



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 04:38 PM BST

PDB ID : 1XRV
Title : Crystal Structure of the novel secretory signalling protein from Porcine (SPP-40) at 2.1Å resolution.
Authors : Srivastava, D.B.; Ethayathulla, A.S.; Singh, N.; Sharma, S.; Singh, T.P.
Deposited on : 2004-10-16
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 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) : 2.13.1

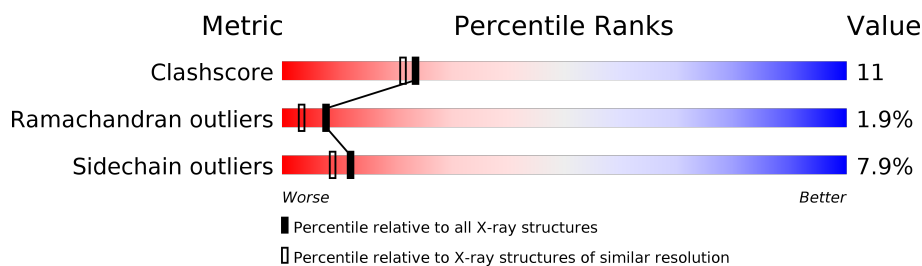
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 on 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	361	
2	B	2	

2 Entry composition [i](#)

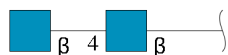
There are 3 unique types of molecules in this entry. The entry contains 3147 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 signal processing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	0	0
			2875	1835	502	529	9			

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

- Molecule 3 is water.

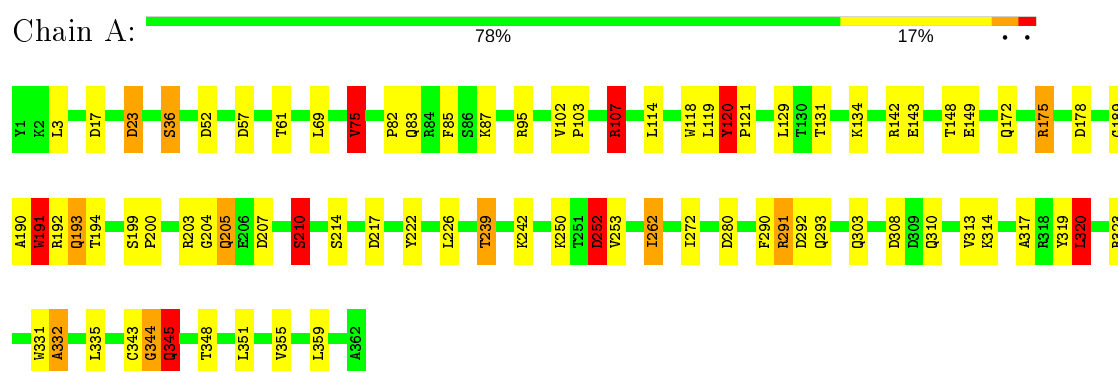
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	244	Total	O	0	0
			244	244		

3 Residue-property plots

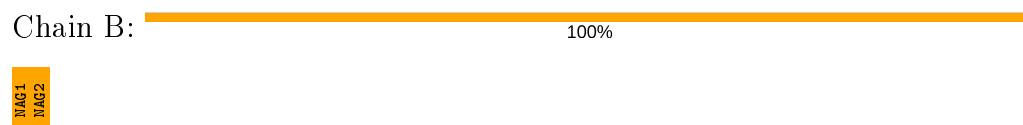
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: signal processing protein



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



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	62.59 Å 66.55 Å 107.47 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.80 – 2.10	Depositor
% Data completeness (in resolution range)	96.8 (56.80-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.188 , 0.228	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3147	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

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

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	0.78	1/2950 (0.0%)	1.03	25/3999 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	SER	C-N	7.08	1.50	1.34

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	ASP	CB-CG-OD2	9.22	126.60	118.30
1	A	210	SER	CA-C-N	-8.11	99.35	117.20
1	A	210	SER	O-C-N	7.90	135.34	122.70
1	A	320	LEU	CA-CB-CG	7.46	132.45	115.30
1	A	23	ASP	CB-CG-OD2	7.45	125.00	118.30
1	A	36	SER	C-N-CA	7.42	140.24	121.70
1	A	331	TRP	C-N-CA	7.01	139.23	121.70
1	A	36	SER	CA-C-N	-6.85	102.14	117.20
1	A	75	VAL	CB-CA-C	-6.75	98.57	111.40
1	A	331	TRP	CA-C-N	-6.75	102.35	117.20
1	A	331	TRP	O-C-N	6.67	133.37	122.70
1	A	217	ASP	CB-CG-OD2	6.44	124.10	118.30
1	A	36	SER	O-C-N	6.39	132.93	122.70
1	A	120	TYR	CB-CG-CD2	6.28	124.77	121.00
1	A	280	ASP	CB-CG-OD2	5.85	123.57	118.30
1	A	191	TRP	CA-CB-CG	5.71	124.56	113.70
1	A	308	ASP	CB-CG-OD2	5.62	123.35	118.30
1	A	120	TYR	CB-CG-CD1	-5.59	117.65	121.00
1	A	52	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	107	ARG	NE-CZ-NH2	-5.56	117.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	107	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	23	ASP	CB-CA-C	5.20	120.79	110.40
1	A	17	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	252	ASP	CB-CG-OD2	5.03	122.83	118.30

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	A	2875	0	2808	63	0
2	B	28	0	25	1	0
3	A	244	0	0	8	0
All	All	3147	0	2833	64	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 11.

All (64) 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:A:250:LYS:HE2	1:A:252:ASP:OD2	1.78	0.84
1:A:191:TRP:CE3	1:A:192:ARG:HG2	2.15	0.81
1:A:348:THR:HG22	3:A:498:HOH:O	1.87	0.74
1:A:57:ASP:O	1:A:61:THR:HG23	1.87	0.74
1:A:222:TYR:O	1:A:226:LEU:HD23	1.86	0.74
1:A:191:TRP:CE3	1:A:192:ARG:CG	2.73	0.71
1:A:148:THR:HG23	3:A:590:HOH:O	1.94	0.67
1:A:222:TYR:O	1:A:226:LEU:CD2	2.43	0.67
1:A:95:ARG:CZ	1:A:131:THR:HG21	2.27	0.64
1:A:343:CYS:O	1:A:344:GLY:C	2.36	0.64
1:A:313:VAL:HG13	1:A:355:VAL:CG2	2.28	0.63
1:A:107:ARG:HD3	1:A:143:GLU:OE2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ALA:HA	1:A:320:LEU:HD13	1.85	0.58
1:A:291:ARG:HG3	1:A:292:ASP:N	2.17	0.58
1:A:190:ALA:HB1	3:A:464:HOH:O	2.04	0.57
1:A:323:ARG:NH1	3:A:431:HOH:O	2.37	0.57
1:A:239:THR:CG2	1:A:335:LEU:HB2	2.35	0.57
1:A:95:ARG:NH2	1:A:131:THR:HG21	2.22	0.54
1:A:82:PRO:HD2	1:A:83:GLN:NE2	2.23	0.54
1:A:242:LYS:HZ1	1:A:272:ILE:HD11	1.73	0.53
1:A:253:VAL:HG22	1:A:290:PHE:HE1	1.72	0.53
1:A:189:GLY:O	1:A:190:ALA:C	2.47	0.53
1:A:313:VAL:HG13	1:A:355:VAL:HG22	1.90	0.52
1:A:203:ARG:HG2	1:A:204:GLY:N	2.24	0.52
1:A:191:TRP:CE3	1:A:192:ARG:HG3	2.45	0.52
1:A:332:ALA:HB3	1:A:335:LEU:HD12	1.92	0.52
1:A:239:THR:HG22	1:A:335:LEU:HB2	1.93	0.50
1:A:199:SER:N	1:A:200:PRO:HD3	2.27	0.50
1:A:310:GLN:O	1:A:314:LYS:HG3	2.11	0.50
1:A:191:TRP:CZ3	1:A:192:ARG:HG2	2.47	0.49
1:A:242:LYS:HE2	3:A:448:HOH:O	2.11	0.49
1:A:149:GLU:CD	3:A:588:HOH:O	2.52	0.48
1:A:102:VAL:HB	1:A:103:PRO:HD3	1.96	0.47
2:B:1:NAG:O4	2:B:2:NAG:O7	2.33	0.47
1:A:323:ARG:NH1	1:A:323:ARG:HG2	2.30	0.47
1:A:95:ARG:CZ	1:A:131:THR:CG2	2.93	0.47
1:A:319:TYR:CZ	1:A:323:ARG:HD2	2.50	0.46
1:A:200:PRO:HB3	1:A:293:GLN:HB3	1.97	0.46
1:A:262:ILE:HD13	1:A:303:GLN:NE2	2.31	0.46
1:A:262:ILE:H	1:A:303:GLN:HE22	1.63	0.45
1:A:313:VAL:CG1	1:A:355:VAL:HG23	2.47	0.45
1:A:291:ARG:HG3	1:A:292:ASP:H	1.82	0.45
1:A:149:GLU:HB2	3:A:588:HOH:O	2.16	0.45
1:A:118:TRP:CD1	1:A:121:PRO:HD3	2.52	0.44
1:A:210:SER:HB3	1:A:214:SER:OG	2.18	0.43
1:A:313:VAL:HG13	1:A:355:VAL:HG23	1.98	0.43
1:A:172:GLN:O	1:A:175:ARG:HG2	2.19	0.43
1:A:192:ARG:O	1:A:194:THR:N	2.47	0.43
1:A:192:ARG:C	1:A:194:THR:H	2.21	0.43
1:A:190:ALA:O	1:A:192:ARG:N	2.52	0.43
1:A:203:ARG:HG2	1:A:204:GLY:H	1.81	0.42
1:A:323:ARG:HH11	1:A:323:ARG:HG2	1.85	0.42
1:A:345:GLN:HB3	1:A:345:GLN:HE21	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:LYS:NZ	1:A:272:ILE:HD11	2.34	0.42
1:A:75:VAL:HG22	1:A:114:LEU:HD11	2.01	0.42
1:A:193:GLN:HE21	1:A:193:GLN:HA	1.85	0.42
1:A:239:THR:HG21	1:A:332:ALA:O	2.20	0.42
1:A:242:LYS:HZ1	1:A:272:ILE:CD1	2.31	0.41
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.65	0.41
1:A:193:GLN:NE2	1:A:193:GLN:HA	2.35	0.41
1:A:344:GLY:O	1:A:345:GLN:O	2.38	0.41
1:A:83:GLN:CD	1:A:83:GLN:H	2.23	0.41
1:A:192:ARG:NH2	3:A:593:HOH:O	2.53	0.41
1:A:242:LYS:NZ	1:A:272:ILE:CD1	2.85	0.40



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	A	359/361 (99%)	334 (93%)	18 (5%)	7 (2%)	 

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	TRP
1	A	345	GLN
1	A	193	GLN
1	A	344	GLY
1	A	120	TYR
1	A	205	GLN
1	A	332	ALA

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	303/303 (100%)	279 (92%)	24 (8%)	12 9

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	23	ASP
1	A	36	SER
1	A	69	LEU
1	A	75	VAL
1	A	85	PHE
1	A	87	LYS
1	A	107	ARG
1	A	120	TYR
1	A	129	LEU
1	A	134	LYS
1	A	142	ARG
1	A	175	ARG
1	A	191	TRP
1	A	205	GLN
1	A	210	SER
1	A	239	THR
1	A	252	ASP
1	A	262	ILE
1	A	291	ARG
1	A	320	LEU
1	A	345	GLN
1	A	351	LEU
1	A	359	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN

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Mol	Chain	Res	Type
1	A	60	ASN
1	A	93	GLN
1	A	193	GLN
1	A	205	GLN
1	A	265	GLN
1	A	294	GLN
1	A	303	GLN
1	A	315	ASN
1	A	345	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	$\# Z > 2$
2	NAG	B	1	1,2	14,14,15	0.68	1 (7%)	17,19,21	1.71	4 (23%)
2	NAG	B	2	2	14,14,15	1.21	2 (14%)	17,19,21	4.13	4 (23%)

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	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	O5-C1	-2.62	1.39	1.43
2	B	2	NAG	O5-C5	-2.37	1.38	1.43
2	B	1	NAG	O5-C1	-2.05	1.40	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	O5-C1-C2	-13.07	90.64	111.29
2	B	2	NAG	O5-C5-C4	-7.04	93.70	110.83
2	B	2	NAG	C1-O5-C5	6.86	121.49	112.19
2	B	1	NAG	O5-C1-C2	-3.92	105.09	111.29
2	B	2	NAG	C3-C4-C5	-3.51	103.98	110.24
2	B	1	NAG	C2-N2-C7	3.39	127.73	122.90
2	B	1	NAG	C8-C7-N2	2.31	120.01	116.10
2	B	1	NAG	O5-C5-C6	2.13	110.55	107.20

There are no chirality outliers.

All (4) torsion outliers are listed below:

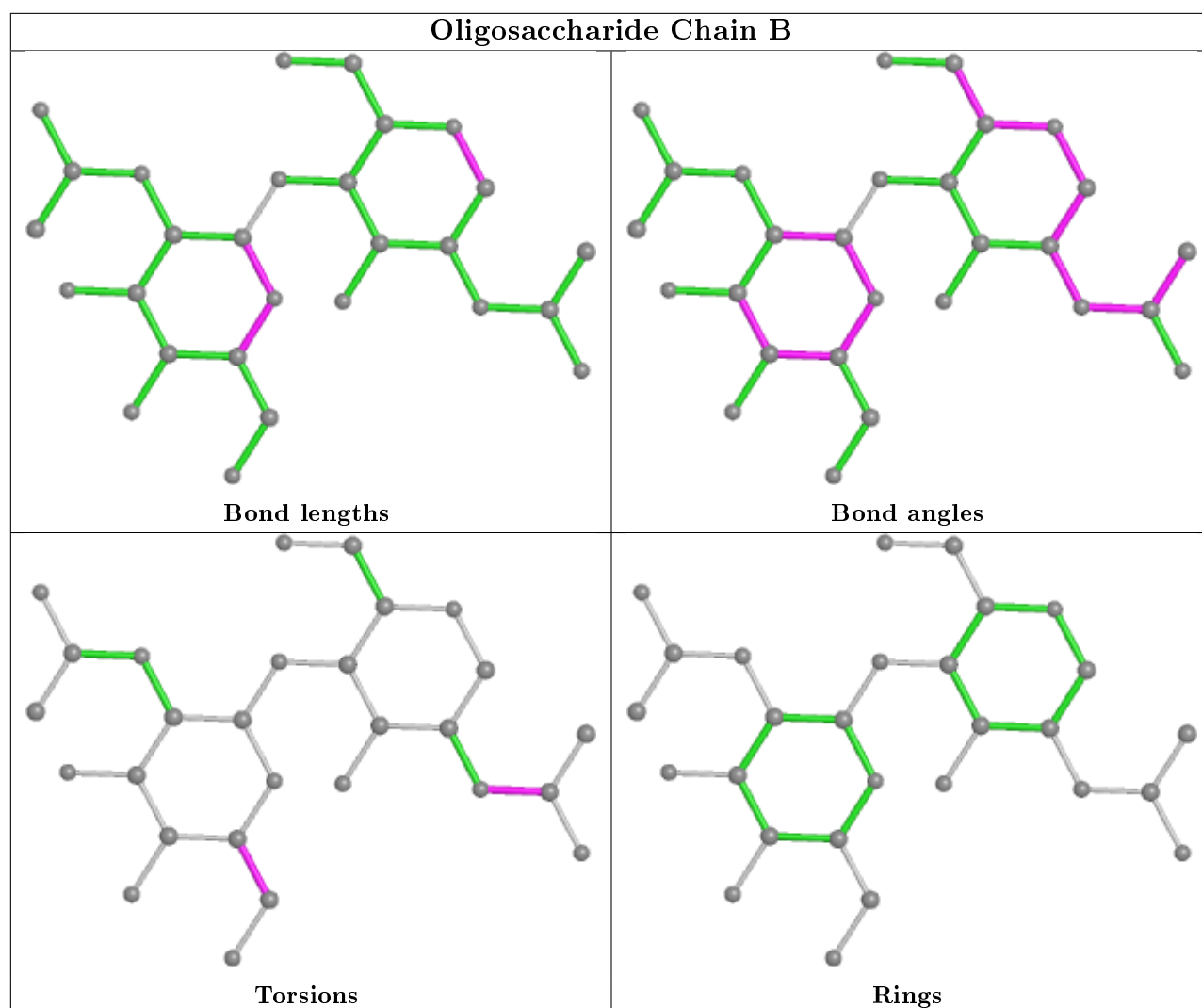
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	2	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	1	0
2	B	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

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.