



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 12:24 PM BST

PDB ID : 1ZB5
Title : Recognition of peptide ligands by signalling protein from porcine mammary gland (SPP-40): Crystal structure of the complex of SPP-40 with a peptide Trp-Pro-Trp at 2.45Å resolution
Authors : Srivastava, D.B.; Ethayathulla, A.S.; Kumar, J.; Singh, N.; Somvanshi, R.K.; Sharma, S.; Dey, S.; Kaur, P.; Singh, T.P.
Deposited on : 2005-04-07
Resolution : 2.45 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

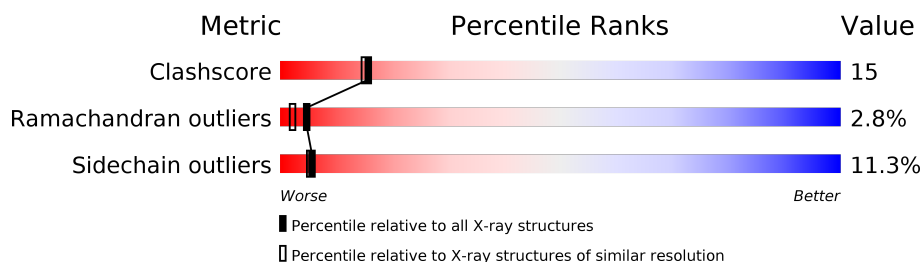
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)

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	3	
2	C	3	
3	D	2	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3113 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.

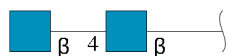
- Molecule 1 is a protein called signal processing protein.

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 a protein called PEPTIDE TRP-PRO-TRP.

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

- Molecule 3 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
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is water.

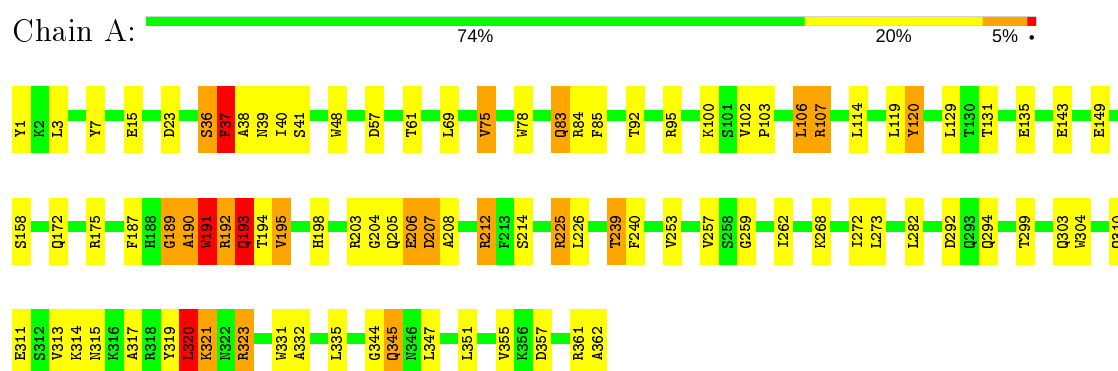
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	138	Total	O	0	0
			138	138		

3 Residue-property plots

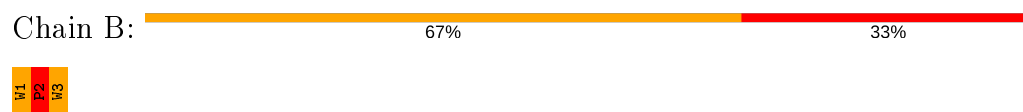
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



- Molecule 2: PEPTIDE TRP-PRO-TRP



- Molecule 3: 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	62.38 Å 66.79 Å 107.66 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.45	Depositor
% Data completeness (in resolution range)	95.2 (20.00-2.45)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.192 , 0.226	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3113	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: 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	0.41	0/2950	0.74	4/3999 (0.1%)
2	B	0.86	0/40	1.16	1/55 (1.8%)
2	C	0.51	0/40	0.54	0/55
All	All	0.42	0/3030	0.75	5/4109 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	LEU	CA-CB-CG	8.92	135.82	115.30
1	A	38	ALA	N-CA-C	-5.83	95.25	111.00
1	A	37	PHE	N-CA-C	5.28	125.26	111.00
1	A	191	TRP	CA-CB-CG	5.25	123.67	113.70
2	B	2	PRO	CA-N-CD	-5.24	104.17	111.50

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	78	0
2	B	36	0	29	6	0
2	C	36	0	29	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	28	0	25	2	0
4	A	138	0	0	7	0
All	All	3113	0	2891	86	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 15.

All (86) 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:357:ASP:O	1:A:361:ARG:HD3	1.77	0.84
1:A:204:GLY:HA2	1:A:292:ASP:HB3	1.60	0.82
1:A:192:ARG:HA	1:A:192:ARG:HE	1.45	0.79
1:A:317:ALA:HA	1:A:320:LEU:HD13	1.67	0.77
1:A:95:ARG:CZ	1:A:131:THR:HG21	2.17	0.74
1:A:191:TRP:O	1:A:191:TRP:HE3	1.73	0.71
1:A:190:ALA:O	1:A:191:TRP:HB3	1.89	0.70
1:A:57:ASP:O	1:A:61:THR:HG23	1.92	0.68
1:A:332:ALA:HB3	1:A:335:LEU:HD12	1.74	0.68
1:A:192:ARG:HA	1:A:192:ARG:NE	2.04	0.68
1:A:192:ARG:O	1:A:194:THR:N	2.26	0.68
1:A:75:VAL:CG2	1:A:114:LEU:HD11	2.26	0.66
1:A:92:THR:HG22	1:A:95:ARG:HH22	1.60	0.66
1:A:239:THR:HG22	1:A:335:LEU:HB2	1.78	0.65
2:B:3:TRP:HE3	2:B:3:TRP:H	1.46	0.63
1:A:319:TYR:CZ	1:A:323:ARG:HD2	2.35	0.62
1:A:92:THR:HG22	1:A:95:ARG:NH2	2.14	0.62
1:A:239:THR:HG21	1:A:332:ALA:O	1.99	0.62
1:A:207:ASP:OD1	1:A:208:ALA:N	2.35	0.60
1:A:253:VAL:HG13	4:A:491:HOH:O	2.01	0.60
1:A:83:GLN:HG2	1:A:84:ARG:N	2.16	0.59
1:A:294:GLN:NE2	1:A:315:ASN:OD1	2.36	0.59
1:A:95:ARG:CZ	1:A:131:THR:CG2	2.82	0.57
1:A:332:ALA:HB1	1:A:335:LEU:HG	1.87	0.56
1:A:317:ALA:HA	1:A:320:LEU:CD1	2.34	0.56
1:A:7:TYR:O	1:A:36:SER:HB2	2.06	0.56
1:A:75:VAL:HG22	1:A:114:LEU:HD11	1.88	0.55
1:A:120:TYR:N	1:A:120:TYR:CD2	2.67	0.55
1:A:239:THR:HG23	1:A:239:THR:O	2.07	0.54
1:A:313:VAL:HG13	1:A:355:VAL:HG22	1.88	0.54
1:A:321:LYS:HE2	1:A:362:ALA:OXT	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:THR:CG2	1:A:335:LEU:HB2	2.37	0.54
1:A:332:ALA:CB	1:A:335:LEU:HD12	2.38	0.53
1:A:313:VAL:HG13	1:A:355:VAL:CG2	2.39	0.53
1:A:208:ALA:O	1:A:212:ARG:HG2	2.09	0.53
1:A:131:THR:HG23	1:A:135:GLU:OE2	2.10	0.52
1:A:193:GLN:HG3	4:A:502:HOH:O	2.09	0.52
1:A:344:GLY:O	1:A:345:GLN:C	2.48	0.52
1:A:204:GLY:HA2	1:A:292:ASP:CB	2.35	0.51
1:A:262:ILE:H	1:A:303:GLN:HE22	1.57	0.50
1:A:323:ARG:NH1	1:A:323:ARG:HG2	2.26	0.50
1:A:361:ARG:O	1:A:362:ALA:HB2	2.10	0.50
1:A:172:GLN:O	1:A:175:ARG:HG2	2.13	0.49
1:A:48:TRP:CE2	3:D:1:NAG:H82	2.48	0.48
1:A:78:TRP:HH2	4:A:413:HOH:O	1.97	0.48
1:A:323:ARG:HH11	1:A:323:ARG:HG2	1.79	0.48
1:A:323:ARG:NH2	4:A:496:HOH:O	2.47	0.48
2:C:1:TRP:CE3	2:C:1:TRP:N	2.81	0.48
1:A:310:GLN:O	1:A:314:LYS:HG3	2.13	0.47
1:A:272:ILE:HG22	1:A:273:LEU:N	2.29	0.47
1:A:198:HIS:CD2	1:A:198:HIS:H	2.30	0.47
1:A:240:PHE:HB3	1:A:335:LEU:HD13	1.97	0.47
1:A:204:GLY:O	1:A:206:GLU:N	2.48	0.47
1:A:37:PHE:HB2	4:A:370:HOH:O	2.14	0.47
1:A:189:GLY:O	1:A:190:ALA:C	2.54	0.46
1:A:189:GLY:O	1:A:190:ALA:O	2.32	0.46
2:B:3:TRP:OXT	2:B:3:TRP:CG	2.68	0.46
2:B:1:TRP:CB	2:B:2:PRO:CD	2.94	0.46
1:A:15:GLU:OE1	1:A:268:LYS:NZ	2.46	0.46
1:A:257:VAL:HG12	1:A:259:GLY:H	1.80	0.45
1:A:1:TYR:CE2	1:A:321:LYS:HD3	2.52	0.45
1:A:107:ARG:HD3	1:A:143:GLU:OE2	2.17	0.45
1:A:345:GLN:HB3	1:A:345:GLN:HE21	1.56	0.45
1:A:192:ARG:HD3	2:B:3:TRP:HB3	1.98	0.45
1:A:39:ASN:CG	1:A:40:ILE:H	2.20	0.44
2:C:1:TRP:N	2:C:1:TRP:HE3	2.15	0.44
1:A:225:ARG:NE	1:A:225:ARG:O	2.51	0.44
1:A:78:TRP:HZ3	1:A:331:TRP:CZ2	2.36	0.44
1:A:191:TRP:O	1:A:191:TRP:CE3	2.63	0.44
1:A:102:VAL:HB	1:A:103:PRO:HD3	1.99	0.43
1:A:195:VAL:HG22	1:A:304:TRP:CE3	2.53	0.43
1:A:15:GLU:HB3	4:A:377:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.71	0.43
1:A:323:ARG:CG	1:A:323:ARG:HH11	2.31	0.43
1:A:83:GLN:HE21	1:A:83:GLN:HB3	1.64	0.43
1:A:187:PHE:HB3	1:A:214:SER:HB3	2.00	0.42
2:B:1:TRP:HB2	2:B:2:PRO:HD2	2.01	0.42
2:C:1:TRP:HB2	2:C:2:PRO:CD	2.50	0.41
1:A:321:LYS:CE	1:A:362:ALA:OXT	2.68	0.41
1:A:319:TYR:OH	1:A:323:ARG:HD2	2.21	0.41
1:A:41:SER:OG	3:D:1:NAG:O5	2.38	0.41
1:A:262:ILE:H	1:A:303:GLN:NE2	2.19	0.41
1:A:102:VAL:HG12	1:A:106:LEU:HD22	2.01	0.41
2:C:1:TRP:HB2	2:C:2:PRO:HD2	2.03	0.41
1:A:192:ARG:NH1	2:B:1:TRP:O	2.53	0.40
1:A:361:ARG:HG3	4:A:460:HOH:O	2.21	0.40

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%)	329 (92%)	22 (6%)	8 (2%)	6	4
2	B	1/3 (33%)	0	0	1 (100%)	0	0
2	C	1/3 (33%)	0	0	1 (100%)	0	0
All	All	361/367 (98%)	329 (91%)	22 (6%)	10 (3%)	5	2

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	TRP
1	A	193	GLN
2	C	2	PRO

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Mol	Chain	Res	Type
1	A	190	ALA
1	A	205	GLN
1	A	206	GLU
2	B	2	PRO
1	A	120	TYR
1	A	37	PHE
1	A	189	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	303/303 (100%)	271 (89%)	32 (11%)	6	6
2	B	3/3 (100%)	1 (33%)	2 (67%)	0	0
2	C	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	309/309 (100%)	274 (89%)	35 (11%)	6	5

All (35) 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	83	GLN
1	A	85	PHE
1	A	100	LYS
1	A	106	LEU
1	A	107	ARG
1	A	129	LEU
1	A	149	GLU
1	A	158	SER
1	A	191	TRP
1	A	192	ARG

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Mol	Chain	Res	Type
1	A	193	GLN
1	A	195	VAL
1	A	203	ARG
1	A	207	ASP
1	A	212	ARG
1	A	225	ARG
1	A	226	LEU
1	A	239	THR
1	A	282	LEU
1	A	299	THR
1	A	311	GLU
1	A	320	LEU
1	A	321	LYS
1	A	323	ARG
1	A	345	GLN
1	A	347	LEU
1	A	351	LEU
2	B	1	TRP
2	B	3	TRP
2	C	1	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	83	GLN
1	A	198	HIS
1	A	294	GLN
1	A	303	GLN
1	A	310	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$
3	NAG	D	1	1,3	14,14,15	2.19	1 (7%)	17,19,21	1.88	4 (23%)
3	NAG	D	2	3	14,14,15	0.42	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
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	NAG	O4-C4	-7.77	1.24	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	NAG	O4-C4-C5	5.41	122.72	109.30
3	D	1	NAG	C3-C4-C5	3.41	116.32	110.24
3	D	1	NAG	C4-C3-C2	2.43	114.58	111.02
3	D	1	NAG	C1-O5-C5	-2.37	108.98	112.19
3	D	2	NAG	C2-N2-C7	-2.10	119.92	122.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

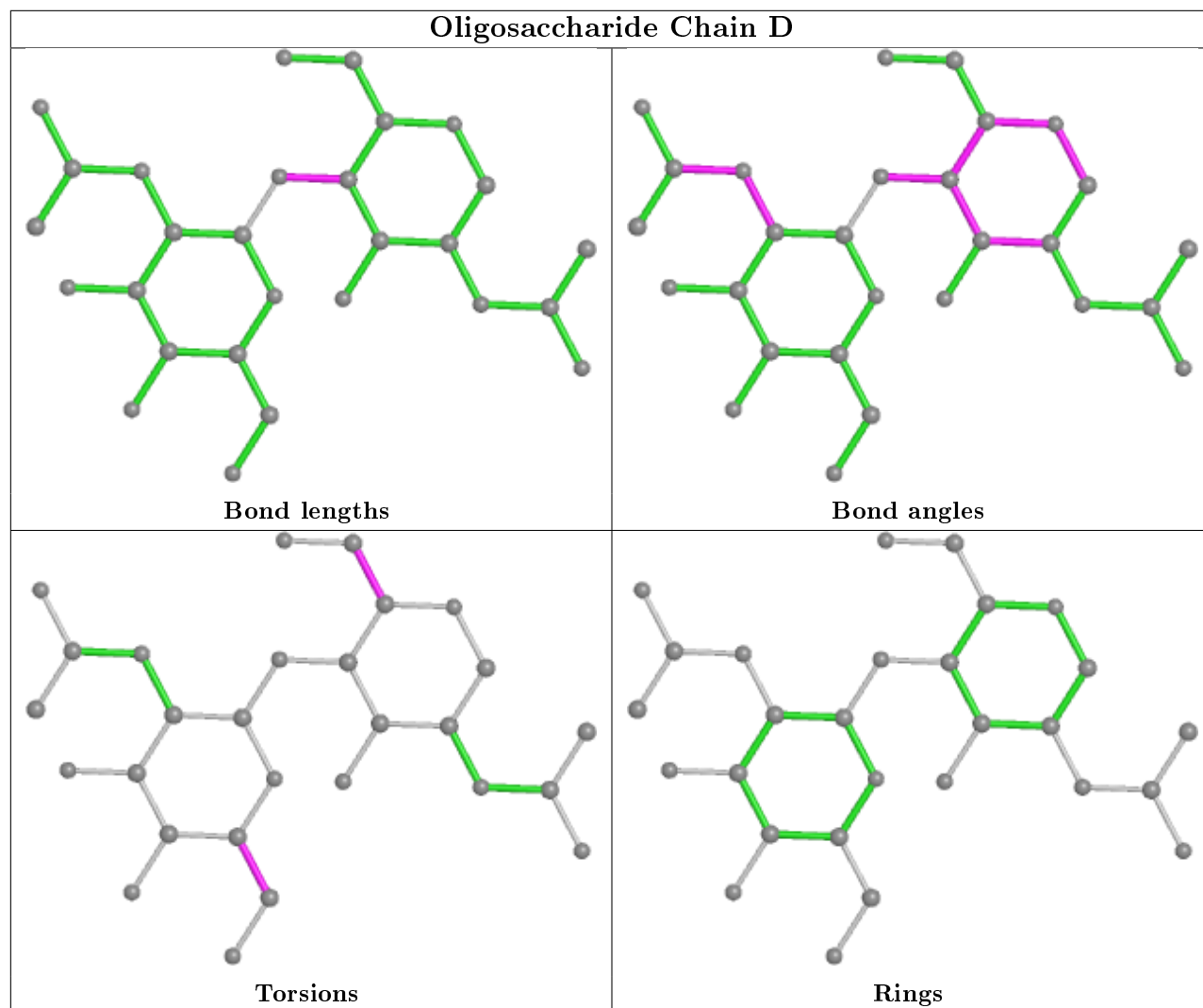
Mol	Chain	Res	Type	Atoms
3	D	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	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.



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.