



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 29, 2024 – 08:12 PM EDT

PDB ID : 4O02  
Title : AlphaVBeta3 integrin in complex with monoclonal antibody FAB fragment.  
Authors : Mahalingam, B.; van Agthoven, J.; Xiong, J.; Arnaout, M.A.  
Deposited on : 2013-12-13  
Resolution : 3.60 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](mailto: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>.

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

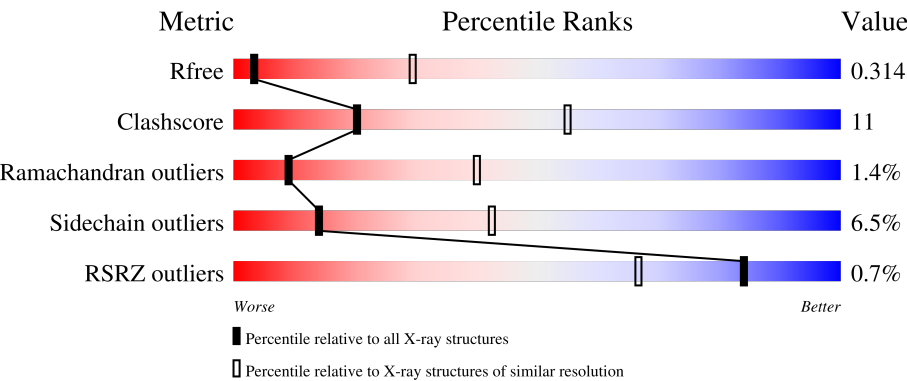
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

# 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 3.60 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 <sub>free</sub>	164625	1563 (3.70-3.50)
Clashscore	180529	1665 (3.70-3.50)
Ramachandran outliers	177936	1641 (3.70-3.50)
Sidechain outliers	177891	1640 (3.70-3.50)
RSRZ outliers	164620	1562 (3.70-3.50)

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  $\geq 3$ , 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	962	
2	B	692	
3	L	214	
4	H	218	
5	C	6	

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Mol	Chain	Length	Quality of chain
6	D	3	 100%
7	E	6	 50%50%
8	F	2	 100%
8	I	2	 50%50%
8	J	2	 100%
9	G	6	 83%17%

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 13526 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
1	A	915	Total	C	N	O	S	0	0	0
			5875	3627	1033	1192	23			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	687	Total	C	N	O	S	0	0	0
			4364	2657	771	871	65			

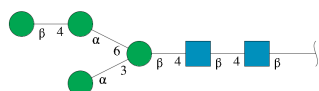
- Molecule 3 is a protein called 17E6 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1453	887	253	307	6			

- Molecule 4 is a protein called 17E6 heavy chain.

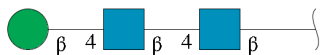
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	218	Total	C	N	O	S	0	0	0
			1440	891	247	293	9			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



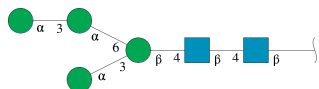
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 6 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
6	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



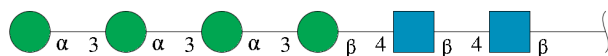
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	E	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



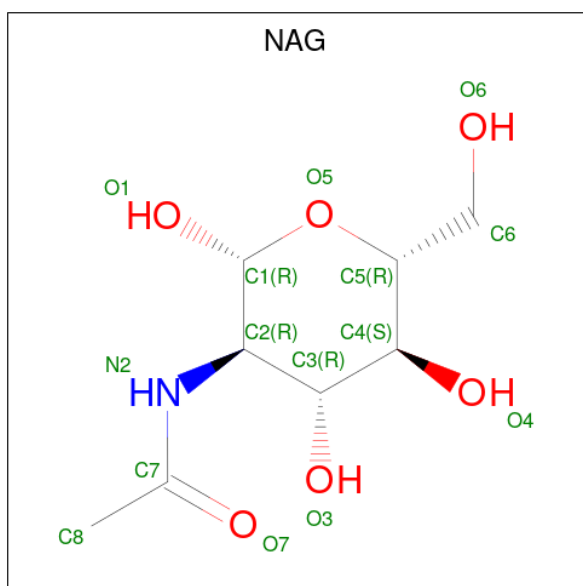
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-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
9	G	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

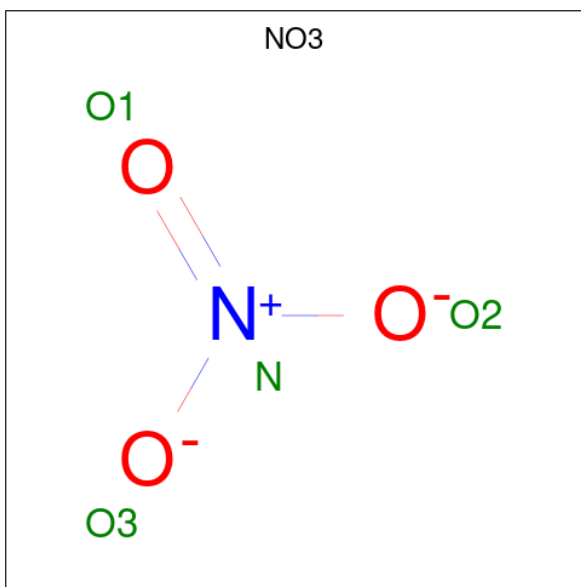


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	B	1	Total	C	N	O	0	0
			14	8	1	5		
10	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 11 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	4	Total	Mn	0	0
			4	4		
11	B	1	Total	Mn	0	0
			1	1		

- Molecule 12 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	N	O	0	0
			4	1	3		
12	A	1	Total	N	O	0	0
			4	1	3		

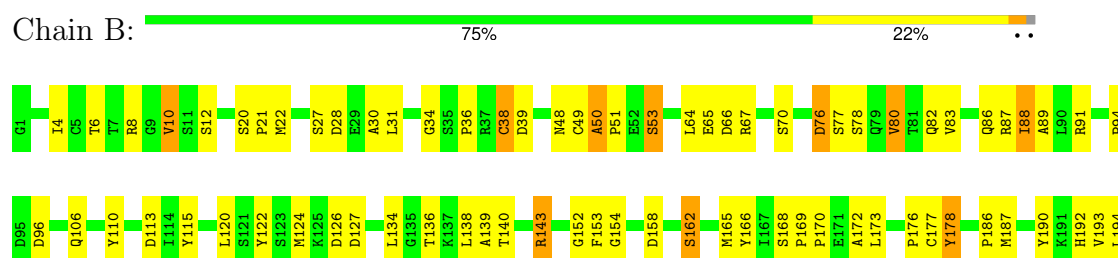
### 3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

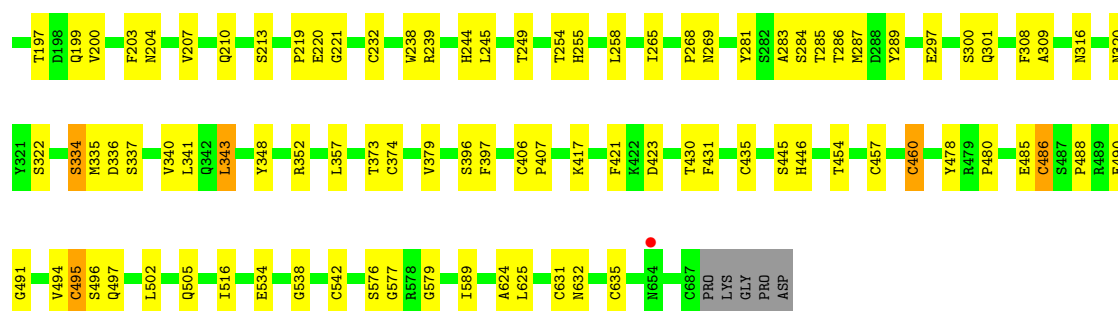
#### • Molecule 1: Integrin alpha-V



#### • Molecule 2: Integrin beta-3

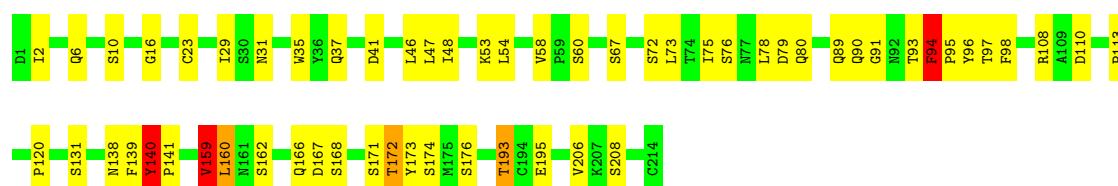






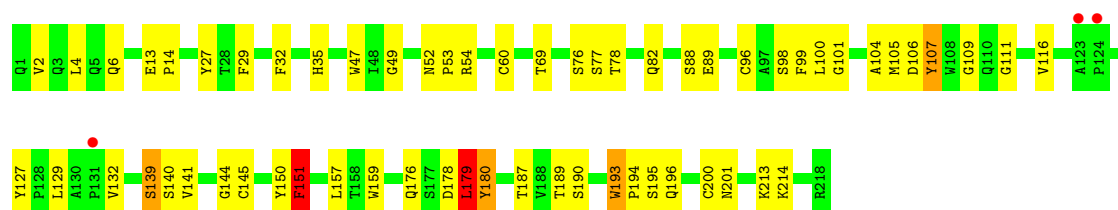
• Molecule 3: 17E6 light chain

Chain L: 73% 24% ..



• Molecule 4: 17E6 heavy chain

Chain H: 72% 25% ..



• Molecule 5: beta-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 33% 67%



• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 100%



• Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50% 50%

  
MAG1  
MAG2  
ENA3  
MAN4  
MAN5  
MAN6

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

  
MAG1  
MAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50% 50%

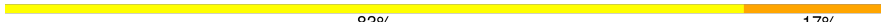
  
MAG1  
MAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%

  
MAG1  
MAG2

- Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  83% 17%

  
MAG1  
MAG2  
ENA3  
MAN4  
MAN5  
MAN6

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.46Å 266.99Å 102.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.86 – 3.60 49.86 – 3.60	Depositor EDS
% Data completeness (in resolution range)	87.6 (49.86-3.60) 87.6 (49.86-3.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.246 , 0.312 0.254 , 0.314	Depositor DCC
$R_{free}$ test set	1563 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	112.3	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 177.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	13526	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	155.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NO3, MN, NAG, MAN

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	0.28	0/5981	0.62	1/8211 (0.0%)
2	B	0.32	1/4438 (0.0%)	0.65	0/6091
3	L	0.29	0/1483	0.62	0/2037
4	H	0.29	0/1475	0.69	1/2027 (0.0%)
All	All	0.30	1/13377 (0.0%)	0.64	2/18366 (0.0%)

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
1	A	0	2
2	B	0	4
3	L	0	3
4	H	0	4
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	335	MET	C-O	5.78	1.34	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	GLY	N-CA-C	-5.39	99.62	113.10
4	H	179	LEU	N-CA-C	5.25	125.16	111.00

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	THR	Peptide
1	A	768	THR	Peptide
2	B	50	ALA	Peptide
2	B	53	SER	Peptide
2	B	8	ARG	Peptide

## 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	5875	0	4346	96	0
2	B	4364	0	3235	104	0
3	L	1453	0	1128	33	0
4	H	1440	0	1084	36	0
5	C	72	0	61	0	0
6	D	39	0	34	0	0
7	E	72	0	61	2	0
8	F	28	0	25	0	0
8	I	28	0	25	1	0
8	J	28	0	25	0	0
9	G	72	0	61	1	0
10	A	14	0	13	0	0
10	B	28	0	26	0	0
11	A	4	0	0	0	0
11	B	1	0	0	0	0
12	A	8	0	0	0	0
All	All	13526	0	10124	263	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.

The worst 5 of 263 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:253:VAL:HG23	1:A:267:PHE:HB2	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:GLU:HG3	1:A:585:ASN:HB3	1.53	0.89
1:A:121:GLU:HA	2:B:169:PRO:HB3	1.57	0.85
1:A:100:SER:HB3	1:A:105:ILE:HG22	1.59	0.83
2:B:31:LEU:HG	2:B:34:GLY:HA3	1.67	0.77

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	911/962 (95%)	815 (90%)	88 (10%)	8 (1%)	14	48
2	B	685/692 (99%)	595 (87%)	79 (12%)	11 (2%)	8	38
3	L	212/214 (99%)	196 (92%)	12 (6%)	4 (2%)	6	35
4	H	216/218 (99%)	190 (88%)	20 (9%)	6 (3%)	4	27
All	All	2024/2086 (97%)	1796 (89%)	199 (10%)	29 (1%)	9	40

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	LYS
1	A	619	ILE
1	A	710	SER
4	H	180	TYR
1	A	453	ILE

### 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	400/816 (49%)	378 (94%)	22 (6%)	18	47
2	B	334/614 (54%)	308 (92%)	26 (8%)	10	36
3	L	125/192 (65%)	115 (92%)	10 (8%)	10	35
4	H	107/183 (58%)	102 (95%)	5 (5%)	22	51
All	All	966/1805 (54%)	903 (94%)	63 (6%)	14	42

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	232	CYS
3	L	160	LEU
2	B	343	LEU
3	L	159	VAL
4	H	96	CYS

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	332	ASN
2	B	313	ASN
4	H	52	ASN
3	L	138	ASN
1	A	314	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 ⓘ

27 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	$\# Z  > 2$
5	NAG	C	1	1,5	14,14,15	0.30	0	17,19,21	0.50	0
5	NAG	C	2	5	14,14,15	0.42	0	17,19,21	0.79	0
5	BMA	C	3	5	11,11,12	1.02	0	15,15,17	1.09	1 (6%)
5	MAN	C	4	5	11,11,12	0.97	1 (9%)	15,15,17	0.88	1 (6%)
5	BMA	C	5	5	11,11,12	0.59	0	15,15,17	0.96	1 (6%)
5	MAN	C	6	5	11,11,12	0.68	0	15,15,17	1.08	2 (13%)
6	NAG	D	1	6,1	14,14,15	0.40	0	17,19,21	0.45	0
6	NAG	D	2	6	14,14,15	0.40	0	17,19,21	0.51	0
6	BMA	D	3	6	11,11,12	0.70	0	15,15,17	0.83	0
7	NAG	E	1	7,1	14,14,15	0.50	0	17,19,21	1.00	1 (5%)
7	NAG	E	2	7	14,14,15	0.42	0	17,19,21	0.44	0
7	BMA	E	3	7	11,11,12	0.65	0	15,15,17	0.96	1 (6%)
7	MAN	E	4	7	11,11,12	0.85	0	15,15,17	1.48	2 (13%)
7	MAN	E	5	7	11,11,12	0.84	0	15,15,17	1.35	2 (13%)
7	MAN	E	6	7	11,11,12	0.53	0	15,15,17	1.05	2 (13%)
8	NAG	F	1	1,8	14,14,15	0.39	0	17,19,21	0.48	0
8	NAG	F	2	8	14,14,15	0.32	0	17,19,21	0.34	0
9	NAG	G	1	1,9	14,14,15	0.25	0	17,19,21	0.55	0
9	NAG	G	2	9	14,14,15	0.64	1 (7%)	17,19,21	0.80	1 (5%)
9	BMA	G	3	9	11,11,12	1.13	1 (9%)	15,15,17	0.88	0
9	MAN	G	4	9	11,11,12	1.21	1 (9%)	15,15,17	1.69	2 (13%)
9	MAN	G	5	9	11,11,12	1.29	2 (18%)	15,15,17	1.57	4 (26%)
9	MAN	G	6	9	11,11,12	0.77	1 (9%)	15,15,17	1.46	2 (13%)
8	NAG	I	1	2,8	14,14,15	0.75	1 (7%)	17,19,21	1.03	1 (5%)
8	NAG	I	2	8	14,14,15	0.38	0	17,19,21	0.93	1 (5%)
8	NAG	J	1	2,8	14,14,15	1.27	1 (7%)	17,19,21	1.61	1 (5%)
8	NAG	J	2	8	14,14,15	0.43	0	17,19,21	0.64	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
5	NAG	C	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	C	2	5	-	4/6/23/26	0/1/1/1
5	BMA	C	3	5	-	0/2/19/22	0/1/1/1
5	MAN	C	4	5	-	1/2/19/22	0/1/1/1
5	BMA	C	5	5	-	0/2/19/22	0/1/1/1
5	MAN	C	6	5	-	2/2/19/22	0/1/1/1
6	NAG	D	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	D	2	6	-	0/6/23/26	0/1/1/1
6	BMA	D	3	6	-	2/2/19/22	0/1/1/1
7	NAG	E	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	E	2	7	-	2/6/23/26	0/1/1/1
7	BMA	E	3	7	-	2/2/19/22	0/1/1/1
7	MAN	E	4	7	-	1/2/19/22	1/1/1/1
7	MAN	E	5	7	-	1/2/19/22	1/1/1/1
7	MAN	E	6	7	-	0/2/19/22	0/1/1/1
8	NAG	F	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	F	2	8	-	2/6/23/26	0/1/1/1
9	NAG	G	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	G	2	9	-	2/6/23/26	0/1/1/1
9	BMA	G	3	9	-	2/2/19/22	0/1/1/1
9	MAN	G	4	9	-	1/2/19/22	1/1/1/1
9	MAN	G	5	9	-	0/2/19/22	0/1/1/1
9	MAN	G	6	9	-	0/2/19/22	0/1/1/1
8	NAG	I	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	I	2	8	-	2/6/23/26	0/1/1/1
8	NAG	J	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	J	2	8	-	2/6/23/26	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	1	NAG	O5-C1	4.64	1.51	1.43
9	G	5	MAN	C1-C2	2.75	1.58	1.52
8	I	1	NAG	O5-C1	2.61	1.48	1.43
5	C	4	MAN	O5-C1	-2.51	1.39	1.43
9	G	5	MAN	C2-C3	2.46	1.56	1.52

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	1	NAG	C1-O5-C5	5.94	120.14	112.19
9	G	4	MAN	C1-O5-C5	5.16	119.10	112.19
7	E	4	MAN	C1-O5-C5	4.64	118.41	112.19
7	E	5	MAN	C1-O5-C5	4.27	117.91	112.19
9	G	6	MAN	C1-O5-C5	3.85	117.35	112.19

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	2	NAG	O5-C5-C6-O6
6	D	3	BMA	O5-C5-C6-O6
8	F	2	NAG	O5-C5-C6-O6
5	C	1	NAG	C4-C5-C6-O6
8	I	2	NAG	C4-C5-C6-O6

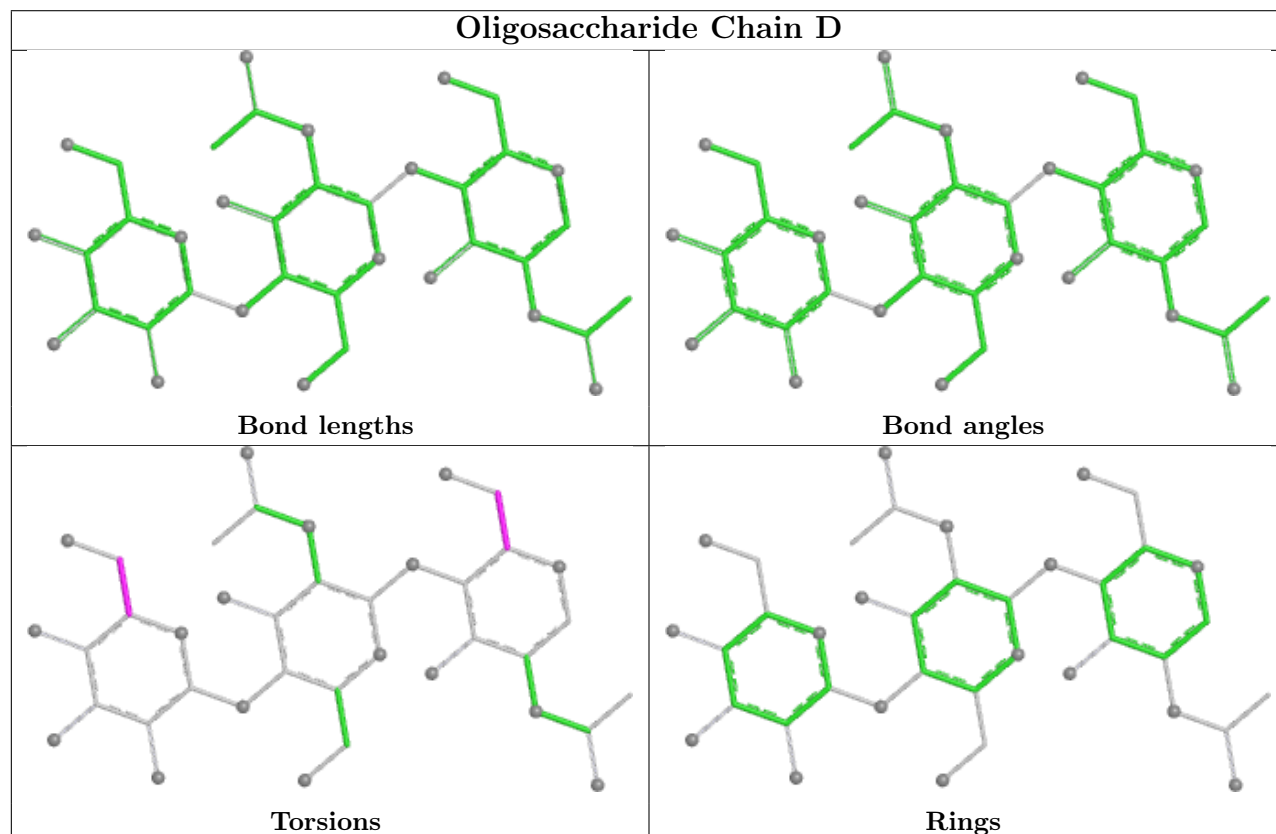
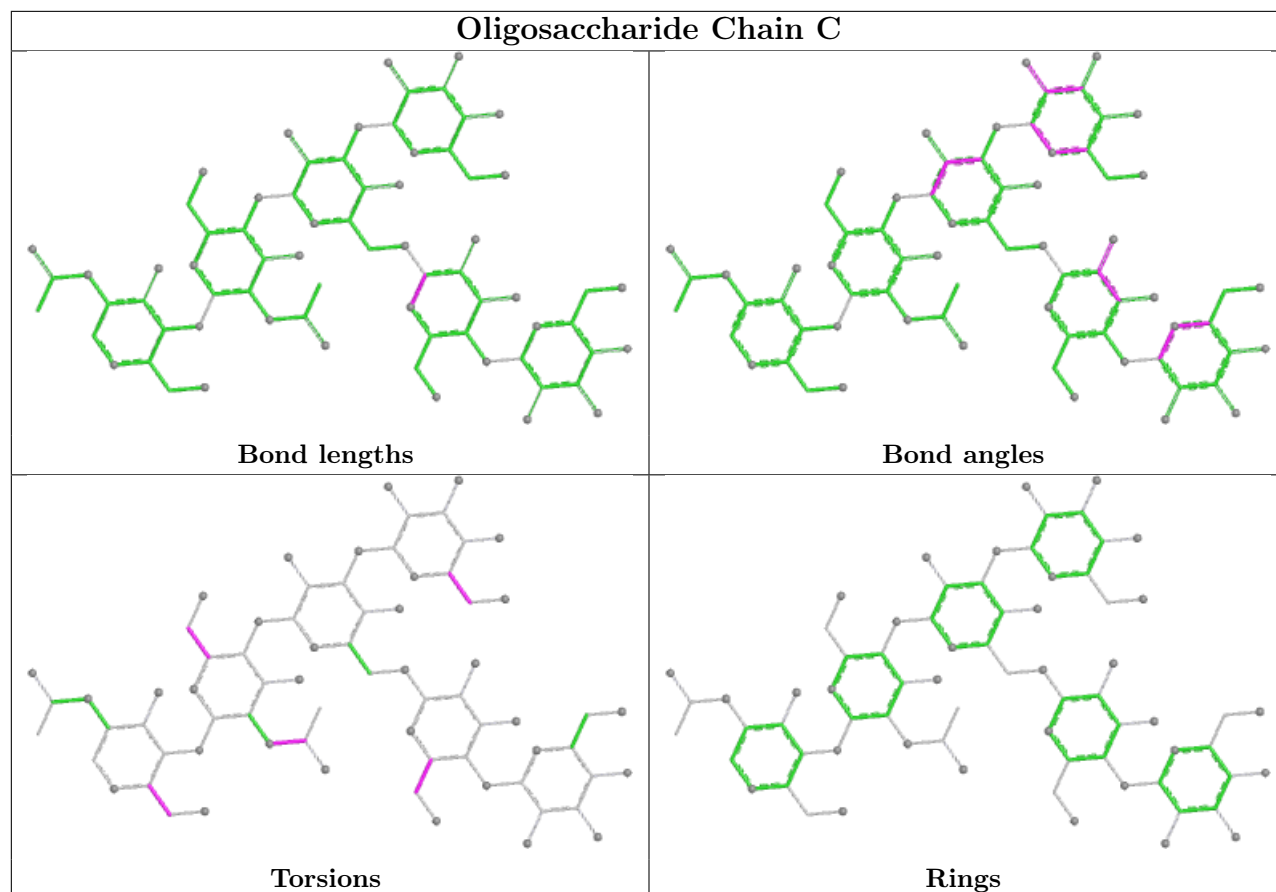
All (3) ring outliers are listed below:

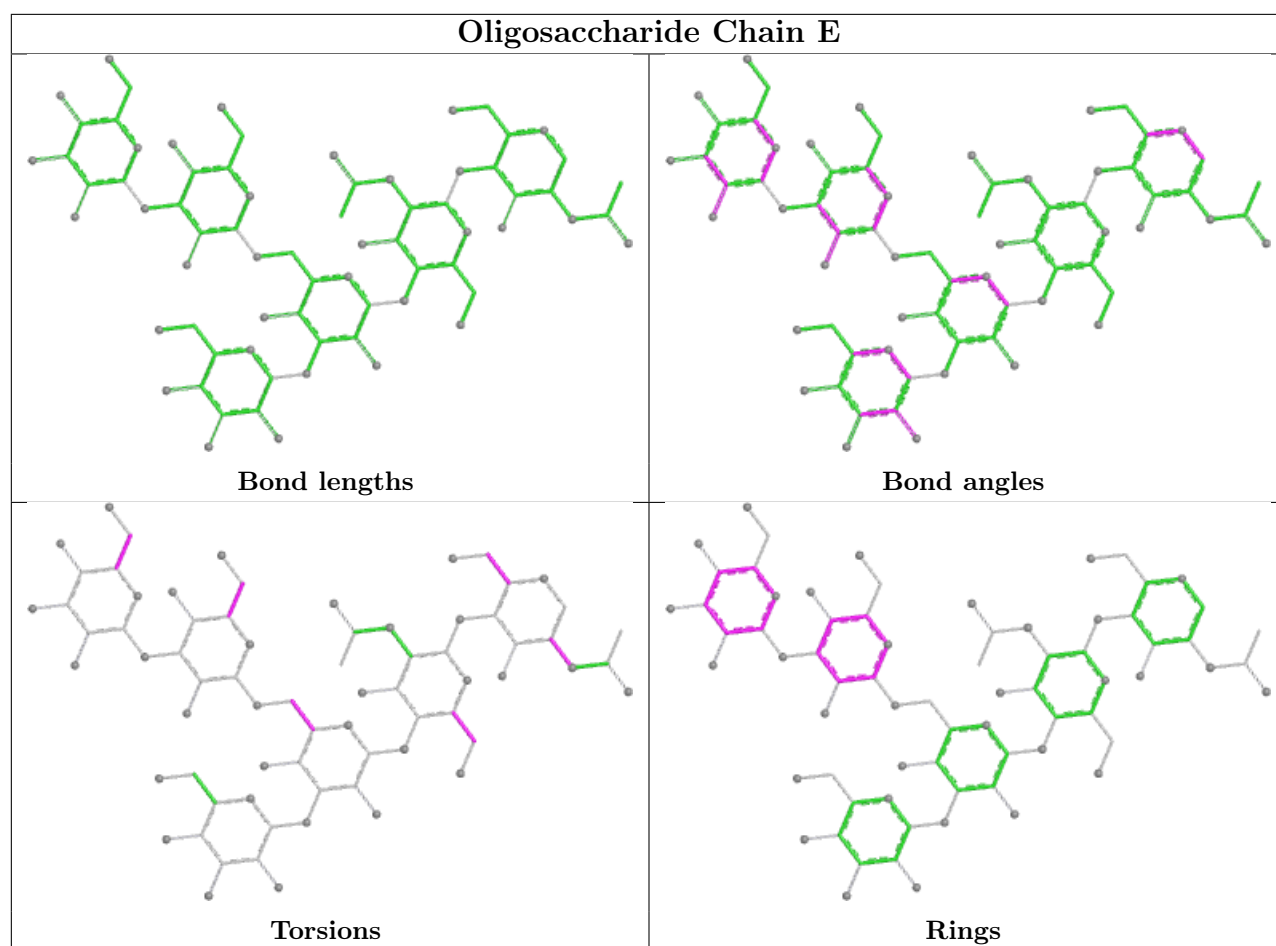
Mol	Chain	Res	Type	Atoms
9	G	4	MAN	C1-C2-C3-C4-C5-O5
7	E	4	MAN	C1-C2-C3-C4-C5-O5
7	E	5	MAN	C1-C2-C3-C4-C5-O5

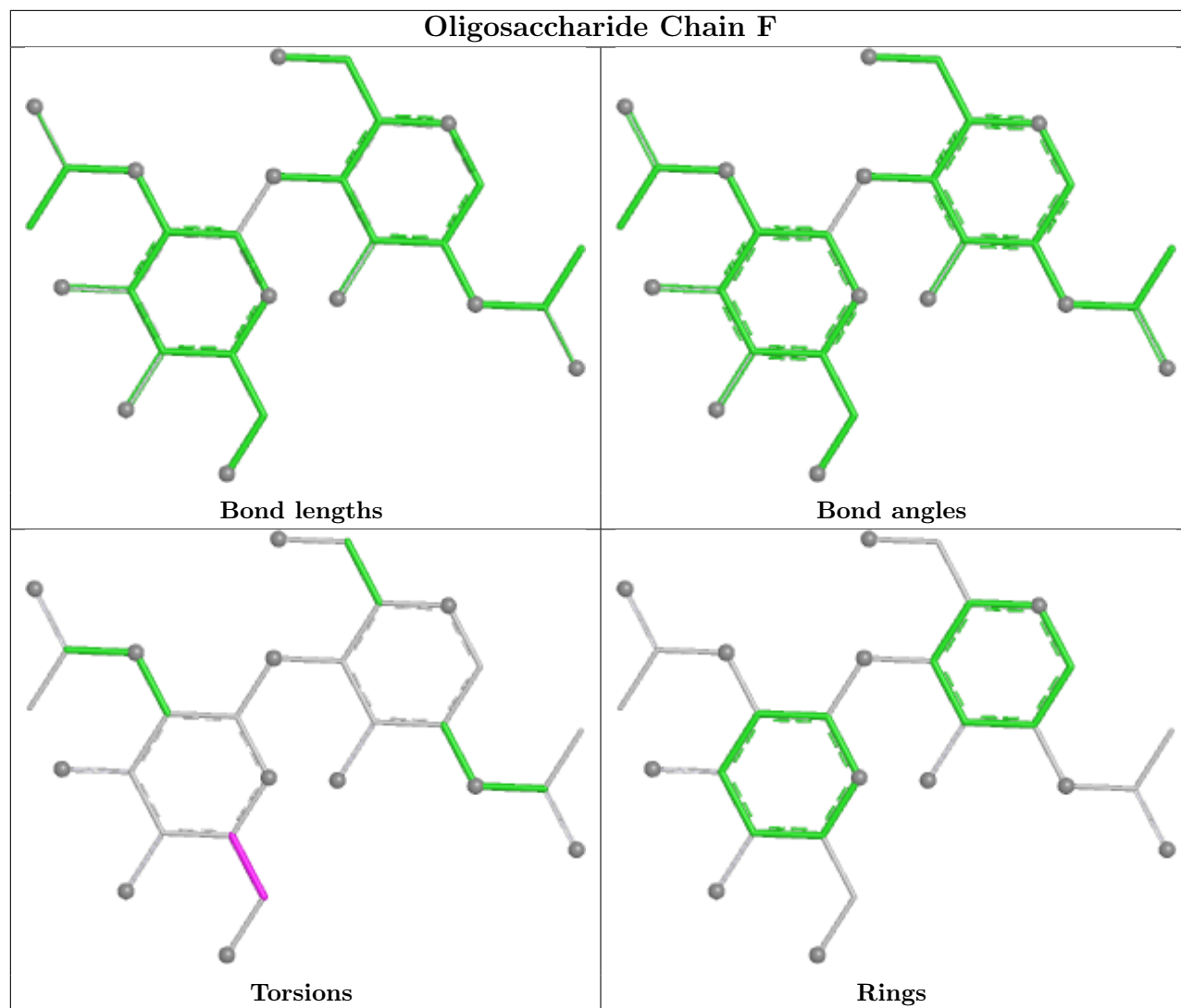
7 monomers are involved in 4 short contacts:

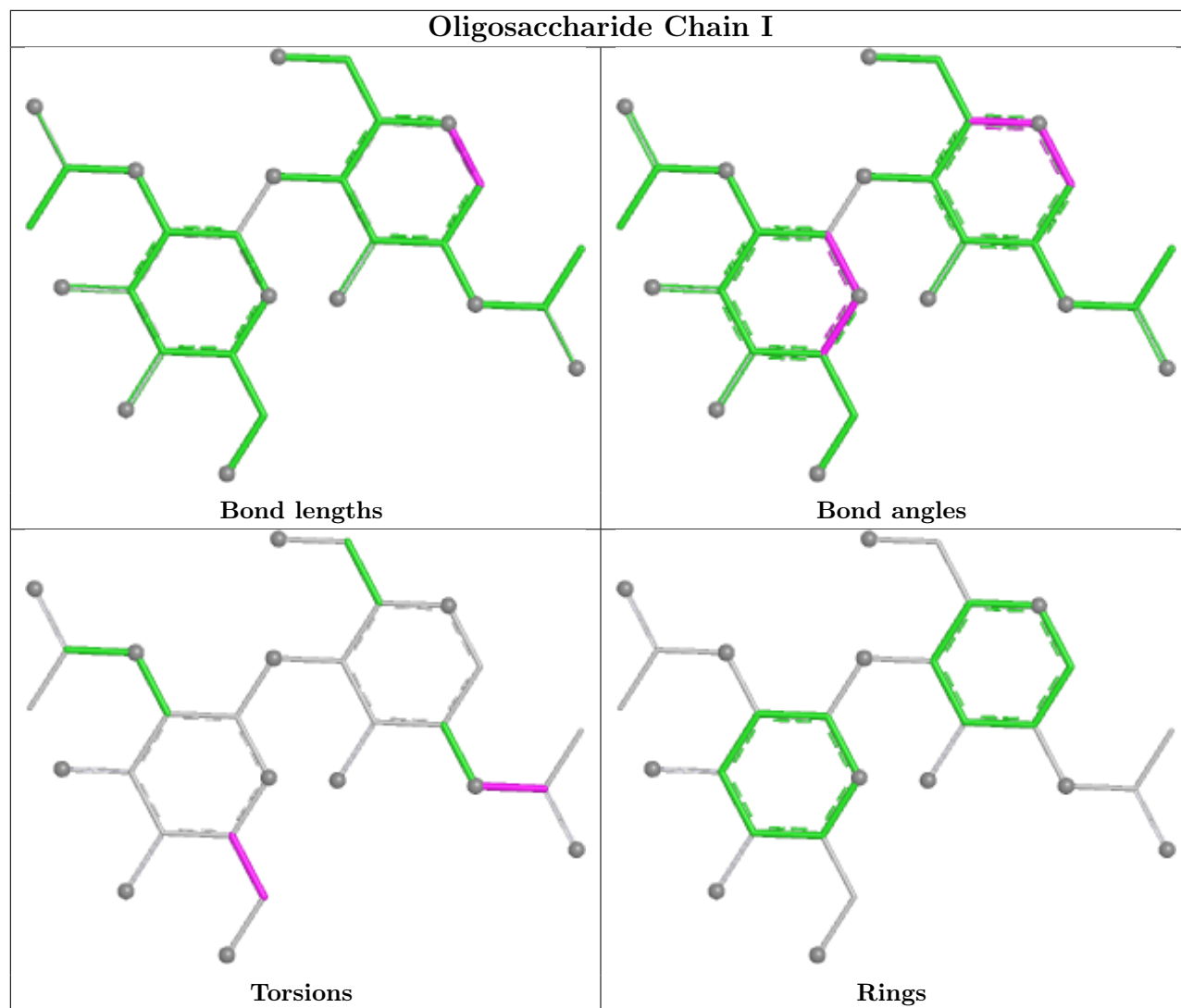
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	4	MAN	1	0
9	G	1	NAG	1	0
7	E	2	NAG	1	0
9	G	2	NAG	1	0
7	E	5	MAN	1	0
8	I	1	NAG	1	0
7	E	1	NAG	1	0

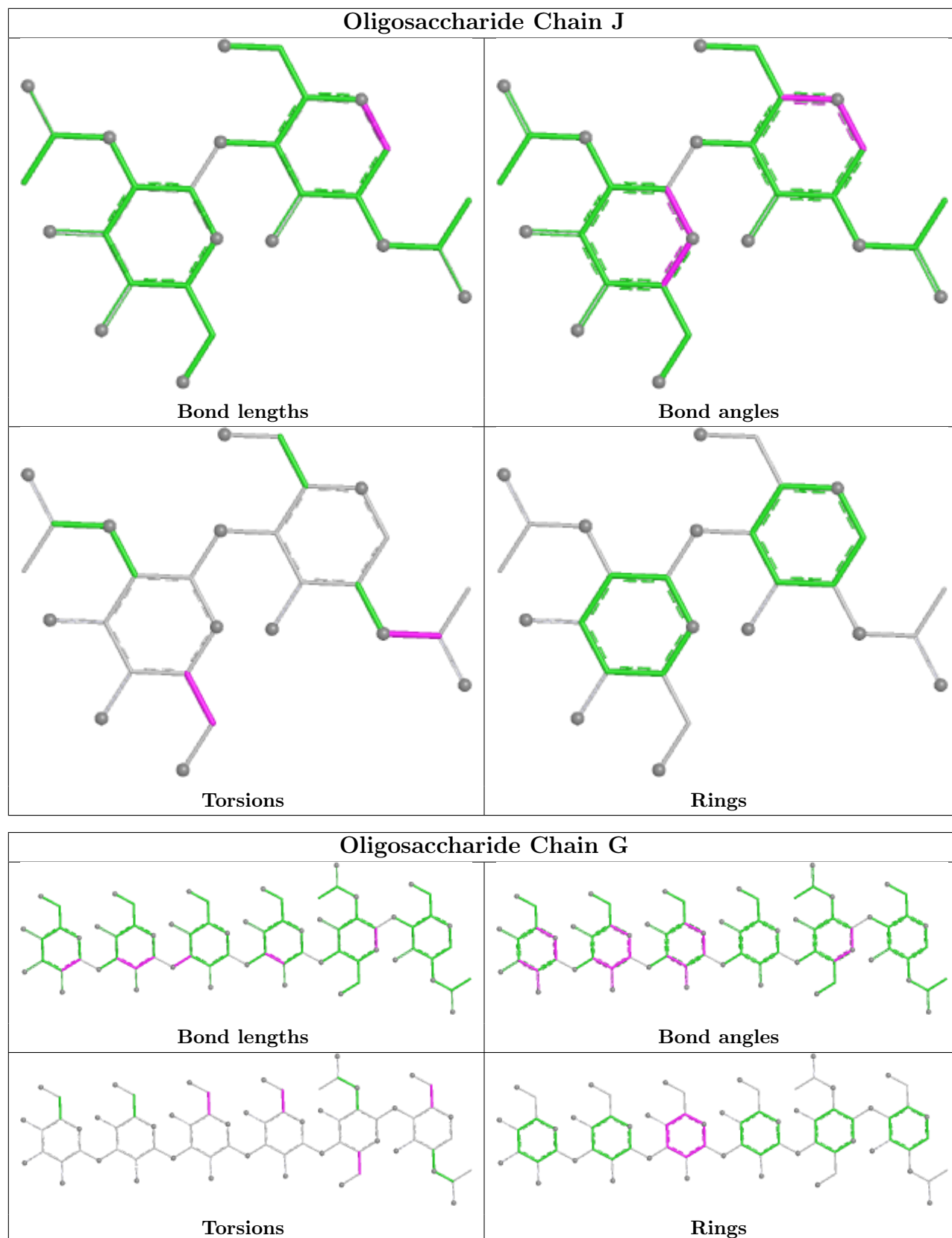
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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
10	NAG	B	706	2	14,14,15	0.33	0	17,19,21	0.56	0
10	NAG	A	1016	1	14,14,15	0.42	0	17,19,21	0.48	0
10	NAG	B	701	2	14,14,15	0.42	0	17,19,21	0.75	1 (5%)
12	NO3	A	1030	-	1,3,3	3.21	1 (100%)	0,3,3	-	-
12	NO3	A	1029	-	1,3,3	3.36	1 (100%)	0,3,3	-	-

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
10	NAG	B	706	2	-	0/6/23/26	0/1/1/1
10	NAG	B	701	2	-	2/6/23/26	0/1/1/1
10	NAG	A	1016	1	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1029	NO3	O1-N	3.36	1.40	1.24
12	A	1030	NO3	O1-N	3.21	1.40	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	701	NAG	C1-O5-C5	2.73	115.85	112.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
10	A	1016	NAG	O5-C5-C6-O6
10	A	1016	NAG	C4-C5-C6-O6
10	B	701	NAG	C4-C5-C6-O6
10	B	701	NAG	O5-C5-C6-O6
10	A	1016	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	915/962 (95%)	-0.27	11 (1%) 76 55	52, 165, 260, 296	0
2	B	687/692 (99%)	-0.27	1 (0%) 92 88	55, 145, 303, 428	0
3	L	214/214 (100%)	-0.39	0 100 100	71, 127, 234, 297	0
4	H	218/218 (100%)	-0.17	3 (1%) 73 52	81, 154, 242, 329	0
All	All	2034/2086 (97%)	-0.27	15 (0%) 84 67	52, 149, 274, 428	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	683	LEU	4.6
4	H	131	PRO	3.6
1	A	681	CYS	3.3
1	A	822	CYS	2.9
2	B	654	ASN	2.8

### 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	NAG	A	1016	14/15	0.54	0.10	190,203,212,212	0
10	NAG	B	706	14/15	0.70	0.09	145,154,161,162	0
10	NAG	B	701	14/15	0.72	0.08	120,143,162,168	0
11	MN	B	707	1/1	0.85	0.11	271,271,271,271	0
11	MN	A	1025	1/1	0.88	0.09	241,241,241,241	0
12	NO3	A	1029	4/4	0.93	0.09	95,98,100,103	0
11	MN	A	1027	1/1	0.94	0.07	187,187,187,187	0
11	MN	A	1026	1/1	0.97	0.06	181,181,181,181	0
12	NO3	A	1030	4/4	0.97	0.09	81,83,84,87	0
11	MN	A	1028	1/1	0.98	0.05	169,169,169,169	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.