WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 4, 2024 – 05:47 pm GMT

PDB ID	:	5BQC
Title	:	Crystal structure of Norrin in complex with the cysteine-rich domain of Frizzled 4 and sucrose octasulfate
Authors	:	Chang, T.-H.; Hsieh, F.-L.; Zebisch, M.; Harlos, K.; Jones, E.Y.
Deposited on	:	2015-05-28
Resolution	:	3.00 Å(reported)

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

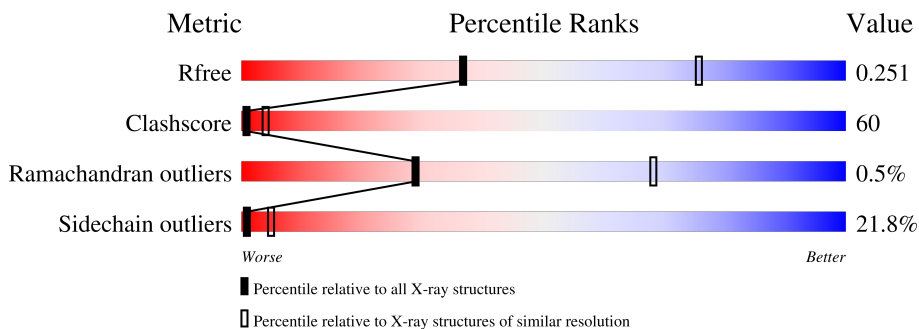|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 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		0.251
Clashscore		60
Ramachandran outliers		0.5%
Sidechain outliers		21.8%

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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 >=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%

Mol	Chain	Length	Quality of chain
1	B	149	26% 46% 12% 17%
2	A	122	32% 34% 16% 18%
3	C	2	100%

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
3	GU4	C	1	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	YYJ	C	2	-	-	X	-
4	NAG	B	202	X	-	-	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 1842 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 Frizzled-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	124	Total 971	C 610	N 165	O 180	S 16	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	39	ASP	-	expression tag	UNP Q9ULV1
B	40	THR	-	expression tag	UNP Q9ULV1
B	41	GLY	-	expression tag	UNP Q9ULV1
B	180	GLY	-	expression tag	UNP Q9ULV1
B	181	THR	-	expression tag	UNP Q9ULV1
B	182	LEU	-	expression tag	UNP Q9ULV1
B	183	GLU	-	expression tag	UNP Q9ULV1
B	184	VAL	-	expression tag	UNP Q9ULV1
B	185	LEU	-	expression tag	UNP Q9ULV1
B	186	PHE	-	expression tag	UNP Q9ULV1
B	187	GLN	-	expression tag	UNP Q9ULV1

- Molecule 2 is a protein called Norrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	100	Total 788	C 480	N 154	O 140	S 14	0	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLY	-	expression tag	UNP Q00604
A	23	PRO	-	expression tag	UNP Q00604
A	24	GLY	-	expression tag	UNP Q00604
A	134	GLY	-	expression tag	UNP Q00604
A	135	THR	-	expression tag	UNP Q00604

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	136	GLU	-	expression tag	UNP Q00604
A	137	THR	-	expression tag	UNP Q00604
A	138	SER	-	expression tag	UNP Q00604
A	139	GLN	-	expression tag	UNP Q00604
A	140	VAL	-	expression tag	UNP Q00604
A	141	ALA	-	expression tag	UNP Q00604
A	142	PRO	-	expression tag	UNP Q00604
A	143	ALA	-	expression tag	UNP Q00604

- Molecule 3 is an oligosaccharide called 1,3,4,6-tetra-O-sulfo-beta-D-fructofuranose-(2-1)-2,3, 4,6-tetra-O-sulfonato-alpha-D-glucopyranose.
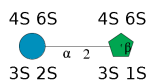
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total 55	C 12	O 35	S 8	0	0	0

- 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
4	B	1	Total 14	C 8	N 1	O 5	0	0

Continued on next page...

Continued from previous page...

| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	14	8	1	5	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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
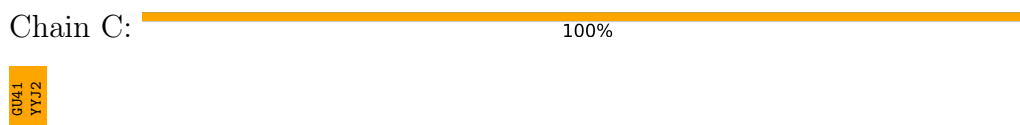
- Molecule 1: Frizzled-4

Chain B:

- Molecule 2: Norrin

Chain A:
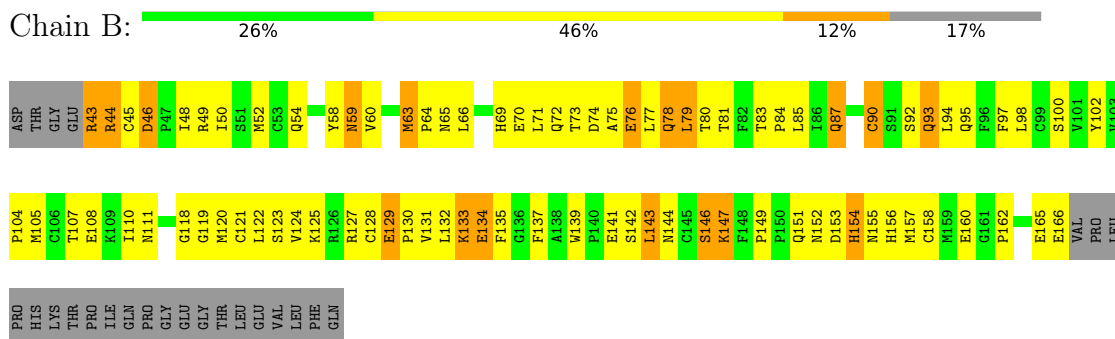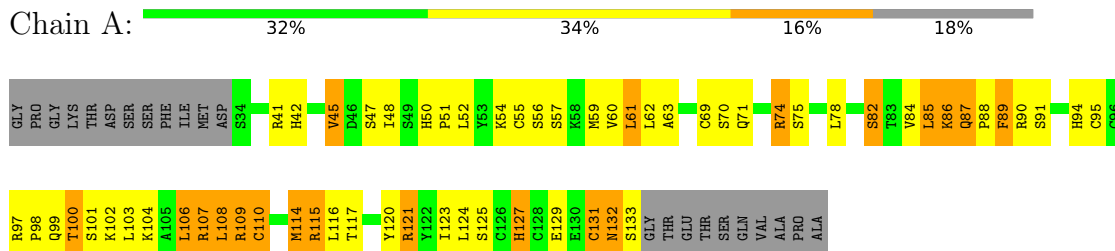
- Molecule 3: 1,3,4,6-tetra-O-sulfo-beta-D-fructofuranose-(2-1)-2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	119.14Å 119.14Å 119.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.34 – 3.00 47.34 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.34-3.00) 100.0 (47.34-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.215 , 0.268 0.262 , 0.251	Depositor DCC
R_{free} test set	483 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å^2)	111.0	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 72.4	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	1842	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[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: GU4, NAG, YYJ

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	B	0.37	0/995	0.54	0/1347
2	A	0.50	0/804	0.57	0/1078
All	All	0.43	0/1799	0.55	0/2425

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	59	ASN	Peptide

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.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	971	0	933	129	0
2	A	788	0	779	83	5
3	C	55	0	6	16	4
4	B	28	0	26	3	0
All	All	1842	0	1744	214	5

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 60.

The worst 5 of 214 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:153:ASP:OD1	1:B:156:HIS:N	1.87	1.08
1:B:110:ILE:HB	2:A:59:MET:HE1	1.36	1.03
2:A:71:GLN:OE1	2:A:94:HIS:ND1	1.97	0.97
2:A:108:LEU:N	2:A:116:LEU:O	1.96	0.97
1:B:152:ASN:OD1	1:B:158:CYS:N	2.00	0.93

All (5) 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)
2:A:107:ARG:NH1	3:C:2:YYJ:O6[10_444]	1.75	0.45
2:A:107:ARG:NH1	3:C:2:YYJ:C5[10_444]	1.97	0.23
2:A:131:CYS:SG	2:A:131:CYS:SG[7_555]	2.00	0.20
2:A:115:ARG:NH2	3:C:2:YYJ:O3S4[10_444]	2.05	0.15
2:A:107:ARG:CZ	3:C:2:YYJ:C6[10_444]	2.14	0.06

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	B	122/149 (82%)	111 (91%)	11 (9%)	0	100	100
2	A	98/122 (80%)	93 (95%)	4 (4%)	1 (1%)	15	53
All	All	220/271 (81%)	204 (93%)	15 (7%)	1 (0%)	29	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	87	GLN

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	B	113/135 (84%)	93 (82%)	20 (18%)	2	9
2	A	93/110 (84%)	68 (73%)	25 (27%)	0	2
All	All	206/245 (84%)	161 (78%)	45 (22%)	1	5

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	85	LEU
2	A	108	LEU
2	A	86	LYS
2	A	100	THR
2	A	110	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	87	GLN
1	B	95	GLN
2	A	71	GLN

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 ⓘ

2 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	$\#|Z| > 2$
3	GU4	C	1	1,3	27,27,28	1.41	2 (7%)	29,43,45	2.12	6 (20%)
3	YYJ	C	2	2,3	27,28,28	1.22	0	28,46,46	1.43	4 (14%)

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
3	GU4	C	1	1,3	-	9/21/38/41	0/1/1/1
3	YYJ	C	2	2,3	-	13/23/42/42	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	GU4	O2-C2	-2.80	1.43	1.47
3	C	1	GU4	O3-C3	-2.75	1.40	1.46

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1	GU4	C1-O5-C5	6.24	120.64	112.19
3	C	1	GU4	O2-C2-C3	5.15	112.35	106.65
3	C	1	GU4	C2-O2-S2	4.19	123.38	117.91
3	C	2	YYJ	C4-O4-S4	3.98	126.56	118.88
3	C	2	YYJ	O2-C2-O5	-3.92	101.94	109.50

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	GU4	C4-O4-S4-O25
3	C	1	GU4	C4-O4-S4-O26
3	C	1	GU4	C4-O4-S4-O24
3	C	1	GU4	C1-C2-O2-S2
3	C	1	GU4	C3-C2-O2-S2

There are no ring outliers.

2 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	GU4	14	0
3	C	2	YYJ	10	4

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 C

Bond lengths

Bond angles

Torsions

Rings
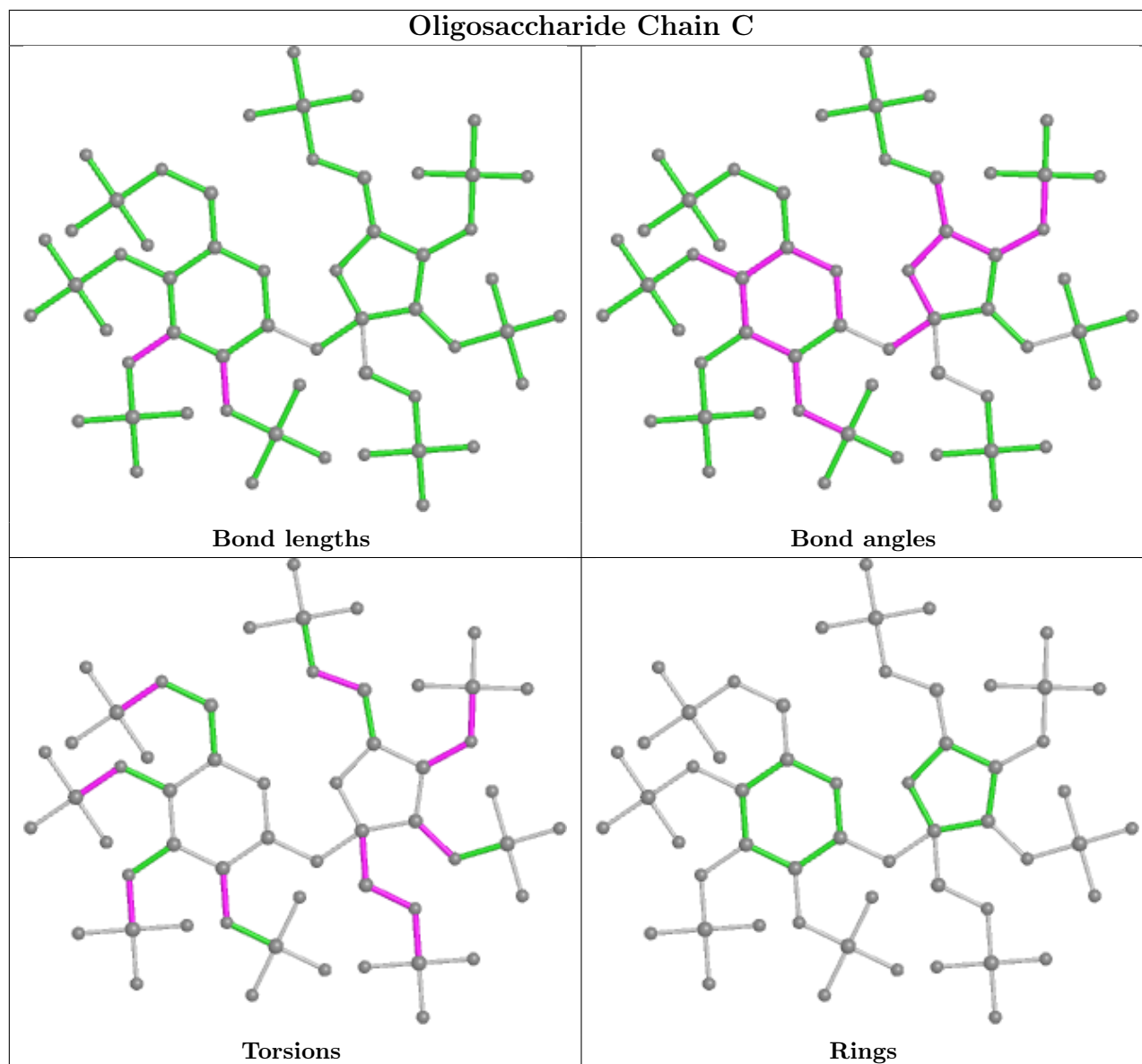
5.6 Ligand geometry ⓘ

2 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	#$|Z| > 2$
4	NAG	B	202	1	14,14,15	0.66	0	17,19,21	1.35	2 (11%)

WORLDWIDE

wwPDB

PROTEIN DATA BANK

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
4	NAG	B	201	1	14,14,15	0.71	0	17,19,21	1.52	3 (17%)

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	B	202	1	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	B	201	1	-	6/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	202	NAG	O5-C1-C2	-4.21	104.64	111.29
4	B	201	NAG	C8-C7-N2	4.00	122.87	116.10
4	B	201	NAG	O7-C7-C8	-2.59	117.25	122.06
4	B	202	NAG	C1-C2-N2	2.19	114.23	110.49
4	B	201	NAG	O5-C1-C2	-2.18	107.84	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	202	NAG	C1

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	201	NAG	O5-C5-C6-O6
4	B	202	NAG	O5-C5-C6-O6
4	B	202	NAG	C4-C5-C6-O6
4	B	201	NAG	C4-C5-C6-O6
4	B	201	NAG	C8-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	202	NAG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	201	NAG	2	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 ⓘ

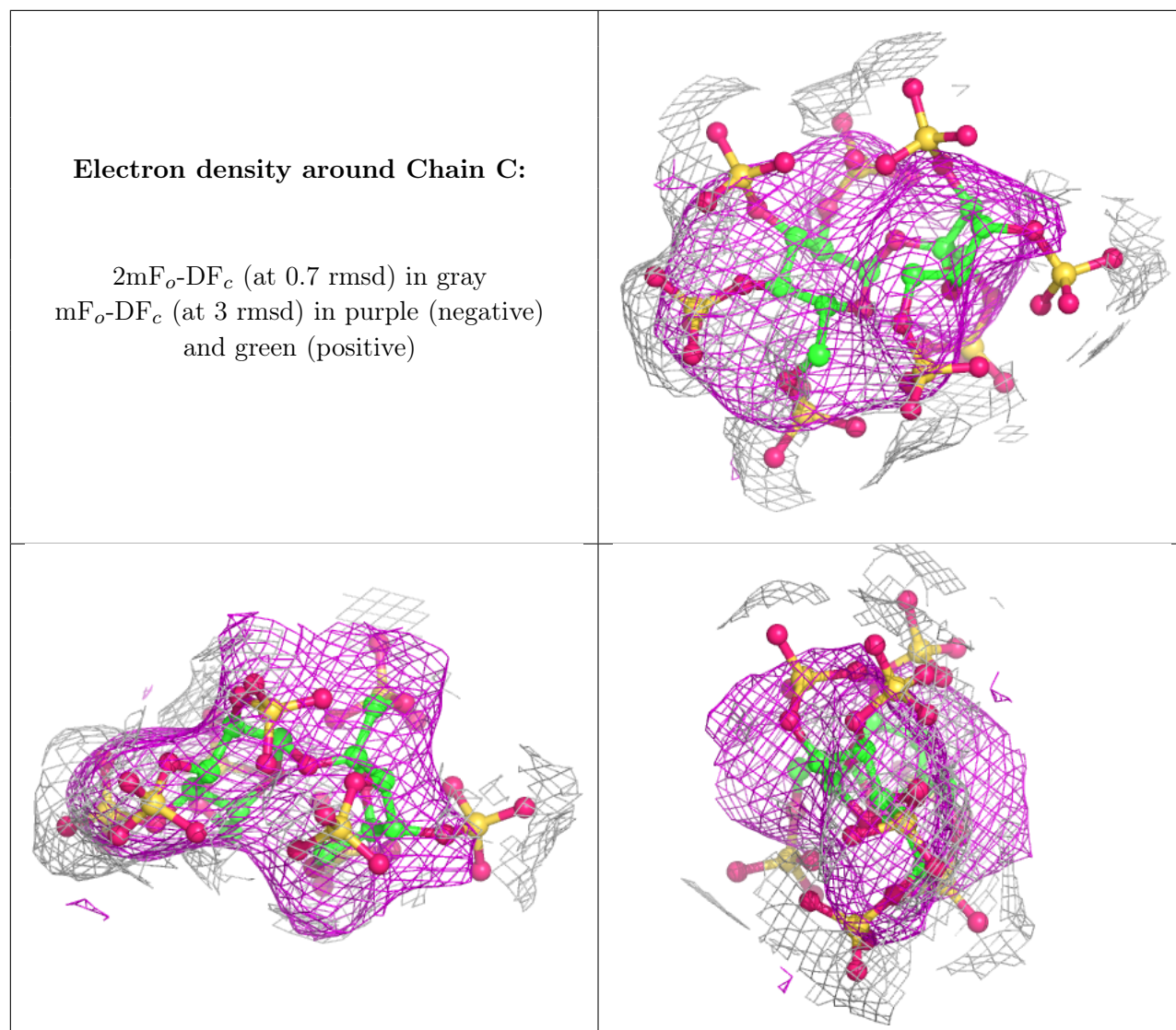Unable to reproduce the depositors R factor - this section is therefore empty.

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

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

6.3 Carbohydrates ⓘ

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

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

Electron density around Chain 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 ⓘ

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

6.5 Other polymers ⓘ

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