WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 16, 2023 – 02:10 PM EDT

PDB ID	:	2AOS
Title	:	Protein-protein Interactions of protective signalling factor: Crystal structure of ternary complex involving signalling protein from goat (SPG-40), tetrasaccharide and a tripeptide Trp-pro-Trp at 2.9 A resolution
Authors	:	Kumar, J.; Ethayathulla, A.S.; Srivastava, D.B.; Somvanshi, R.K.; Singh, N.; Sharma, S.; Dey, S.; Bhushan, A.; Kaur, P.; Singh, T.P.
Deposited on	:	2005-08-14
Resolution	:	2.90 Å(reported)

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

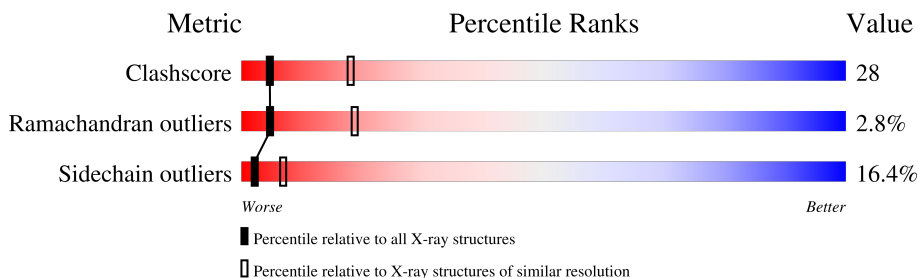|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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
Clashscore		28
Ramachandran outliers		2.8%
Sidechain outliers		16.4%

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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	361	58% 34% 8% •
2	D	3	67% 33%
3	B	4	100%
4	C	3	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	NAG	B	1	-	-	X	-
3	NAG	B	2	-	-	X	-

2   Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 3107 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 Signaling protein from goat, SPG-40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total 2877	C 1836	N 508	O 524	S 9	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	VAL	ILE	SEE REMARK 999	GB 19526603
A	131	ALA	GLY	SEE REMARK 999	GB 19526603
A	205	ASN	GLN	SEE REMARK 999	GB 19526603
A	206	SER	GLU	SEE REMARK 999	GB 19526603
A	?	-	ASP	SEE REMARK 999	GB 19526603
A	361	ARG	GLU	SEE REMARK 999	GB 19526603

- Molecule 2 is a protein called Trp-Pro-Trp tripeptide.

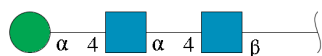| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total 36	C 27	N 5	O 4	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(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
3	B	4	Total 56	C 32	N 4	O 20	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-

alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	97	97	97	0	0
5	D	2	Total	O	0	0
			2	2		

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.

Note EDS was not executed.

• Molecule 1: Signaling protein from goat, SPG-40

Chain A:
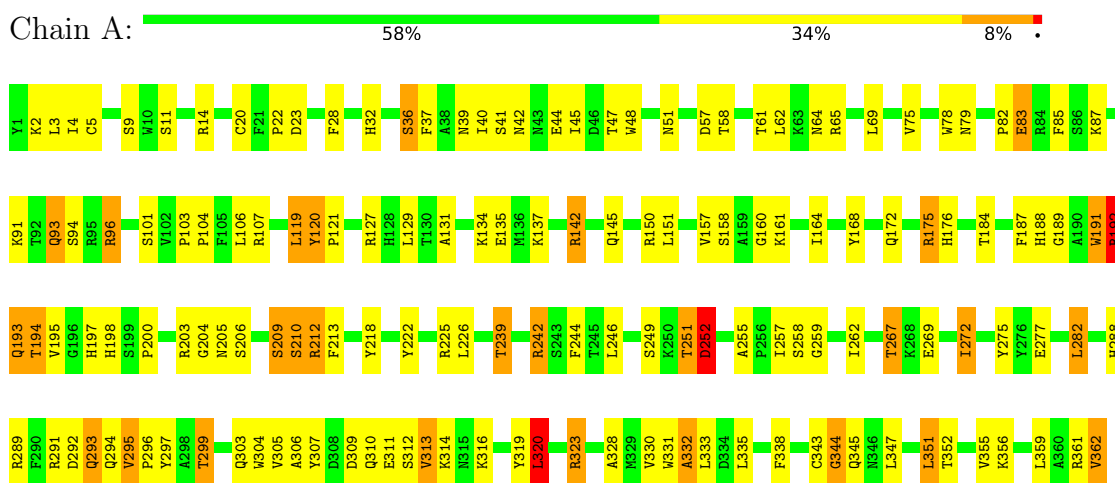
• Molecule 2: Trp-Pro-Trp tripeptide

Chain D:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gl ucopyranose

Chain B:
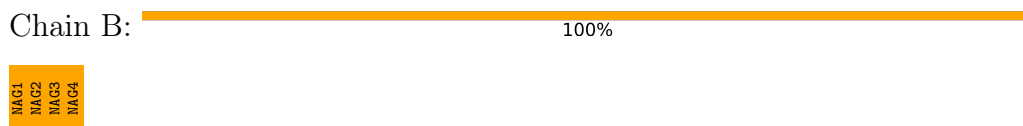
• Molecule 4: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

wwPDB X-ray Structure Validation Summary Report
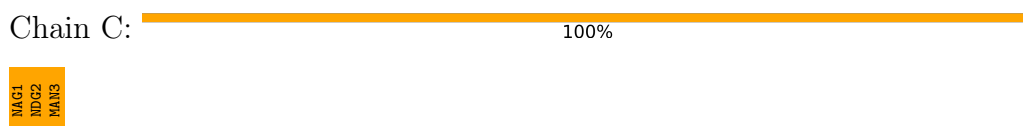
4 Data and refinement statistics ⓘ

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.87Å 66.51Å 107.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.00 – 2.90	Depositor
% Data completeness (in resolution range)	98.1 (56.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.192 , 0.239	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3107	wwPDB-VP
Average B, all atoms (Å²)	42.0	wwPDB-VP

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, NDG

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	0.71	0/2953	0.84	3/4001 (0.1%)
2	D	1.00	0/40	1.53	1/55 (1.8%)
All	All	0.71	0/2993	0.85	4/4056 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	119	LEU	CA-CB-CG	-6.62	100.07	115.30
1	A	320	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	36	SER	C-N-CA	5.22	134.76	121.70
2	D	2	PRO	N-CA-C	5.07	125.29	112.10

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	A	2877	0	2818	142	0
2	D	36	0	29	18	0
3	B	56	0	49	20	0
4	C	39	0	33	6	0
5	A	97	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	2	0	0	0	0
All	All	3107	0	2929	167	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 28.

The worst 5 of 167 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:D:1:TRP:H3	2:D:2:PRO:HD3	1.23	1.04
1:A:82:PRO:HG3	2:D:1:TRP:HB2	1.40	1.03
1:A:204:GLY:HA2	1:A:292:ASP:HB3	1.41	1.01
1:A:78:TRP:CD1	2:D:1:TRP:HZ2	1.79	1.01
1:A:82:PRO:HD3	2:D:1:TRP:HD1	1.27	0.98

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	359/361 (99%)	320 (89%)	29 (8%)	10 (3%)	5	19
2	D	1/3 (33%)	1 (100%)	0	0	100	100
All	All	360/364 (99%)	321 (89%)	29 (8%)	10 (3%)	5	19

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	TRP
1	A	192	ARG
1	A	205	ASN

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Mol	Chain	Res	Type
1	A	332	ALA
1	A	344	GLY

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	A	302/302 (100%)	255 (84%)	47 (16%)	2	8
2	D	3/3 (100%)	0	3 (100%)	0	0
All	All	305/305 (100%)	255 (84%)	50 (16%)	2	7

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251	THR
1	A	293	GLN
2	D	3	TRP
1	A	252	ASP
1	A	272	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	HIS
1	A	288	HIS
1	A	303	GLN
1	A	293	GLN
1	A	79	ASN

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
3	NAG	B	1	3	14,14,15	0.75	0	17,19,21	2.35	7 (41%)
3	NAG	B	2	3	14,14,15	1.39	3 (21%)	17,19,21	2.10	7 (41%)
3	NAG	B	3	3	14,14,15	1.33	1 (7%)	17,19,21	2.40	5 (29%)
3	NAG	B	4	3	14,14,15	0.91	1 (7%)	17,19,21	1.86	5 (29%)
4	NAG	C	1	4	14,14,15	0.95	1 (7%)	17,19,21	3.80	5 (29%)
4	NDG	C	2	4	14,14,15	0.74	0	17,19,21	3.75	12 (70%)
4	MAN	C	3	4	11,11,12	1.11	0	15,15,17	2.66	5 (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
3	NAG	B	1	3	-	3/6/23/26	0/1/1/1
3	NAG	B	2	3	-	6/6/23/26	0/1/1/1
3	NAG	B	3	3	-	3/6/23/26	0/1/1/1
3	NAG	B	4	3	-	2/6/23/26	0/1/1/1
4	NAG	C	1	4	-	0/6/23/26	0/1/1/1
4	NDG	C	2	4	-	2/6/23/26	0/1/1/1
4	MAN	C	3	4	-	2/2/19/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3	NAG	C1-C2	3.74	1.57	1.52
3	B	2	NAG	C1-C2	2.66	1.56	1.52
3	B	2	NAG	O5-C5	-2.48	1.38	1.43
4	C	1	NAG	O5-C1	-2.47	1.39	1.43
3	B	2	NAG	C4-C3	2.24	1.58	1.52

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1	NAG	C2-N2-C7	-14.06	102.89	122.90
4	C	2	NDG	C2-N2-C7	-9.42	109.50	122.90
3	B	3	NAG	O5-C1-C2	7.09	122.48	111.29
4	C	2	NDG	C1-O5-C5	6.53	121.04	112.19
4	C	3	MAN	O5-C1-C2	6.42	120.68	110.77

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	4	NAG	O7-C7-N2-C2
3	B	4	NAG	C8-C7-N2-C2
3	B	2	NAG	O5-C5-C6-O6
4	C	3	MAN	C4-C5-C6-O6
3	B	2	NAG	C4-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3	MAN	2	0
3	B	1	NAG	14	0
3	B	2	NAG	14	0
4	C	1	NAG	4	0
3	B	3	NAG	3	0
3	B	4	NAG	2	0
4	C	2	NDG	2	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 B

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings
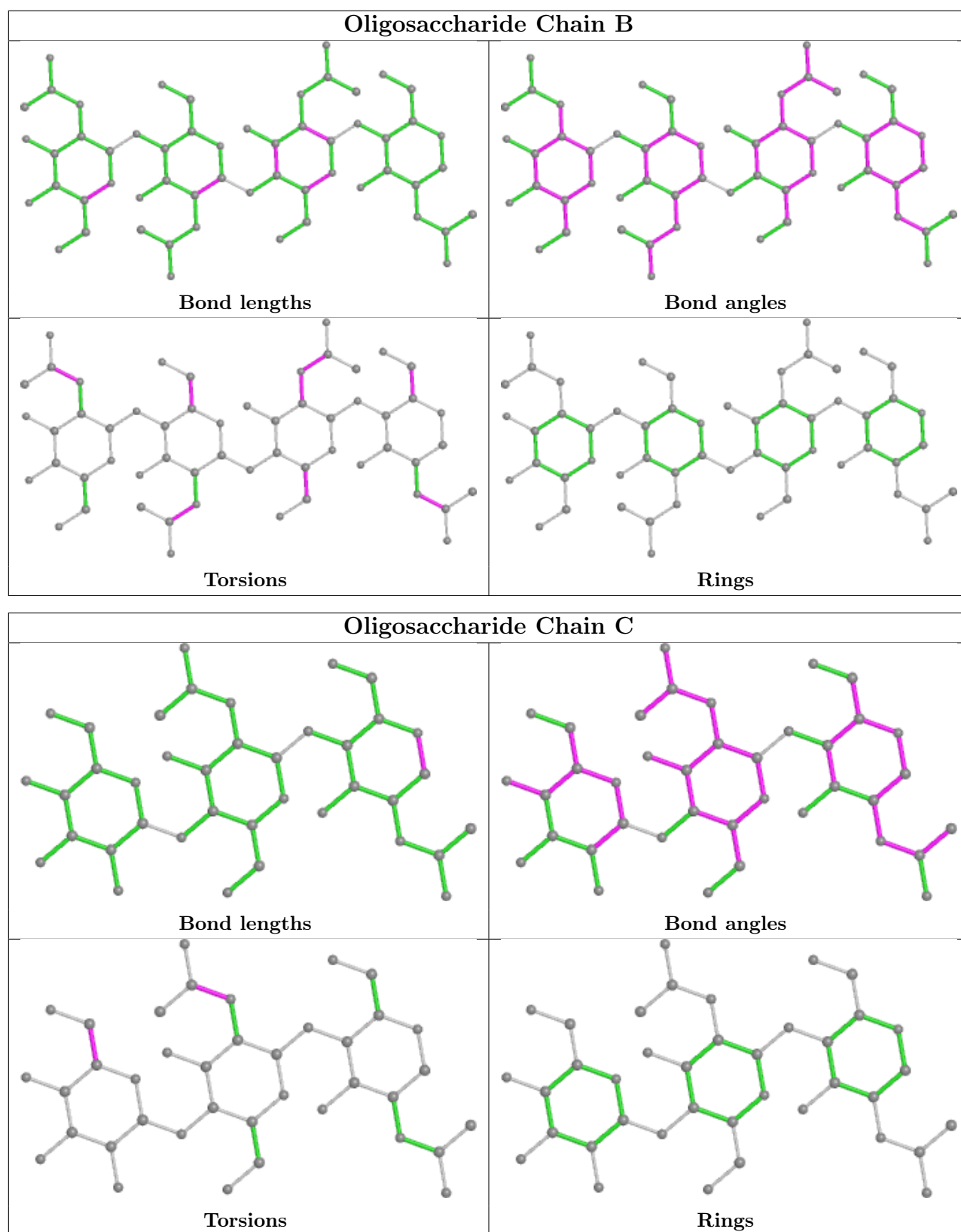
5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.