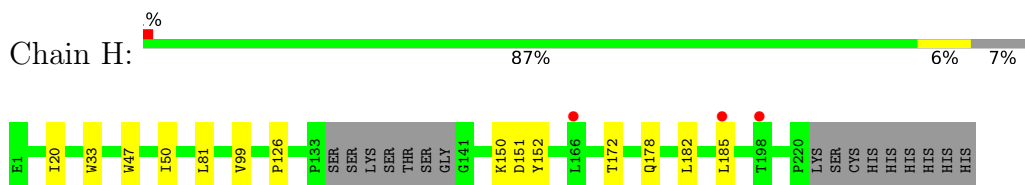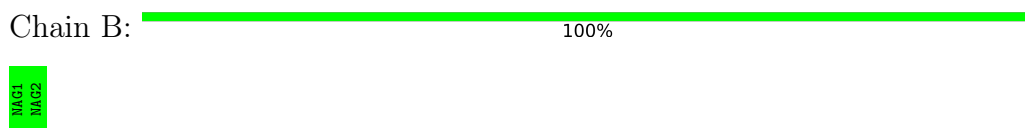

• Molecule 2: C47B222 Fab Light Chain
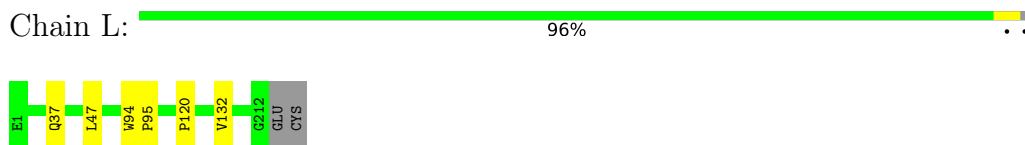
• Molecule 3: Leukocyte surface antigen CD47

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

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

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.57Å 72.93Å 72.70Å 90.00° 108.97° 90.00°	Depositor
Resolution (Å)	32.22 – 2.30 50.03 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.3 (32.22-2.30) 98.4 (50.03-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 2.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.201 , 0.255 0.203 , 0.255	Depositor DCC
R_{free} test set	1332 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	0.918	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.5	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4197	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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: NAG, 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	H	0.20	0/1621	0.37	0/2217
2	L	0.21	0/1592	0.37	0/2178
3	C	0.21	0/870	0.38	0/1184
All	All	0.21	0/4083	0.37	0/5579

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 ⓘ

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	H	1578	0	1493	7	0
2	L	1554	0	1441	3	0
3	C	856	0	795	9	0
4	A	28	0	25	0	0
4	B	28	0	25	0	0
5	L	6	0	8	0	0
6	C	42	0	39	2	0
7	C	20	0	0	0	0
7	H	46	0	0	0	0
7	L	39	0	0	0	0
All	All	4197	0	3826	19	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 2.

The worst 5 of 19 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:H:126:PRO:HB3	1:H:152:TYR:HB3	1.82	0.62
3:C:12:PHE:HB3	6:C:202:NAG:H82	1.82	0.61
2:L:94:TRP:CD2	2:L:95:PRO:HA	2.40	0.56
3:C:40:TRP:HB2	3:C:48:TYR:HB3	1.87	0.55
2:L:37:GLN:HB3	2:L:47:LEU:HD11	1.88	0.55

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	H	209/229 (91%)	202 (97%)	7 (3%)	0	100	100
2	L	210/214 (98%)	200 (95%)	10 (5%)	0	100	100
3	C	112/129 (87%)	104 (93%)	8 (7%)	0	100	100
All	All	531/572 (93%)	506 (95%)	25 (5%)	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	H	166/195 (85%)	166 (100%)	0	100	100
2	L	153/184 (83%)	153 (100%)	0	100	100
3	C	89/118 (75%)	89 (100%)	0	100	100
All	All	408/497 (82%)	408 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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 ⓘ

4 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	$\#|Z| > 2$
4	NAG	A	1	3,4	14,14,15	0.47	0	17,19,21	1.35	1 (5%)
4	NAG	A	2	4	14,14,15	0.18	0	17,19,21	0.55	0
4	NAG	B	1	3,4	14,14,15	0.25	0	17,19,21	0.44	0
4	NAG	B	2	4	14,14,15	0.38	0	17,19,21	0.50	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.

WORLDWIDE
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PROTEIN DATA BANK

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1	3,4	-	3/6/23/26	0/1/1/1
4	NAG	A	2	4	-	4/6/23/26	0/1/1/1
4	NAG	B	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	B	2	4	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1	NAG	O5-C1-C2	-4.04	104.91	111.29

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1	NAG	O5-C5-C6-O6
4	A	1	NAG	C8-C7-N2-C2
4	A	1	NAG	O7-C7-N2-C2
4	B	1	NAG	C4-C5-C6-O6
4	A	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.

Oligosaccharide Chain A

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain B
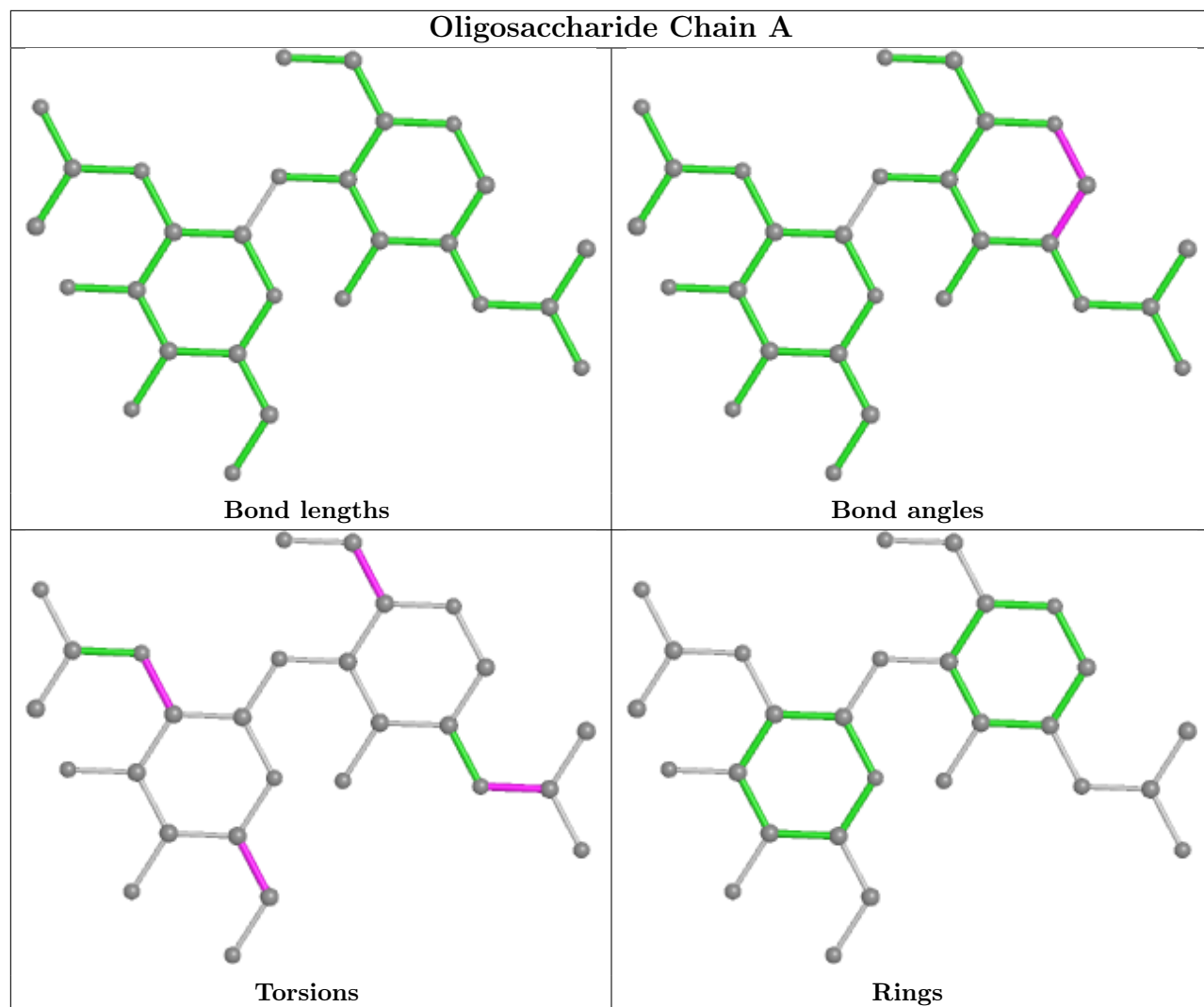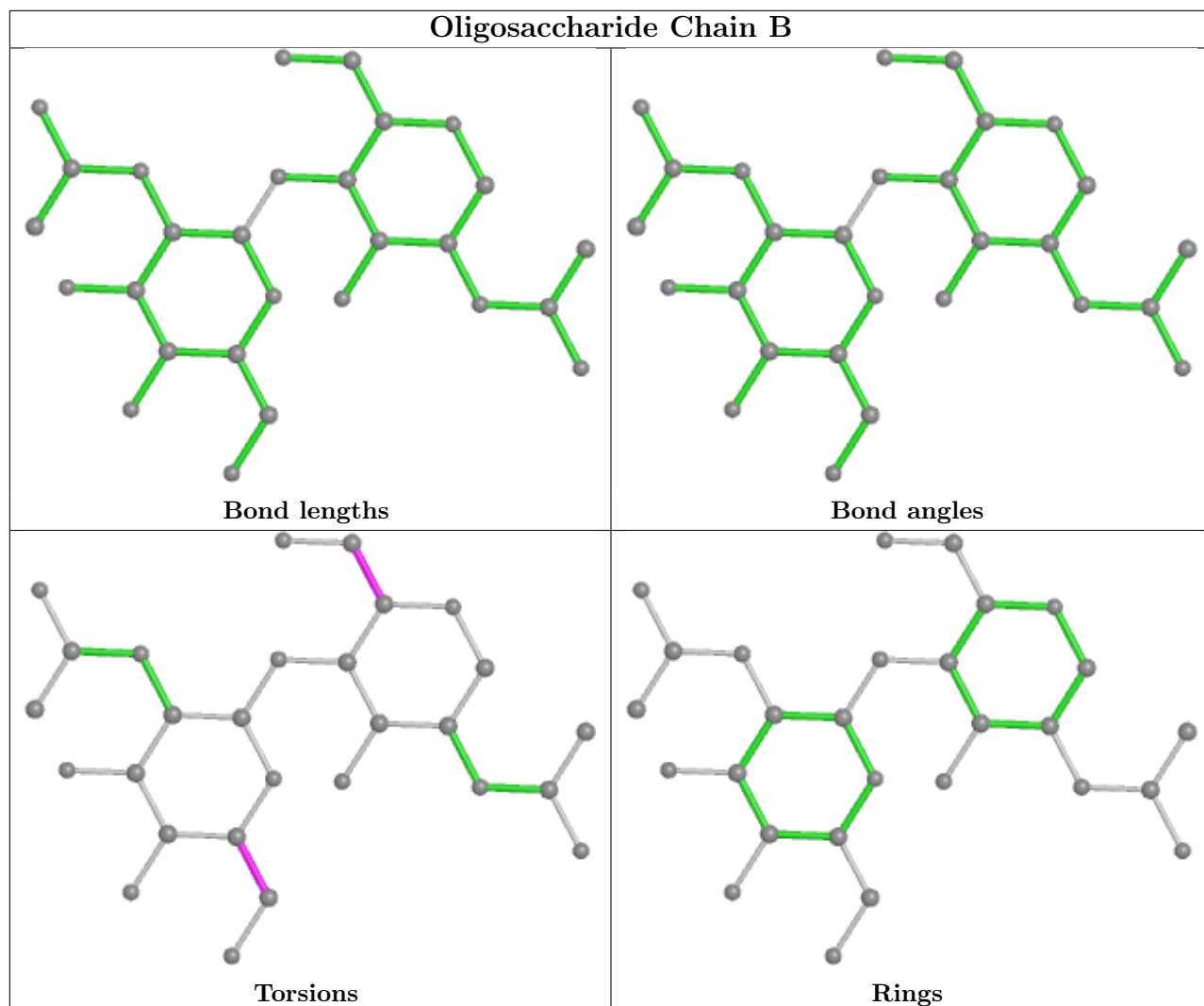
5.6 Ligand geometry ⓘ

4 ligands 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	$\#|Z| > 2$
6	NAG	C	203	3	14,14,15	0.22	0	17,19,21	0.38	0
5	GOL	L	301	-	5,5,5	0.36	0	5,5,5	0.30	0
6	NAG	C	202	3	14,14,15	0.24	0	17,19,21	0.41	0
6	NAG	C	201	3	14,14,15	0.29	0	17,19,21	0.62	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
6	NAG	C	203	3	-	0/6/23/26	0/1/1/1
5	GOL	L	301	-	-	2/4/4/4	-
6	NAG	C	202	3	-	2/6/23/26	0/1/1/1
6	NAG	C	201	3	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	301	GOL	O1-C1-C2-C3
6	C	201	NAG	C8-C7-N2-C2
6	C	201	NAG	O7-C7-N2-C2
6	C	202	NAG	O5-C5-C6-O6
6	C	202	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	202	NAG	1	0
6	C	201	NAG	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	H	213/229 (93%)	0.13	3 (1%)	75	80	44, 62, 83, 102	0
2	L	212/214 (99%)	0.20	0	100	100	43, 66, 92, 125	0
3	C	114/129 (88%)	0.17	0	100	100	47, 65, 93, 115	0
All	All	539/572 (94%)	0.16	3 (0%)	89	92	43, 64, 91, 125	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	166	LEU	2.3
1	H	198	THR	2.2
1	H	185	LEU	2.0

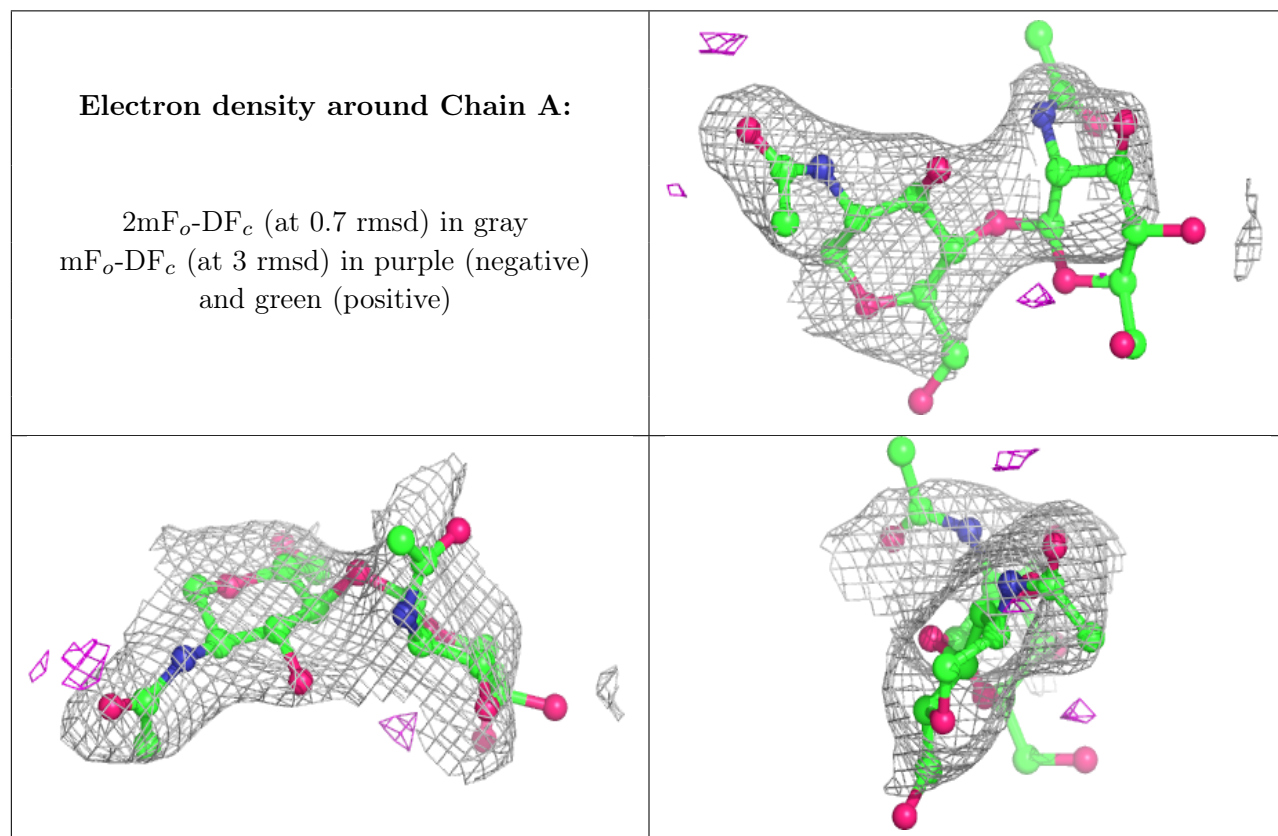## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

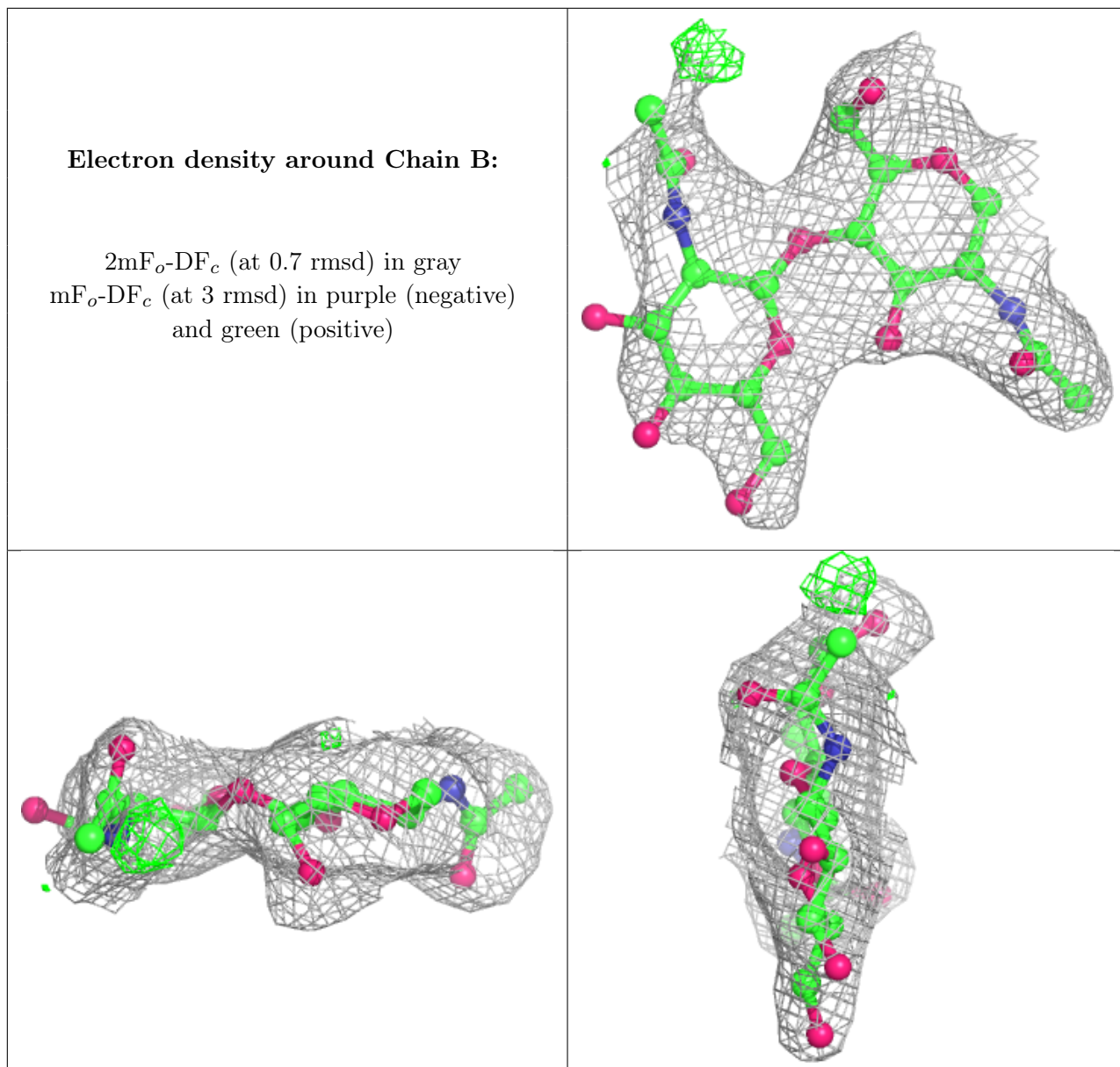There are no non-standard protein/DNA/RNA residues in this entry.

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
4	NAG	A	2	14/15	0.68	0.29	127,133,144,146	0
4	NAG	B	2	14/15	0.81	0.21	100,123,129,129	0
4	NAG	B	1	14/15	0.90	0.13	65,86,97,108	0
4	NAG	A	1	14/15	0.91	0.13	79,89,100,116	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:

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

Electron density around Chain B:

$2mF_o\text{-}DF_c$ (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	C	201	14/15	0.68	0.32	96,108,117,120	0
6	NAG	C	202	14/15	0.80	0.27	59,84,102,108	0
5	GOL	L	301	6/6	0.90	0.24	81,88,91,93	0
6	NAG	C	203	14/15	0.91	0.12	63,79,90,96	0

6.5 Other polymers ⓘ

There are no such residues in this entry.