



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2025 – 02:02 PM JST

PDB ID : 9L2K / pdb_00009l2k
Title : The crystal structure of SFTSV Gn and SD22 antibody complex
Authors : Shi, W.F.; Quan, C.S.; Qi, J.X.
Deposited on : 2024-12-17
Resolution : 2.78 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

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 : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

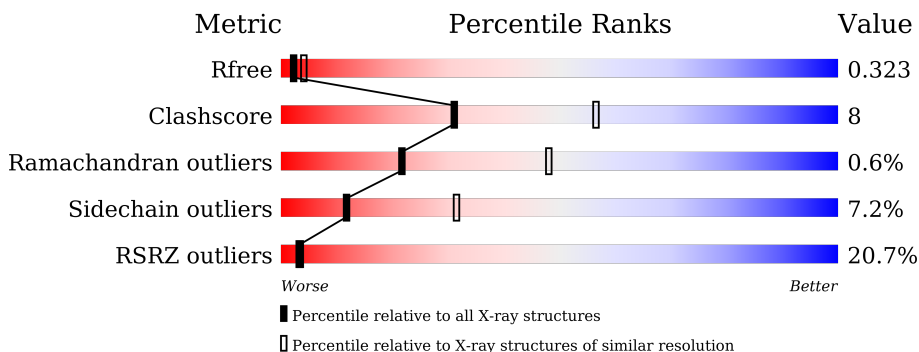
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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}	164625	4924 (2.80-2.76)
Clashscore	180529	5458 (2.80-2.76)
Ramachandran outliers	177936	5386 (2.80-2.76)
Sidechain outliers	177891	5388 (2.80-2.76)
RSRZ outliers	164620	4926 (2.80-2.76)

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 $\leq 5\%$. 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	344	<div> <div>17%</div> <div> <div>73%</div> <div>19%</div> <div>• 7%</div> </div> </div>
2	H	223	<div> <div>12%</div> <div> <div>40%</div> <div>13%</div> <div>• 46%</div> </div> </div>
3	L	214	<div> <div>13%</div> <div> <div>42%</div> <div>8%</div> <div>50%</div> </div> </div>
4	B	3	<div> <div>100%</div> </div>
5	C	2	<div> <div>50%</div> <div>50%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4262 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 Envelopment polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2462	1539	428	469	26			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A1S6K8S9
A	2	GLY	-	expression tag	UNP A0A1S6K8S9
A	3	TRP	-	expression tag	UNP A0A1S6K8S9
A	4	SER	-	expression tag	UNP A0A1S6K8S9
A	5	CYS	-	expression tag	UNP A0A1S6K8S9
A	6	ILE	-	expression tag	UNP A0A1S6K8S9
A	7	ILE	-	expression tag	UNP A0A1S6K8S9
A	8	LEU	-	expression tag	UNP A0A1S6K8S9
A	9	PHE	-	expression tag	UNP A0A1S6K8S9
A	10	LEU	-	expression tag	UNP A0A1S6K8S9
A	11	VAL	-	expression tag	UNP A0A1S6K8S9
A	12	ALA	-	expression tag	UNP A0A1S6K8S9
A	13	THR	-	expression tag	UNP A0A1S6K8S9
A	14	ALA	-	expression tag	UNP A0A1S6K8S9
A	15	THR	-	expression tag	UNP A0A1S6K8S9
A	16	GLY	-	expression tag	UNP A0A1S6K8S9
A	17	VAL	-	expression tag	UNP A0A1S6K8S9
A	18	HIS	-	expression tag	UNP A0A1S6K8S9
A	339	HIS	-	expression tag	UNP A0A1S6K8S9
A	340	HIS	-	expression tag	UNP A0A1S6K8S9
A	341	HIS	-	expression tag	UNP A0A1S6K8S9
A	342	HIS	-	expression tag	UNP A0A1S6K8S9
A	343	HIS	-	expression tag	UNP A0A1S6K8S9
A	344	HIS	-	expression tag	UNP A0A1S6K8S9

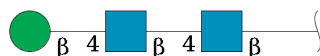
- Molecule 2 is a protein called SD22 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	121	Total	C	N	O	S	0	0	0
			921	582	157	179	3			

- Molecule 3 is a protein called SD22 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	108	Total	C	N	O	S	0	0	0
			812	510	137	162	3			

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

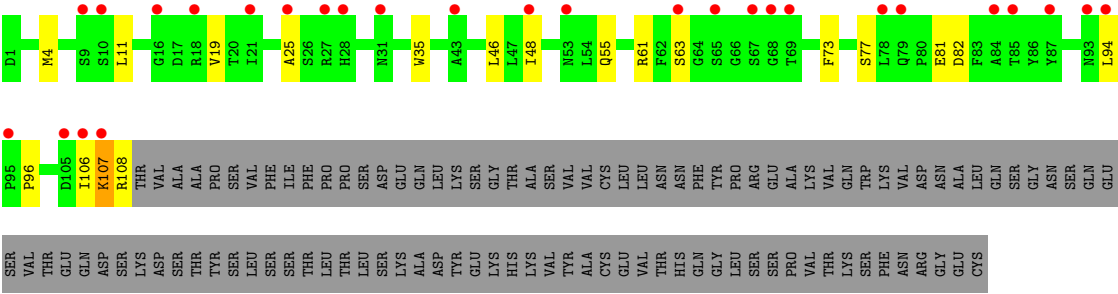


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 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
5	C	2	Total	C	N	O	0	0	0
			28	16	2	10			



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

Chain B: 100%



● Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	64.47Å 70.35Å 177.47Å 90.00° 90.18° 90.00°	Depositor
Resolution (Å)	41.94 – 2.78 41.94 – 2.79	Depositor EDS
% Data completeness (in resolution range)	84.3 (41.94-2.78) 84.3 (41.94-2.79)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	44.44 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.304 , 0.312 0.309 , 0.323	Depositor DCC
R_{free} test set	990 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 23.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	4262	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, BMA

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	0.18	0/2526	0.43	1/3408 (0.0%)
2	H	0.16	0/944	0.46	1/1279 (0.1%)
3	L	0.20	0/833	0.39	0/1136
All	All	0.18	0/4303	0.43	2/5823 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	ARG	CB-CA-C	-6.45	104.63	110.44
2	H	103	PHE	CA-CB-CG	6.22	120.02	113.80

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	2462	0	2331	33	0
2	H	921	0	858	27	0
3	L	812	0	755	18	0
4	B	39	0	34	0	0
5	C	28	0	25	1	0
All	All	4262	0	4003	67	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 8.

The worst 5 of 67 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:H:103:PHE:CE1	3:L:94:LEU:HD11	2.02	0.93
2:H:103:PHE:CZ	3:L:94:LEU:HD11	2.05	0.92
1:A:22:SER:OG	1:A:79:SER:HB2	1.93	0.69
2:H:103:PHE:HE1	3:L:94:LEU:HD11	1.56	0.66
1:A:74:GLN:HG3	1:A:75:ARG:HG3	1.78	0.66

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	319/344 (93%)	301 (94%)	15 (5%)	3 (1%)	14	38
2	H	119/223 (53%)	114 (96%)	5 (4%)	0	100	100
3	L	106/214 (50%)	102 (96%)	4 (4%)	0	100	100
All	All	544/781 (70%)	517 (95%)	24 (4%)	3 (1%)	22	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	A	46	SER
1	A	301	GLU

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	272/294 (92%)	252 (93%)	20 (7%)	11	30
2	H	97/188 (52%)	91 (94%)	6 (6%)	15	39
3	L	87/187 (46%)	80 (92%)	7 (8%)	10	27
All	All	456/669 (68%)	423 (93%)	33 (7%)	12	31

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	77	SER
3	L	81	GLU
3	L	108	ARG
1	A	245	LYS
1	A	239	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
2	H	39	GLN
3	L	38	HIS
3	L	55	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

5 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	B	1	1,4	14,14,15	0.42	0	17,19,21	0.47	0
4	NAG	B	2	4	14,14,15	0.23	0	17,19,21	0.36	0
4	BMA	B	3	4	11,11,12	0.53	0	15,15,17	0.68	0
5	NAG	C	1	1,5	14,14,15	0.36	0	17,19,21	0.97	2 (11%)
5	NAG	C	2	5	14,14,15	0.40	0	17,19,21	0.69	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
4	NAG	B	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	B	2	4	-	0/6/23/26	0/1/1/1
4	BMA	B	3	4	-	0/2/19/22	0/1/1/1
5	NAG	C	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1	NAG	C1-O5-C5	2.68	115.83	112.19
5	C	2	NAG	C1-O5-C5	2.09	115.02	112.19
5	C	1	NAG	C2-N2-C7	2.08	125.86	122.90

There are no chirality outliers.

All (1) torsion outliers are listed below:

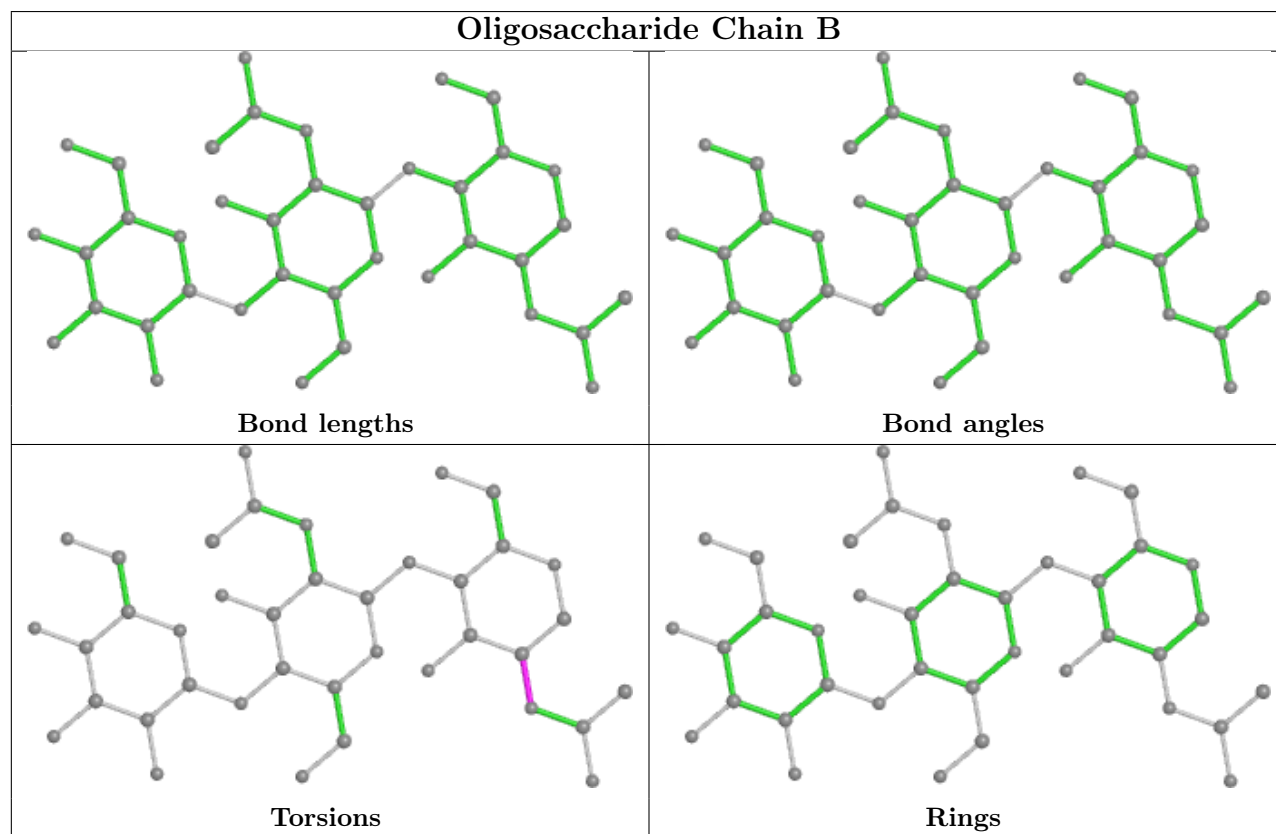
Mol	Chain	Res	Type	Atoms
4	B	1	NAG	C1-C2-N2-C7

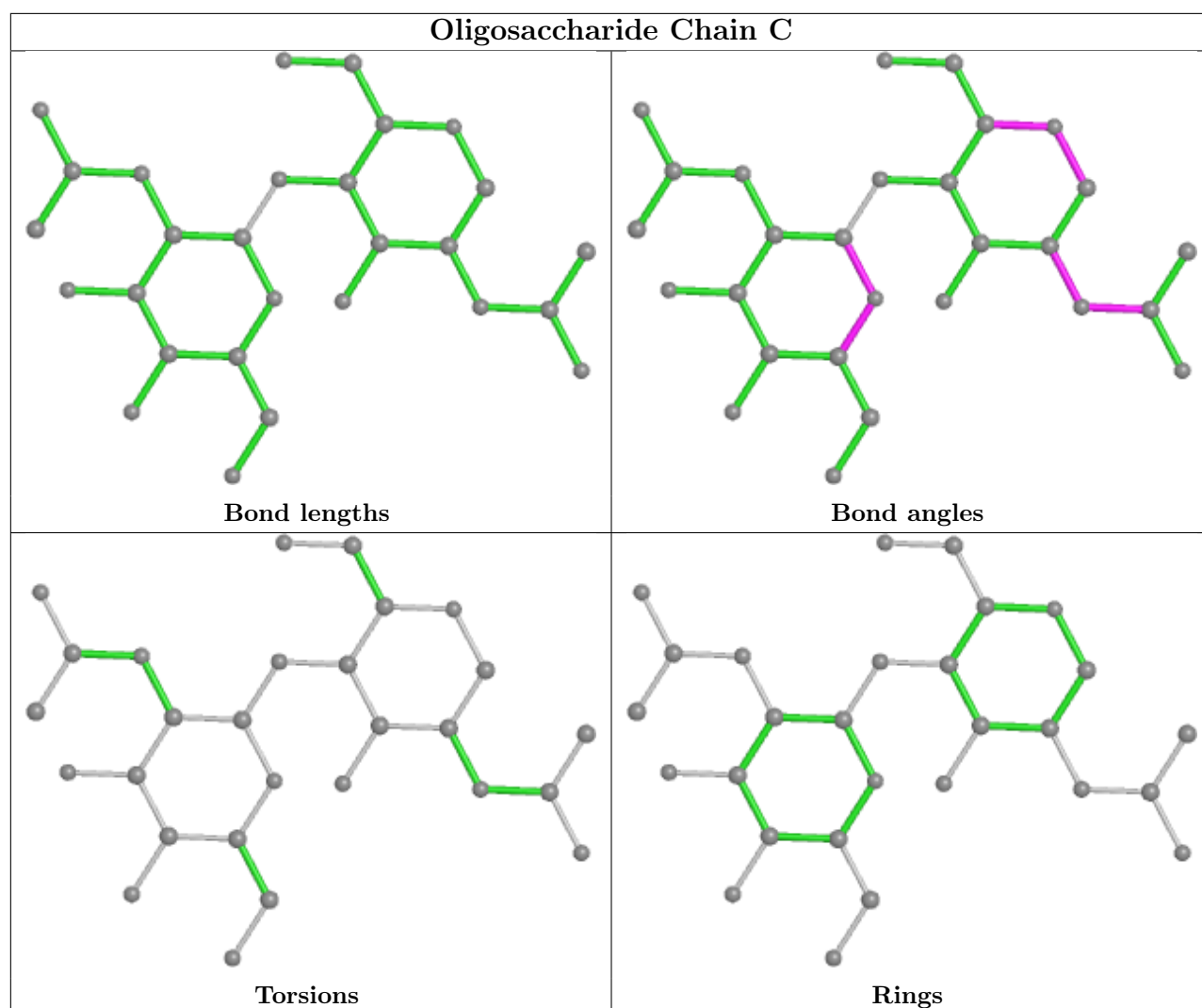
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1	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](#)

There are no ligands in this entry.

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, 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(Å ²)	Q<0.9
1	A	321/344 (93%)	1.21	60 (18%) 4 4	22, 38, 76, 144	0
2	H	121/223 (54%)	1.14	26 (21%) 3 3	31, 44, 59, 71	0
3	L	108/214 (50%)	1.48	28 (25%) 2 2	30, 49, 60, 72	0
All	All	550/781 (70%)	1.25	114 (20%) 3 3	22, 41, 66, 144	0

The worst 5 of 114 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	299	THR	10.3
1	A	300	SER	8.3
3	L	94	LEU	6.6
1	A	302	ALA	6.3
1	A	338	LEU	5.6

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](#)

SUGAR-RSR INFOmissingINFO

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.