



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2023 – 06:57 PM EDT

PDB ID : 1L5G
Title : CRYSTAL STRUCTURE OF THE EXTRACELLULAR SEGMENT OF INTEGRIN AVB3 IN COMPLEX WITH AN ARG-GLY-ASP LIGAND
Authors : Xiong, J.-P.; Stehle, T.; Zhang, R.; Joachimiak, A.; Frech, M.; Goodman, S.L.; Arnaout, M.A.
Deposited on : 2002-03-06
Resolution : 3.20 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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

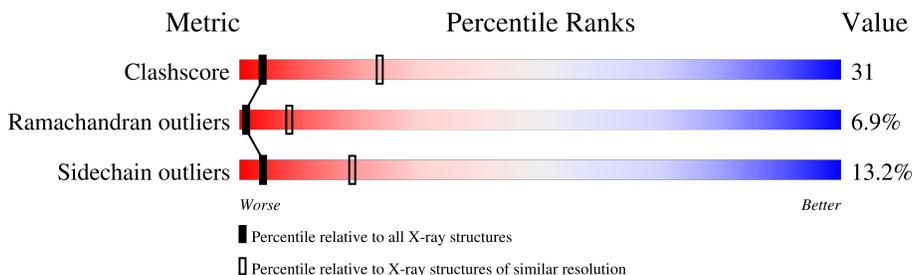
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

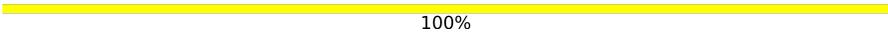
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	957	47% 41% 8% . .
2	B	692	29% 37% 10% . 22%
3	C	5	20% 40% 40%
4	D	2	50% 50%
4	E	2	100%
4	F	2	50% 50%
4	H	2	50% 50%
5	G	2	100%

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Mol	Chain	Length	Quality of chain
5	I	2	 50% 50%
5	J	2	 100%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 11700 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 INTEGRIN ALPHA V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	927	7216	4568	1224	1389	35	0	0	0

- Molecule 2 is a protein called INTEGRIN BETA-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	539	4182	2594	700	842	46	0	0	0

- Molecule 3 is a protein called CYCLIC ARG-GLY-ASP PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	5	42	27	8	7	0	0	0

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



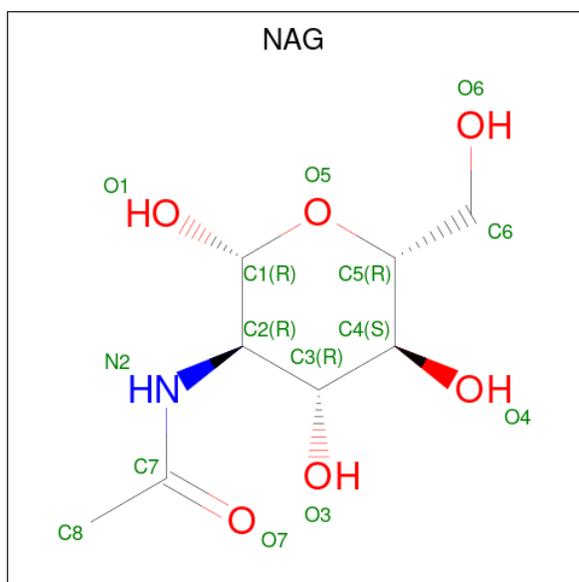
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	2	28	16	2	10	0	0	0
4	E	2	28	16	2	10	0	0	0
4	F	2	28	16	2	10	0	0	0
4	H	2	28	16	2	10	0	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

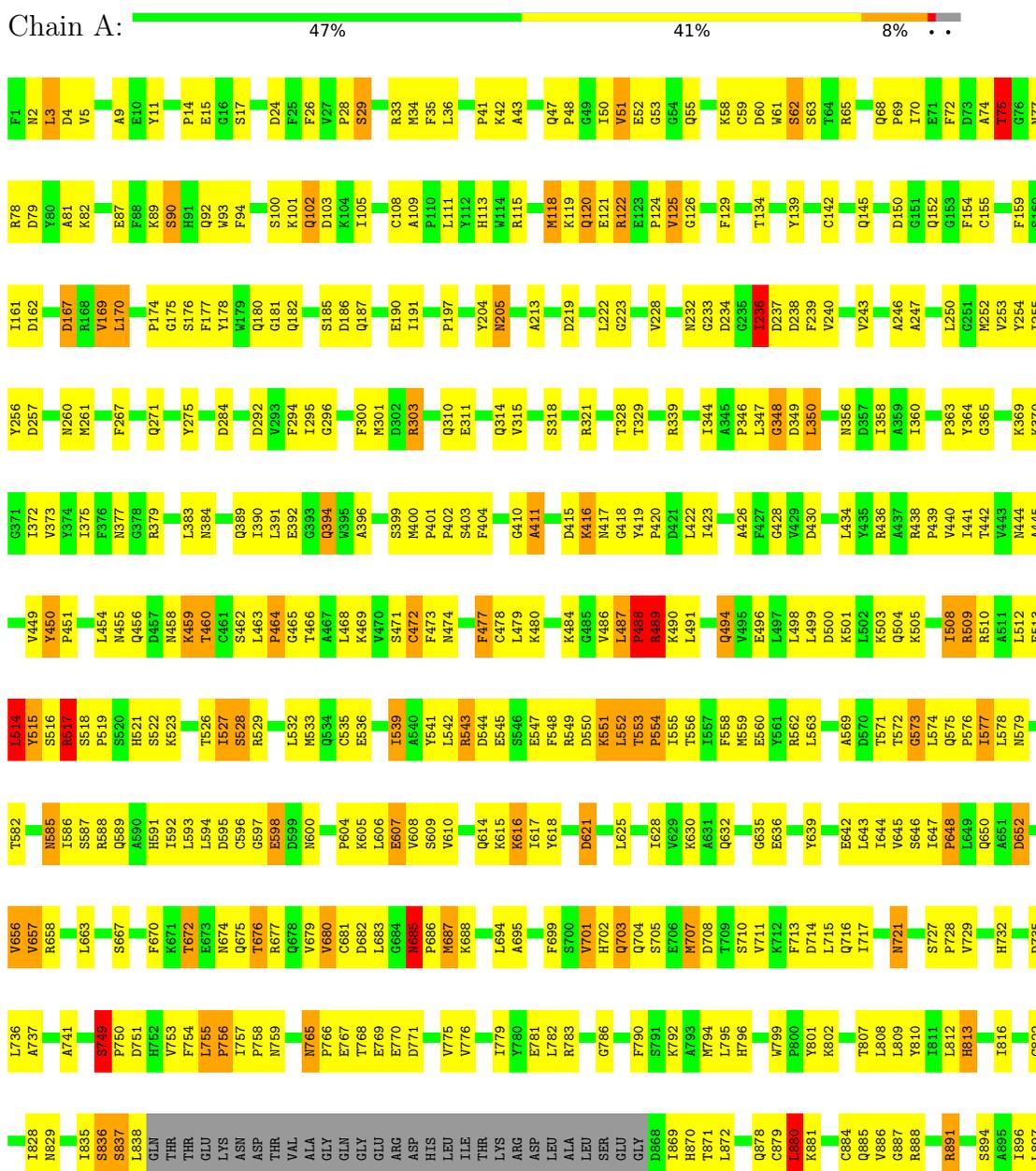
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	5	Total 5	Mn 5	0	0
7	B	3	Total 3	Mn 3	0	0

3 Residue-property plots [i](#)

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.

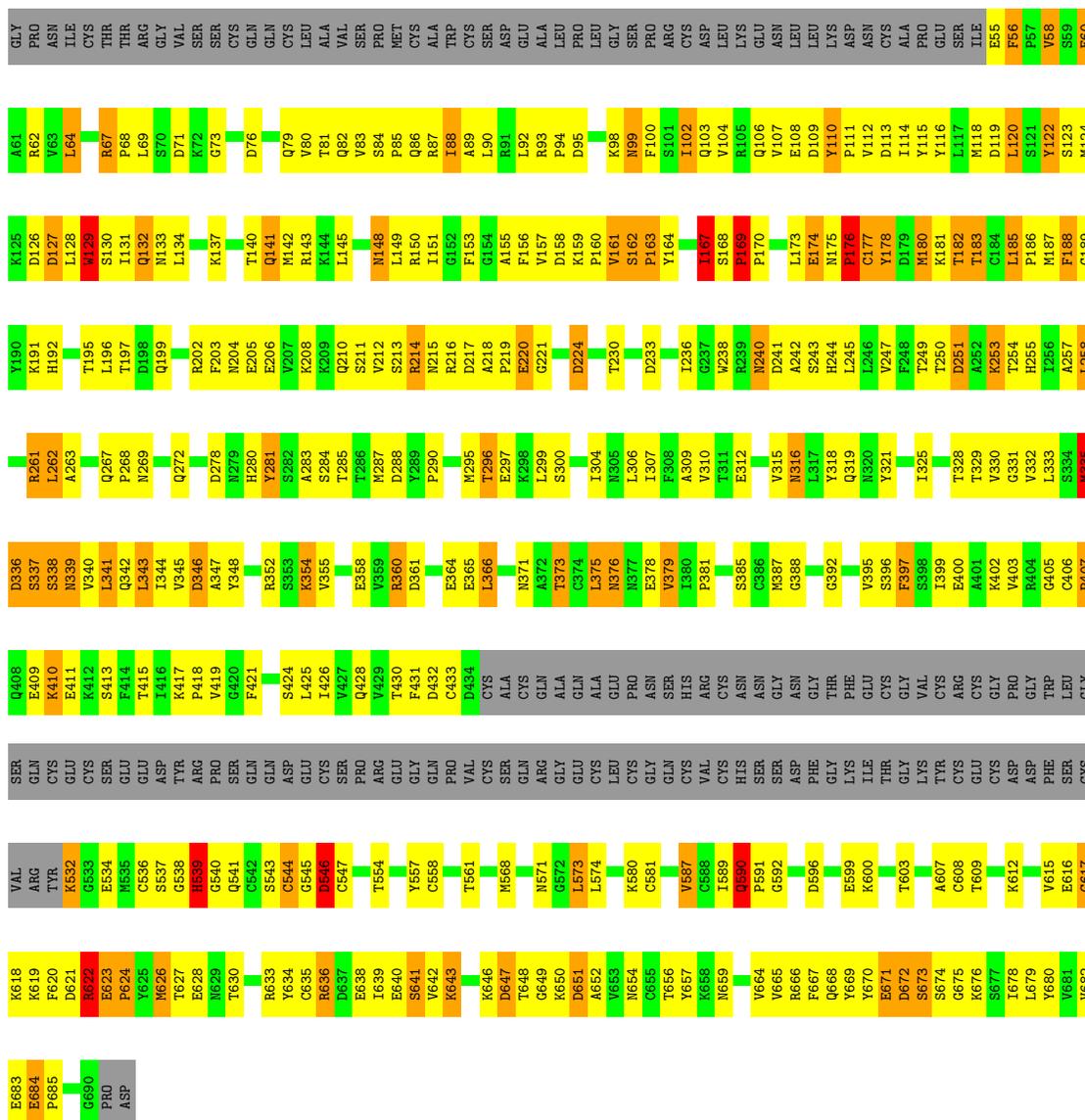
- Molecule 1: INTEGRIN ALPHA V





- Molecule 2: INTEGRIN BETA-3

Chain B: 29% 37% 10% 22%



- Molecule 3: CYCLIC ARG-GLY-ASP PEPTIDE

Chain C: 20% 40% 40%



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

Chain D:  50% 50%

MAG1
MAG2

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

Chain E:  100%

MAG1
MAG2

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

Chain F:  50% 50%

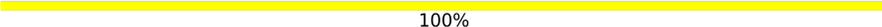
MAG1
MAG2

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

Chain H:  50% 50%

MAG1
MAG2

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

Chain G:  100%

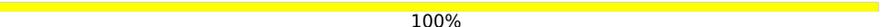
MAG1
MAG2

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

Chain I:  50% 50%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	129.79Å 129.79Å 308.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.248 , 0.328	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	11700	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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, NDG, MVA, MN

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	0.48	1/7372 (0.0%)	0.83	13/9994 (0.1%)
2	B	0.48	0/4256	0.85	7/5754 (0.1%)
3	C	0.49	0/34	0.77	0/43
All	All	0.48	1/11662 (0.0%)	0.84	20/15791 (0.1%)

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
3	C	1	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	THR	CA-CB	6.56	1.70	1.53

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	75	THR	N-CA-CB	7.91	125.33	110.30
2	B	336	ASP	N-CA-C	-7.27	91.38	111.00
1	A	553	THR	N-CA-C	-7.17	91.65	111.00
1	A	907	THR	N-CA-C	-7.16	91.68	111.00
1	A	460	THR	N-CA-C	7.02	129.94	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	5004	PHE	CA

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	7216	0	7035	396	0
2	B	4182	0	4029	300	0
3	C	42	0	39	8	0
4	D	28	0	25	5	0
4	E	28	0	25	0	0
4	F	28	0	25	3	0
4	H	28	0	25	3	0
5	G	28	0	24	7	0
5	I	28	0	24	0	0
5	J	28	0	24	8	0
6	A	28	0	26	8	0
6	B	28	0	26	5	0
7	A	5	0	0	0	0
7	B	3	0	0	0	0
All	All	11700	0	11327	708	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 31.

The worst 5 of 708 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)
5:G:1:NAG:H2	5:G:1:NAG:H61	1.34	1.06
1:A:487:LEU:HD23	1:A:488:PRO:HD3	1.37	1.05
1:A:236:ILE:HD13	1:A:236:ILE:H	1.21	1.02
2:B:69:LEU:HD22	2:B:80:VAL:HA	1.46	0.95
2:B:371:ASN:ND2	6:B:3371:NAG:H62	1.81	0.95

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	923/957 (96%)	743 (80%)	125 (14%)	55 (6%)	1	12
2	B	535/692 (77%)	392 (73%)	98 (18%)	45 (8%)	1	5
3	C	3/5 (60%)	2 (67%)	0	1 (33%)	0	0
All	All	1461/1654 (88%)	1137 (78%)	223 (15%)	101 (7%)	1	8

5 of 101 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ARG
1	A	236	ILE
1	A	396	ALA
1	A	411	ALA
1	A	487	LEU

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	787/812 (97%)	707 (90%)	80 (10%)	7	29
2	B	484/616 (79%)	396 (82%)	88 (18%)	1	8
3	C	3/3 (100%)	3 (100%)	0	100	100
All	All	1274/1431 (89%)	1106 (87%)	168 (13%)	4	19

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	224	ASP
2	B	430	THR
2	B	261	ARG
2	B	343	LEU
2	B	561	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	927	ASN
2	B	215	ASN
1	A	935	ASN
2	B	141	GLN
2	B	267	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](#)

1 non-standard protein/DNA/RNA residue is 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	MVA	C	5005	3	6,7,8	1.31	1 (16%)	7,8,10	0.93	0

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	MVA	C	5005	3	-	1/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5005	MVA	CN-N	-2.54	1.40	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	5005	MVA	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	5005	MVA	3	0

5.5 Carbohydrates [i](#)

14 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	D	1	1,4	14,14,15	0.49	0	17,19,21	0.66	0
4	NAG	D	2	4	14,14,15	0.41	0	17,19,21	0.78	1 (5%)
4	NAG	E	1	1,4	14,14,15	0.52	0	17,19,21	0.81	0
4	NAG	E	2	4	14,14,15	0.40	0	17,19,21	0.66	0
4	NAG	F	1	1,4	14,14,15	0.75	0	17,19,21	0.66	0
4	NAG	F	2	4	14,14,15	0.54	0	17,19,21	0.72	0
5	NAG	G	1	1,5	14,14,15	0.48	0	17,19,21	0.72	0
5	NDG	G	2	5	14,14,15	0.67	0	17,19,21	0.54	0
4	NAG	H	1	1,4	14,14,15	0.50	0	17,19,21	1.33	2 (11%)
4	NAG	H	2	4	14,14,15	0.43	0	17,19,21	0.57	0
5	NAG	I	1	5,2	14,14,15	0.80	0	17,19,21	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NDG	I	2	5	14,14,15	0.78	1 (7%)	17,19,21	1.04	2 (11%)
5	NAG	J	1	5,2	14,14,15	0.62	0	17,19,21	0.73	0
5	NDG	J	2	5	14,14,15	0.47	0	17,19,21	0.77	0

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	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1
5	NAG	G	1	1,5	-	0/6/23/26	0/1/1/1
5	NDG	G	2	5	-	4/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
5	NAG	I	1	5,2	-	2/6/23/26	0/1/1/1
5	NDG	I	2	5	-	1/6/23/26	0/1/1/1
5	NAG	J	1	5,2	-	2/6/23/26	0/1/1/1
5	NDG	J	2	5	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	2	NDG	C1-C2	2.17	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	NAG	C3-C4-C5	3.25	116.04	110.24
4	H	1	NAG	C4-C3-C2	3.09	115.55	111.02
5	I	2	NDG	C1-O5-C5	2.69	115.84	112.19
5	I	2	NDG	C2-N2-C7	-2.23	119.73	122.90
4	D	2	NAG	C2-N2-C7	-2.18	119.79	122.90

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

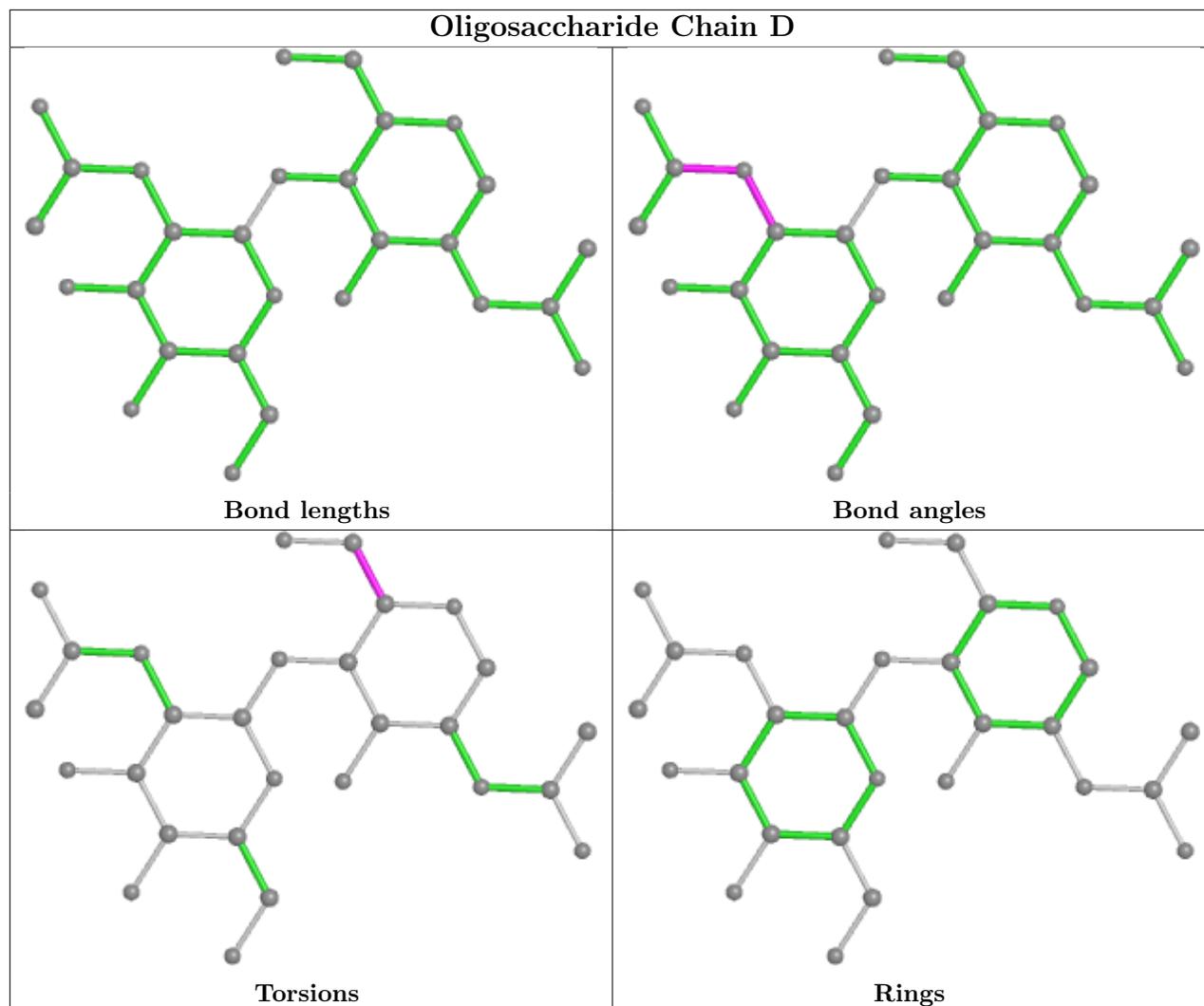
Mol	Chain	Res	Type	Atoms
5	G	2	NDG	C3-C2-N2-C7
4	H	2	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6

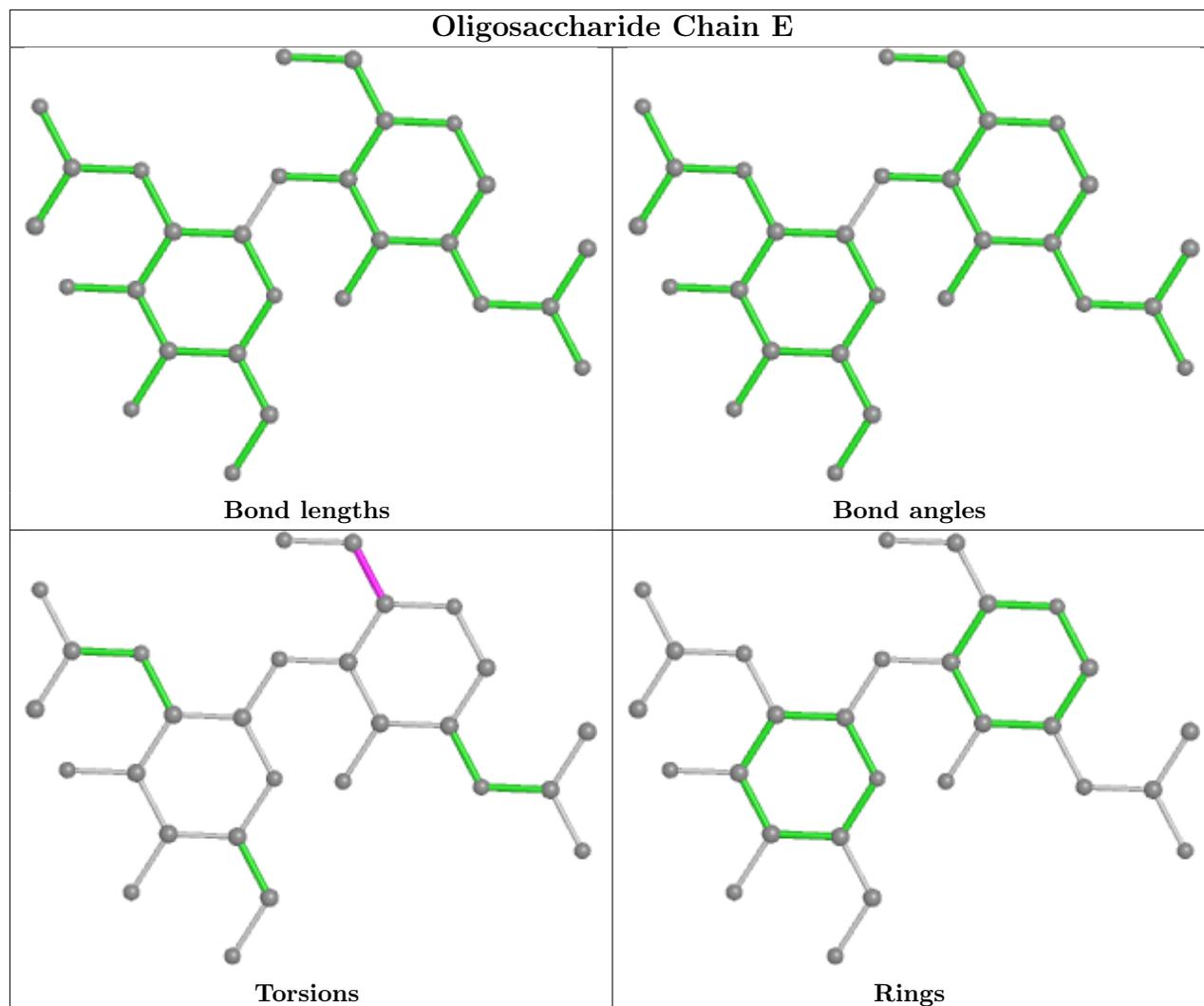
There are no ring outliers.

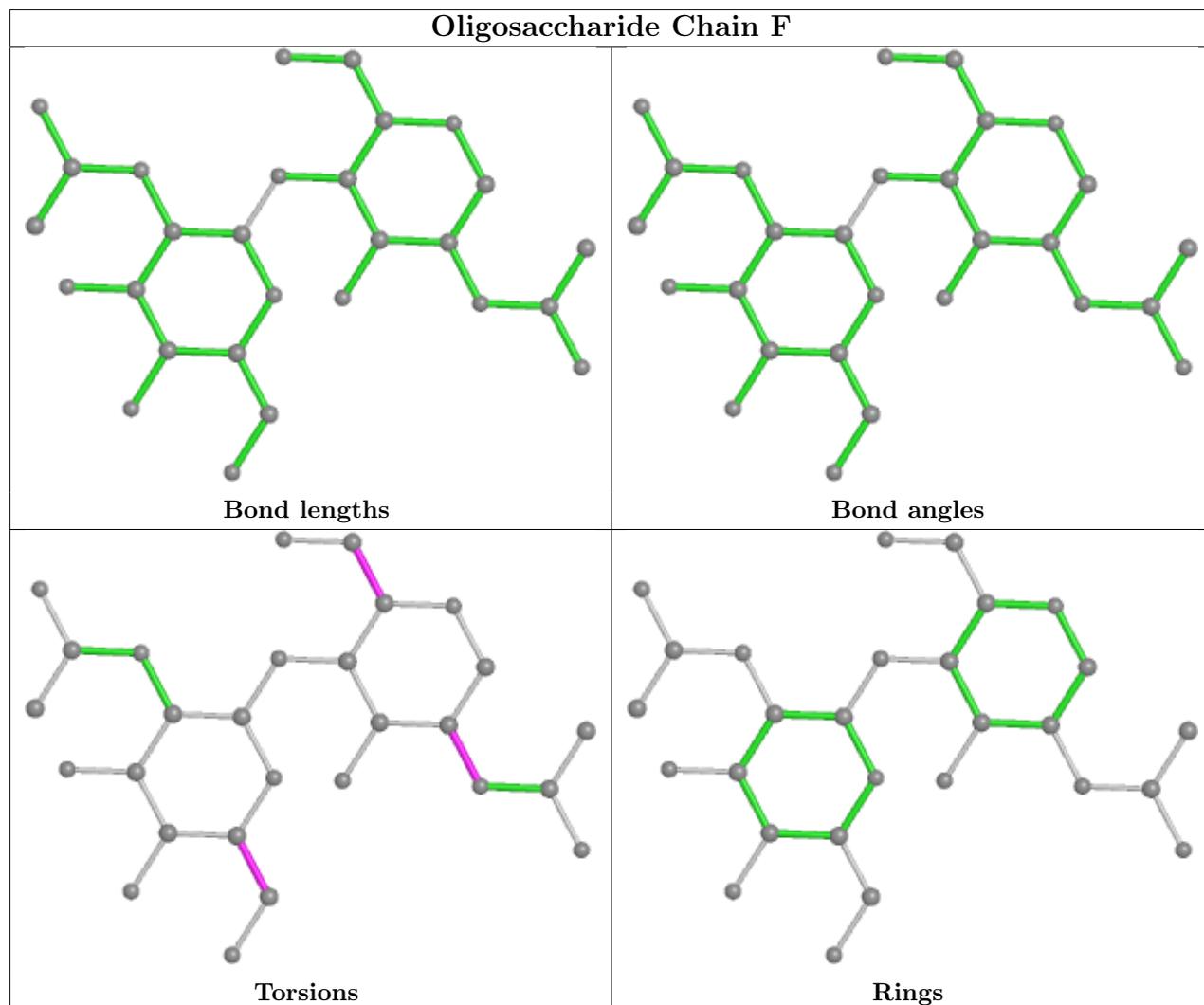
8 monomers are involved in 26 short contacts:

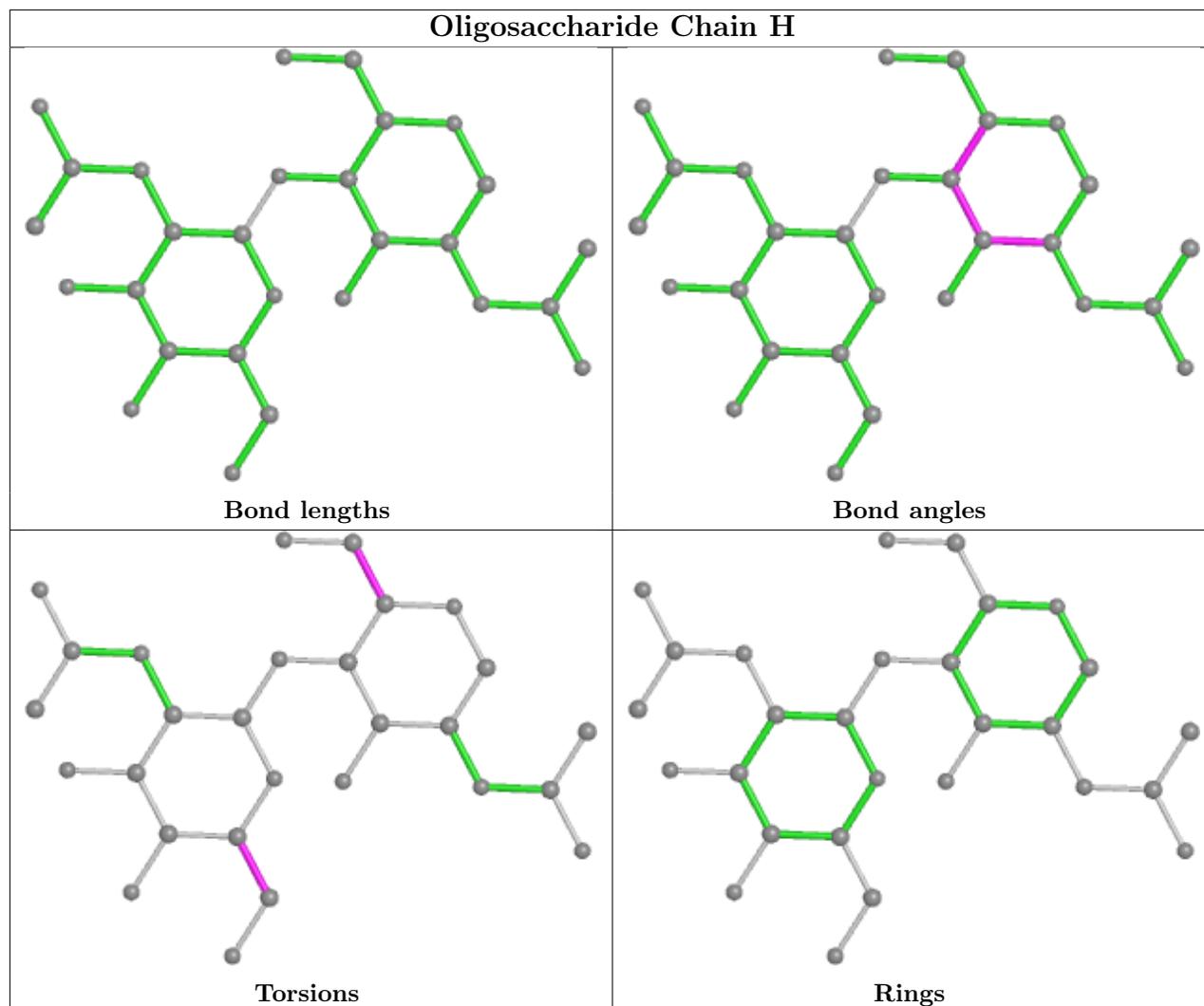
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	1	NAG	3	0
4	H	1	NAG	3	0
5	J	2	NDG	4	0
4	D	2	NAG	5	0
4	F	1	NAG	3	0
4	D	1	NAG	2	0
5	G	2	NDG	4	0
5	J	1	NAG	4	0

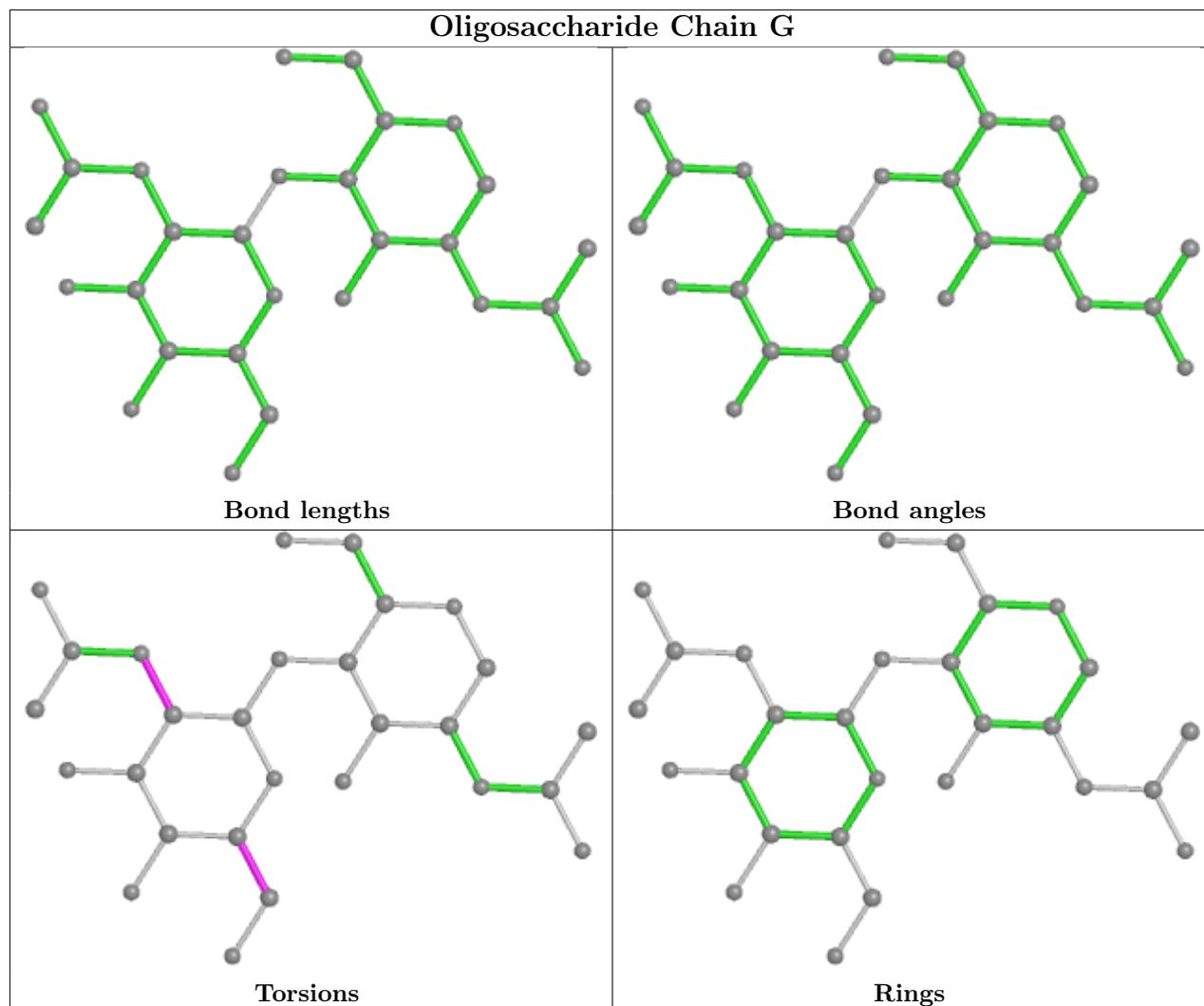
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

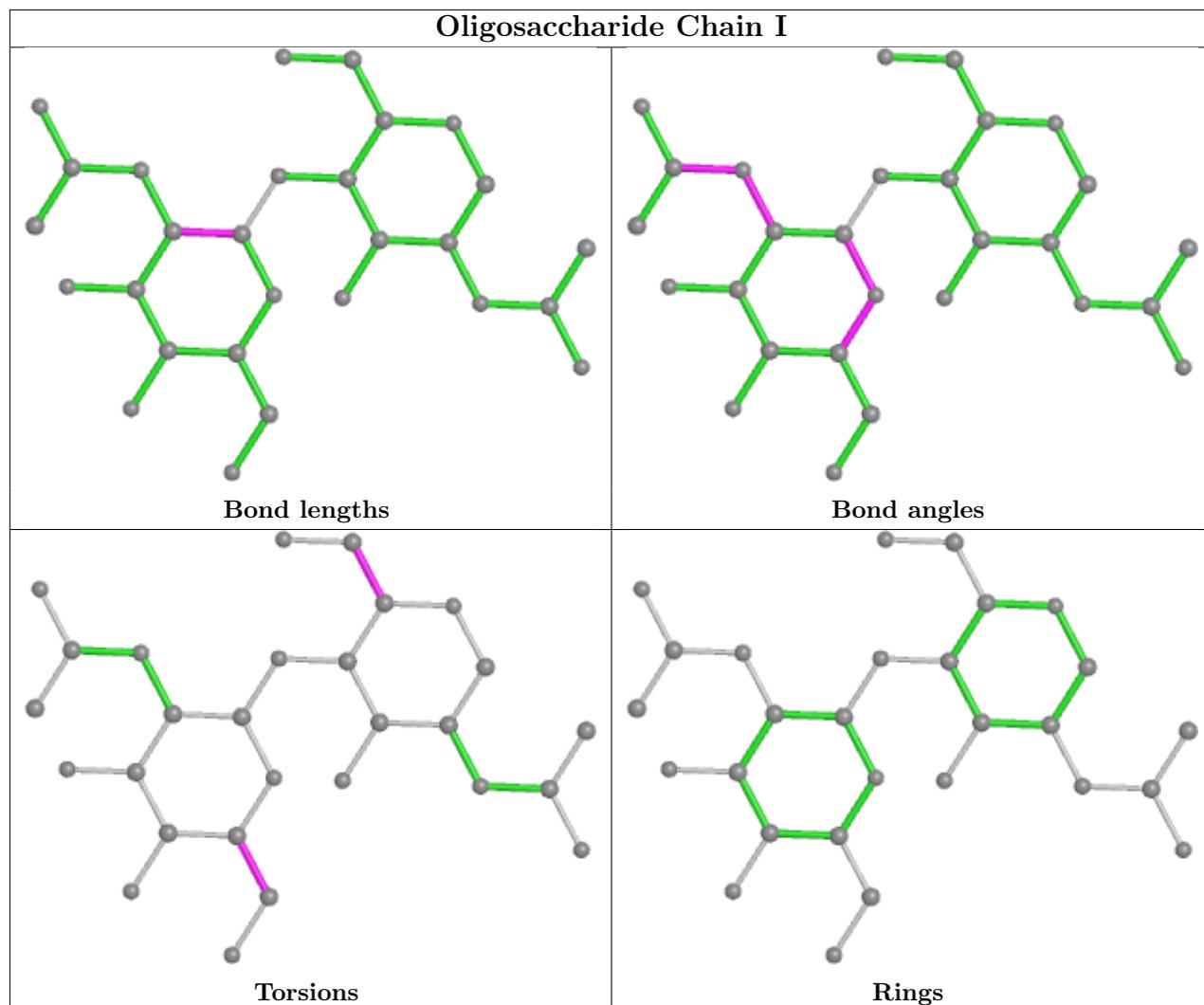


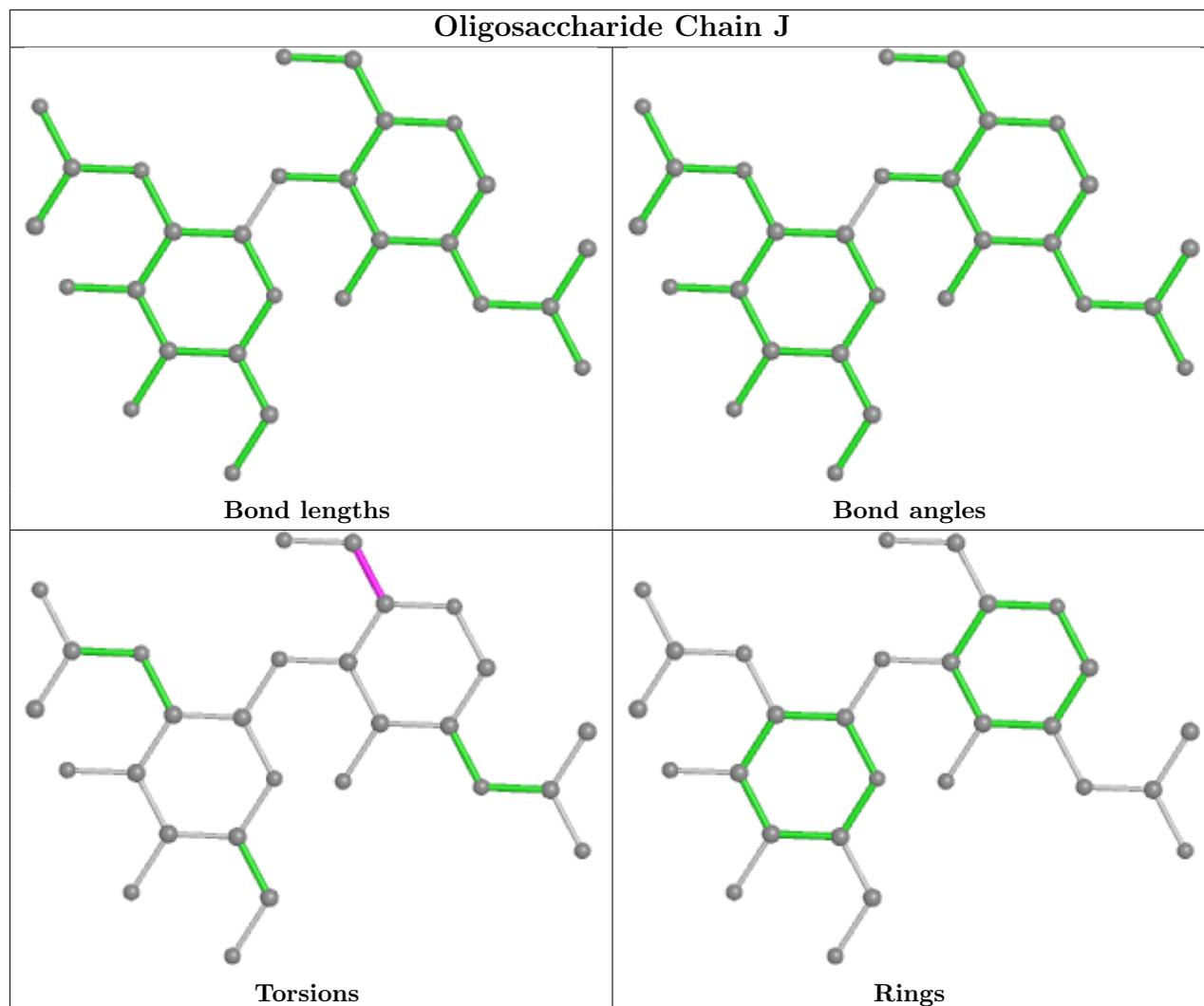












5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
6	NAG	A	2260	1	14,14,15	0.66	0	17,19,21	0.70	0
6	NAG	B	3371	2	14,14,15	0.51	0	17,19,21	0.63	0
6	NAG	B	3320	2	14,14,15	0.56	0	17,19,21	0.84	1 (5%)
6	NAG	A	2458	1	14,14,15	0.47	0	17,19,21	0.79	0

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
6	NAG	A	2260	1	-	4/6/23/26	0/1/1/1
6	NAG	B	3371	2	-	4/6/23/26	0/1/1/1
6	NAG	B	3320	2	-	0/6/23/26	0/1/1/1
6	NAG	A	2458	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	3320	NAG	C2-N2-C7	-2.02	120.03	122.90

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2260	NAG	C4-C5-C6-O6
6	B	3371	NAG	C1-C2-N2-C7
6	A	2260	NAG	O5-C5-C6-O6
6	B	3371	NAG	O5-C5-C6-O6
6	A	2458	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2260	NAG	3	0
6	B	3371	NAG	4	0
6	B	3320	NAG	1	0
6	A	2458	NAG	5	0

5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.