



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 19, 2024 – 12:09 PM EDT

PDB ID : 4ZNE  
Title : IgG1 Fc-FcγRI ecd complex  
Authors : Oganessian, V.Y.; Dall'Acqua, W.F.  
Deposited on : 2015-05-04  
Resolution : 2.42 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](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

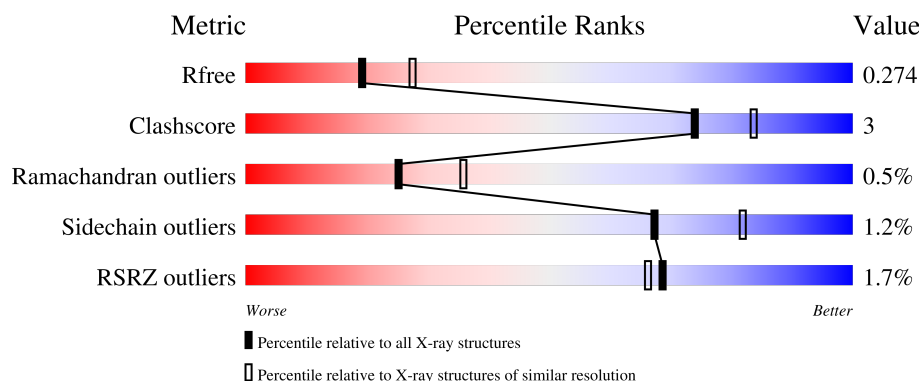
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 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.



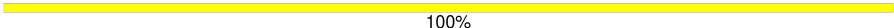

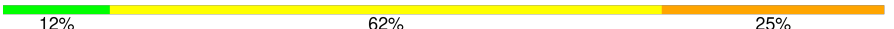
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	5670 (2.44-2.40)
Clashscore	180529	6299 (2.44-2.40)
Ramachandran outliers	177936	6232 (2.44-2.40)
Sidechain outliers	177891	6233 (2.44-2.40)
RSRZ outliers	164620	5670 (2.44-2.40)

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	267	 3% 78% 11% • 9%
2	E	227	 93% • 5%
2	J	227	 83% 9% 8%
3	B	3	 100%
4	C	2	 50% 50%

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Mol	Chain	Length	Quality of chain
5	D	2	 100%
6	F	8	 12% 88%
6	G	8	 12% 62% 25%

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
5	NAG	D	2	X	-	-	-
6	MAN	F	3	X	-	-	-
6	MAN	G	3	X	-	-	-
7	NAG	A	305	X	-	-	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5767 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.

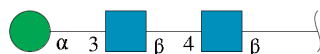
- Molecule 1 is a protein called High affinity immunoglobulin gamma Fc receptor I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1932	1228	333	363	8			

- Molecule 2 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	215	Total	C	N	O	S	0	0	0
			1711	1090	287	328	6			
2	J	209	Total	C	N	O	S	0	0	0
			1668	1061	281	320	6			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



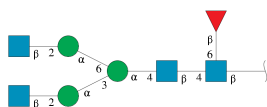
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	2	Total	C	N	O	0	0	0
			25	14	1	10			

- Molecule 5 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
5	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	8	Total	C	N	O	0	0	0
			99	56	4	39			
6	G	8	Total	C	N	O	0	0	0
			99	56	4	39			

- Molecule 7 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
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Zn	0	0
			1	1		
8	E	1	Total	Zn	0	0
			1	1		
8	J	1	Total	Zn	0	0
			1	1		

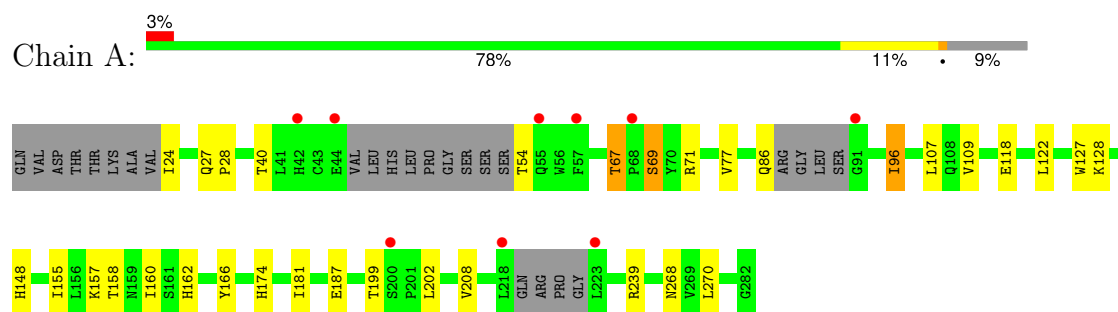
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	16	Total	O	0	0
			16	16		
9	E	64	Total	O	0	0
			64	64		
9	J	55	Total	O	0	0
			55	55		

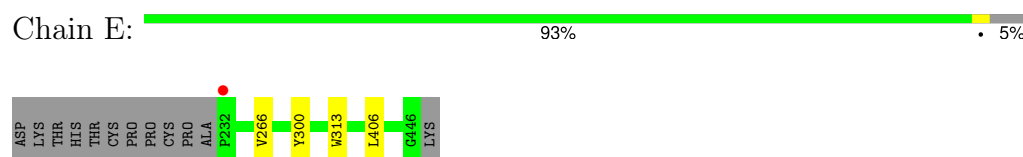
### 3 Residue-property plots [i](#)

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 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.

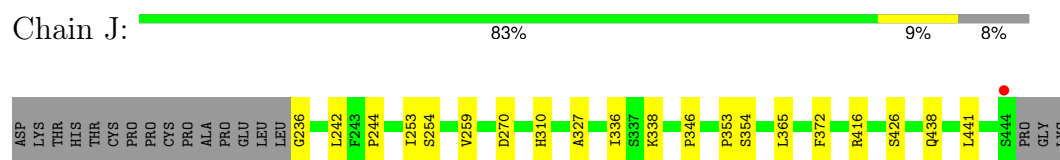
- Molecule 1: High affinity immunoglobulin gamma Fc receptor I



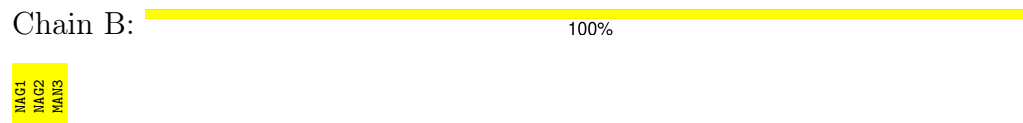
- Molecule 2: Ig gamma-1 chain C region



- Molecule 2: Ig gamma-1 chain C region



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



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



MAG1  
MAG2

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

Chain D:  100%


MAG1  
MAG2

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

Chain F:  12% 88%

MAG1  
MAG2  
MAN3  
MAN4  
MAG5  
MAG6  
MAG7  
FUL8

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

Chain G:  12% 62% 25%

MAG1  
MAG2  
MAN3  
MAN4  
MAG5  
MAG6  
MAG7  
FUL8



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.74Å 126.75Å 71.84Å 90.00° 118.44° 90.00°	Depositor
Resolution (Å)	86.55 – 2.42 86.55 – 2.42	Depositor EDS
% Data completeness (in resolution range)	98.6 (86.55-2.42) 98.7 (86.55-2.42)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.201 , 0.254 0.228 , 0.274	Depositor DCC
$R_{free}$ test set	1947 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.0	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 25.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5767	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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: FUL, NAG, ZN, 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	0.67	0/1976	0.72	0/2680
2	E	0.67	1/1759 (0.1%)	0.70	0/2397
2	J	0.66	0/1714	0.68	1/2335 (0.0%)
All	All	0.66	1/5449 (0.0%)	0.70	1/7412 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	313	TRP	CD2-CE2	5.70	1.48	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	416	ARG	NE-CZ-NH2	-5.31	117.64	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	THR	Peptide
1	A	27	GLN	Peptide

## 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	1932	0	1887	18	0
2	E	1711	0	1679	2	0
2	J	1668	0	1633	14	0
3	B	39	0	34	0	0
4	C	25	0	22	0	0
5	D	28	0	25	0	0
6	F	99	0	85	0	0
6	G	99	0	85	1	0
7	A	28	0	26	0	0
8	A	1	0	0	0	0
8	E	1	0	0	0	0
8	J	1	0	0	0	0
9	A	16	0	0	1	0
9	E	64	0	0	0	0
9	J	55	0	0	1	0
All	All	5767	0	5476	33	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 3.

All (33) 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:J:244:PRO:HB3	2:J:336:ILE:HD11	1.78	0.66
1:A:67:THR:HG22	1:A:69:SER:H	1.60	0.66
1:A:109:VAL:HG12	1:A:122:LEU:HD23	1.77	0.65
1:A:107:LEU:HD21	1:A:166:TYR:HB3	1.80	0.64
1:A:174:HIS:ND1	9:A:401:HOH:O	2.32	0.59
1:A:24:ILE:HB	1:A:96:ILE:HD12	1.86	0.56
1:A:270:LEU:C	1:A:270:LEU:HD23	2.27	0.54
1:A:109:VAL:HG13	1:A:181:ILE:CD1	2.38	0.54
2:J:353:PRO:HD3	2:J:365:LEU:HD23	1.91	0.52
6:G:1:NAG:H61	6:G:8:FUL:O2	2.10	0.51
2:E:406:LEU:C	2:E:406:LEU:HD12	2.32	0.50
1:A:40:THR:HG22	1:A:71:ARG:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:HIS:HB3	2:J:236:GLY:HA3	1.95	0.49
1:A:160:ILE:HD11	1:A:187:GLU:N	2.29	0.48
1:A:67:THR:HG22	1:A:69:SER:N	2.28	0.48
2:J:346:PRO:HB3	2:J:372:PHE:HB3	1.95	0.48
2:J:253:ILE:CD1	2:J:310:HIS:CD2	2.97	0.47
2:E:266:VAL:HB	2:E:300:TYR:HB2	1.98	0.46
1:A:118:GLU:O	1:A:158:THR:HG23	2.16	0.46
1:A:148:HIS:HB3	2:J:236:GLY:CA	2.47	0.45
2:J:338:LYS:NZ	9:J:602:HOH:O	2.38	0.45
2:J:426:SER:CB	2:J:438:GLN:HG2	2.47	0.44
1:A:155:ILE:HG21	1:A:162:HIS:CD2	2.53	0.44
2:J:426:SER:HB3	2:J:438:GLN:HG2	2.00	0.44
2:J:242:LEU:HD11	2:J:259:VAL:CG1	2.48	0.43
1:A:157:LYS:HE2	1:A:268:ASN:HB2	1.99	0.43
2:J:353:PRO:HD3	2:J:365:LEU:CD2	2.49	0.43
1:A:107:LEU:CD2	1:A:166:TYR:HB3	2.48	0.43
2:J:270:ASP:OD1	2:J:327:ALA:HB2	2.19	0.42
2:J:365:LEU:HB3	2:J:441:LEU:HD23	2.01	0.42
1:A:54:THR:HG23	1:A:86:GLN:O	2.21	0.41
1:A:127:TRP:CE3	1:A:128:LYS:HE2	2.56	0.41
2:J:253:ILE:HD13	2:J:310:HIS:CD2	2.57	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	234/267 (88%)	224 (96%)	7 (3%)	3 (1%)	10	13
2	E	213/227 (94%)	210 (99%)	3 (1%)	0	100	100
2	J	207/227 (91%)	201 (97%)	6 (3%)	0	100	100
All	All	654/721 (91%)	635 (97%)	16 (2%)	3 (0%)	25	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	PRO
1	A	239	ARG
1	A	67	THR

### 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	215/236 (91%)	210 (98%)	5 (2%)	45	64
2	E	199/210 (95%)	199 (100%)	0	100	100
2	J	194/210 (92%)	192 (99%)	2 (1%)	73	85
All	All	608/656 (93%)	601 (99%)	7 (1%)	67	82

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	SER
1	A	77	VAL
1	A	96	ILE
1	A	202	LEU
1	A	208	VAL
2	J	254	SER
2	J	354	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	ASN
2	E	361	ASN
2	E	389	ASN
2	E	438	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

15 non-standard protein/DNA/RNA residues 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
6	NAG	F	7	6	14,14,15	0.75	0	17,19,21	0.98	1 (5%)
3	NAG	B	2	3	14,14,15	0.88	0	17,19,21	2.29	6 (35%)
5	NAG	D	2	5	14,14,15	1.48	2 (14%)	17,19,21	2.17	5 (29%)
6	NAG	F	2	6	14,14,15	0.52	0	17,19,21	1.54	3 (17%)
6	NAG	G	1	2,6	14,14,15	0.57	0	17,19,21	1.88	4 (23%)
7	NAG	A	305	1	14,14,15	1.33	1 (7%)	17,19,21	1.77	4 (23%)
6	NAG	F	1	2,6	14,14,15	0.51	0	17,19,21	1.86	2 (11%)
5	NAG	D	1	1,5	14,14,15	0.79	0	17,19,21	1.72	4 (23%)
3	NAG	B	1	3,1	14,14,15	0.67	0	17,19,21	1.58	3 (17%)
7	NAG	A	304	1	14,14,15	0.60	0	17,19,21	1.69	5 (29%)
6	NAG	G	5	6	14,14,15	0.54	0	17,19,21	1.11	2 (11%)
6	NAG	G	7	6	14,14,15	0.50	0	17,19,21	1.28	2 (11%)
6	NAG	F	5	6	14,14,15	0.51	0	17,19,21	0.94	0
6	NAG	G	2	6	14,14,15	0.63	0	17,19,21	1.05	1 (5%)
4	NAG	C	1	4,1	14,14,15	0.66	0	17,19,21	1.26	2 (11%)

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	F	7	6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	2	3	-	4/6/23/26	0/1/1/1
5	NAG	D	2	5	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1
6	NAG	G	1	2,6	-	2/6/23/26	0/1/1/1
7	NAG	A	305	1	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	F	1	2,6	-	0/6/23/26	0/1/1/1
5	NAG	D	1	1,5	-	2/6/23/26	0/1/1/1
3	NAG	B	1	3,1	-	0/6/23/26	0/1/1/1
7	NAG	A	304	1	-	0/6/23/26	0/1/1/1
6	NAG	G	5	6	-	2/6/23/26	0/1/1/1
6	NAG	G	7	6	-	2/6/23/26	0/1/1/1
6	NAG	F	5	6	-	4/6/23/26	0/1/1/1
6	NAG	G	2	6	-	2/6/23/26	0/1/1/1
4	NAG	C	1	4,1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	305	NAG	C1-C2	3.73	1.57	1.52
5	D	2	NAG	C1-C2	3.35	1.56	1.52
5	D	2	NAG	C3-C2	2.08	1.56	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	NAG	C1-O5-C5	7.07	121.67	112.19
6	F	1	NAG	C1-O5-C5	5.63	119.73	112.19
5	D	2	NAG	C4-C3-C2	5.10	118.49	111.02
6	G	1	NAG	C1-O5-C5	5.03	118.92	112.19
7	A	305	NAG	C4-C3-C2	4.67	117.86	111.02
5	D	2	NAG	C1-O5-C5	3.72	117.17	112.19
7	A	305	NAG	O5-C1-C2	3.62	116.89	111.29
6	G	1	NAG	O5-C5-C6	3.41	114.29	107.66
3	B	1	NAG	C1-O5-C5	3.40	116.74	112.19
6	G	1	NAG	C6-C5-C4	-3.38	104.72	113.02
5	D	1	NAG	C4-C3-C2	3.36	115.95	111.02
5	D	1	NAG	C2-N2-C7	3.25	127.26	122.90
6	F	2	NAG	C2-N2-C7	3.20	127.19	122.90
7	A	304	NAG	C1-C2-N2	3.17	115.42	110.43
5	D	2	NAG	C2-N2-C7	3.14	127.11	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	7	NAG	O5-C5-C6	3.10	113.69	107.66
3	B	2	NAG	O3-C3-C2	3.07	115.78	109.40
5	D	1	NAG	C1-C2-N2	3.07	115.26	110.43
5	D	2	NAG	C3-C4-C5	3.04	115.73	110.23
7	A	304	NAG	O5-C1-C2	-3.03	106.60	111.29
7	A	304	NAG	C4-C3-C2	2.99	115.40	111.02
4	C	1	NAG	C4-C3-C2	2.93	115.31	111.02
3	B	1	NAG	O5-C1-C2	-2.92	106.77	111.29
6	F	2	NAG	O7-C7-N2	2.92	127.14	121.98
3	B	2	NAG	C3-C4-C5	2.91	115.51	110.23
5	D	2	NAG	O5-C5-C4	2.80	117.63	110.83
3	B	1	NAG	C1-C2-N2	2.59	114.52	110.43
4	C	1	NAG	O5-C5-C4	-2.54	104.65	110.83
6	F	7	NAG	C4-C3-C2	-2.51	107.34	111.02
6	G	2	NAG	O7-C7-C8	-2.46	117.68	122.05
6	F	1	NAG	C6-C5-C4	-2.44	107.03	113.02
7	A	304	NAG	C1-O5-C5	2.44	115.45	112.19
7	A	305	NAG	C3-C4-C5	2.39	114.57	110.23
6	G	5	NAG	C3-C4-C5	2.37	114.53	110.23
3	B	2	NAG	C2-N2-C7	2.36	126.06	122.90
6	G	1	NAG	O6-C6-C5	2.31	119.21	111.33
3	B	2	NAG	C4-C3-C2	-2.31	107.63	111.02
7	A	305	NAG	C2-N2-C7	2.30	125.98	122.90
6	G	7	NAG	O5-C1-C2	-2.27	107.77	111.29
6	F	2	NAG	O7-C7-C8	-2.27	118.02	122.05
5	D	1	NAG	O7-C7-N2	2.25	125.96	121.98
6	G	5	NAG	C8-C7-N2	2.20	119.77	116.12
7	A	304	NAG	C3-C4-C5	2.05	113.94	110.23
3	B	2	NAG	O5-C5-C4	2.03	115.77	110.83

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	305	NAG	C1
5	D	2	NAG	C1

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1	NAG	C1-C2-N2-C7
6	G	7	NAG	O5-C5-C6-O6
3	B	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	G	1	NAG	O5-C5-C6-O6
6	G	7	NAG	C4-C5-C6-O6
6	F	5	NAG	C4-C5-C6-O6
6	G	1	NAG	C4-C5-C6-O6
3	B	2	NAG	C4-C5-C6-O6
6	G	2	NAG	O5-C5-C6-O6
6	F	5	NAG	C8-C7-N2-C2
6	F	5	NAG	O7-C7-N2-C2
6	G	5	NAG	C8-C7-N2-C2
6	G	5	NAG	O7-C7-N2-C2
6	F	5	NAG	O5-C5-C6-O6
6	G	2	NAG	C4-C5-C6-O6
5	D	1	NAG	C3-C2-N2-C7
3	B	2	NAG	C1-C2-N2-C7
5	D	2	NAG	C1-C2-N2-C7
3	B	2	NAG	C3-C2-N2-C7
5	D	2	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	1	NAG	1	0

## 5.5 Carbohydrates

23 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	3,1	14,14,15	0.67	0	17,19,21	1.58	3 (17%)
3	NAG	B	2	3	14,14,15	0.88	0	17,19,21	2.29	6 (35%)
3	MAN	B	3	3	11,11,12	0.73	0	15,15,17	2.51	3 (20%)
4	NAG	C	1	4,1	14,14,15	0.66	0	17,19,21	1.26	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MAN	C	2	4	11,11,12	0.60	0	15,15,17	0.74	0
5	NAG	D	1	1,5	14,14,15	0.79	0	17,19,21	1.72	4 (23%)
5	NAG	D	2	5	14,14,15	1.48	2 (14%)	17,19,21	2.17	5 (29%)
6	NAG	F	1	2,6	14,14,15	0.51	0	17,19,21	1.86	2 (11%)
6	NAG	F	2	6	14,14,15	0.52	0	17,19,21	1.54	3 (17%)
6	MAN	F	3	6	11,11,12	0.31	0	15,15,17	1.26	2 (13%)
6	MAN	F	4	6	11,11,12	0.82	0	15,15,17	0.93	1 (6%)
6	NAG	F	5	6	14,14,15	0.51	0	17,19,21	0.94	0
6	MAN	F	6	6	11,11,12	0.77	0	15,15,17	1.23	1 (6%)
6	NAG	F	7	6	14,14,15	0.75	0	17,19,21	0.98	1 (5%)
6	FUL	F	8	6	10,10,11	0.82	0	14,14,16	2.36	4 (28%)
6	NAG	G	1	2,6	14,14,15	0.57	0	17,19,21	1.88	4 (23%)
6	NAG	G	2	6	14,14,15	0.63	0	17,19,21	1.05	1 (5%)
6	MAN	G	3	6	11,11,12	0.33	0	15,15,17	1.30	1 (6%)
6	MAN	G	4	6	11,11,12	0.69	0	15,15,17	0.98	1 (6%)
6	NAG	G	5	6	14,14,15	0.54	0	17,19,21	1.11	2 (11%)
6	MAN	G	6	6	11,11,12	0.62	0	15,15,17	0.93	0
6	NAG	G	7	6	14,14,15	0.50	0	17,19,21	1.28	2 (11%)
6	FUL	G	8	6	10,10,11	0.59	0	14,14,16	1.83	5 (35%)

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	3,1	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	4/6/23/26	0/1/1/1
3	MAN	B	3	3	-	1/2/19/22	0/1/1/1
4	NAG	C	1	4,1	-	0/6/23/26	0/1/1/1
4	MAN	C	2	4	-	0/2/19/22	0/1/1/1
5	NAG	D	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	D	2	5	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	F	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1
6	MAN	F	3	6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	F	4	6	-	2/2/19/22	0/1/1/1
6	NAG	F	5	6	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	F	6	6	-	0/2/19/22	0/1/1/1
6	NAG	F	7	6	-	0/6/23/26	0/1/1/1
6	FUL	F	8	6	-	-	0/1/1/1
6	NAG	G	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	G	2	6	-	2/6/23/26	0/1/1/1
6	MAN	G	3	6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	G	4	6	-	2/2/19/22	0/1/1/1
6	NAG	G	5	6	-	2/6/23/26	0/1/1/1
6	MAN	G	6	6	-	0/2/19/22	0/1/1/1
6	NAG	G	7	6	-	2/6/23/26	0/1/1/1
6	FUL	G	8	6	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	2	NAG	C1-C2	3.35	1.56	1.52
5	D	2	NAG	C3-C2	2.08	1.56	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3	MAN	C1-O5-C5	7.31	121.98	112.19
3	B	2	NAG	C1-O5-C5	7.07	121.67	112.19
6	F	1	NAG	C1-O5-C5	5.63	119.73	112.19
5	D	2	NAG	C4-C3-C2	5.10	118.49	111.02
3	B	3	MAN	C1-C2-C3	5.07	117.03	109.64
6	G	1	NAG	C1-O5-C5	5.03	118.92	112.19
6	F	8	FUL	C1-C2-C3	4.62	116.37	109.64
6	G	8	FUL	C1-C2-C3	-4.01	103.81	109.64
6	F	8	FUL	O3-C3-C2	-3.97	101.96	110.05
6	F	8	FUL	C1-O5-C5	3.85	122.04	112.97
5	D	2	NAG	C1-O5-C5	3.72	117.17	112.19
6	F	8	FUL	O5-C1-C2	3.41	118.92	110.79
6	G	1	NAG	O5-C5-C6	3.41	114.29	107.66
6	F	6	MAN	O2-C2-C3	-3.40	103.11	110.15
3	B	1	NAG	C1-O5-C5	3.40	116.74	112.19
6	G	1	NAG	C6-C5-C4	-3.38	104.72	113.02
5	D	1	NAG	C4-C3-C2	3.36	115.95	111.02
5	D	1	NAG	C2-N2-C7	3.25	127.26	122.90
6	F	2	NAG	C2-N2-C7	3.20	127.19	122.90
5	D	2	NAG	C2-N2-C7	3.14	127.11	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	3	MAN	C1-C2-C3	3.10	114.16	109.64
6	G	7	NAG	O5-C5-C6	3.10	113.69	107.66
3	B	2	NAG	O3-C3-C2	3.07	115.78	109.40
5	D	1	NAG	C1-C2-N2	3.07	115.26	110.43
5	D	2	NAG	C3-C4-C5	3.04	115.73	110.23
4	C	1	NAG	C4-C3-C2	2.93	115.31	111.02
3	B	1	NAG	O5-C1-C2	-2.92	106.77	111.29
6	F	2	NAG	O7-C7-N2	2.92	127.14	121.98
6	G	8	FUL	O2-C2-C1	2.92	115.91	109.22
3	B	2	NAG	C3-C4-C5	2.91	115.51	110.23
5	D	2	NAG	O5-C5-C4	2.80	117.63	110.83
6	G	8	FUL	O5-C1-C2	-2.77	104.18	110.79
6	F	4	MAN	O2-C2-C3	-2.71	104.53	110.15
3	B	1	NAG	C1-C2-N2	2.59	114.52	110.43
6	F	3	MAN	O4-C4-C3	-2.56	104.34	110.38
6	F	3	MAN	C1-O5-C5	2.54	115.59	112.19
4	C	1	NAG	O5-C5-C4	-2.54	104.65	110.83
6	F	7	NAG	C4-C3-C2	-2.51	107.34	111.02
3	B	3	MAN	O5-C1-C2	2.49	116.73	110.79
6	G	2	NAG	O7-C7-C8	-2.46	117.68	122.05
6	F	1	NAG	C6-C5-C4	-2.44	107.03	113.02
6	G	4	MAN	O2-C2-C3	-2.40	105.18	110.15
6	G	5	NAG	C3-C4-C5	2.37	114.53	110.23
3	B	2	NAG	C2-N2-C7	2.36	126.06	122.90
6	G	1	NAG	O6-C6-C5	2.31	119.21	111.33
3	B	2	NAG	C4-C3-C2	-2.31	107.63	111.02
6	G	7	NAG	O5-C1-C2	-2.27	107.77	111.29
6	F	2	NAG	O7-C7-C8	-2.27	118.02	122.05
5	D	1	NAG	O7-C7-N2	2.25	125.96	121.98
6	G	5	NAG	C8-C7-N2	2.20	119.77	116.12
6	G	8	FUL	O5-C5-C6	2.16	112.09	107.40
6	G	8	FUL	C2-C3-C4	-2.05	107.25	110.86
3	B	2	NAG	O5-C5-C4	2.03	115.77	110.83

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	D	2	NAG	C1
6	F	3	MAN	C1
6	G	3	MAN	C1

All (25) torsion outliers are listed below:

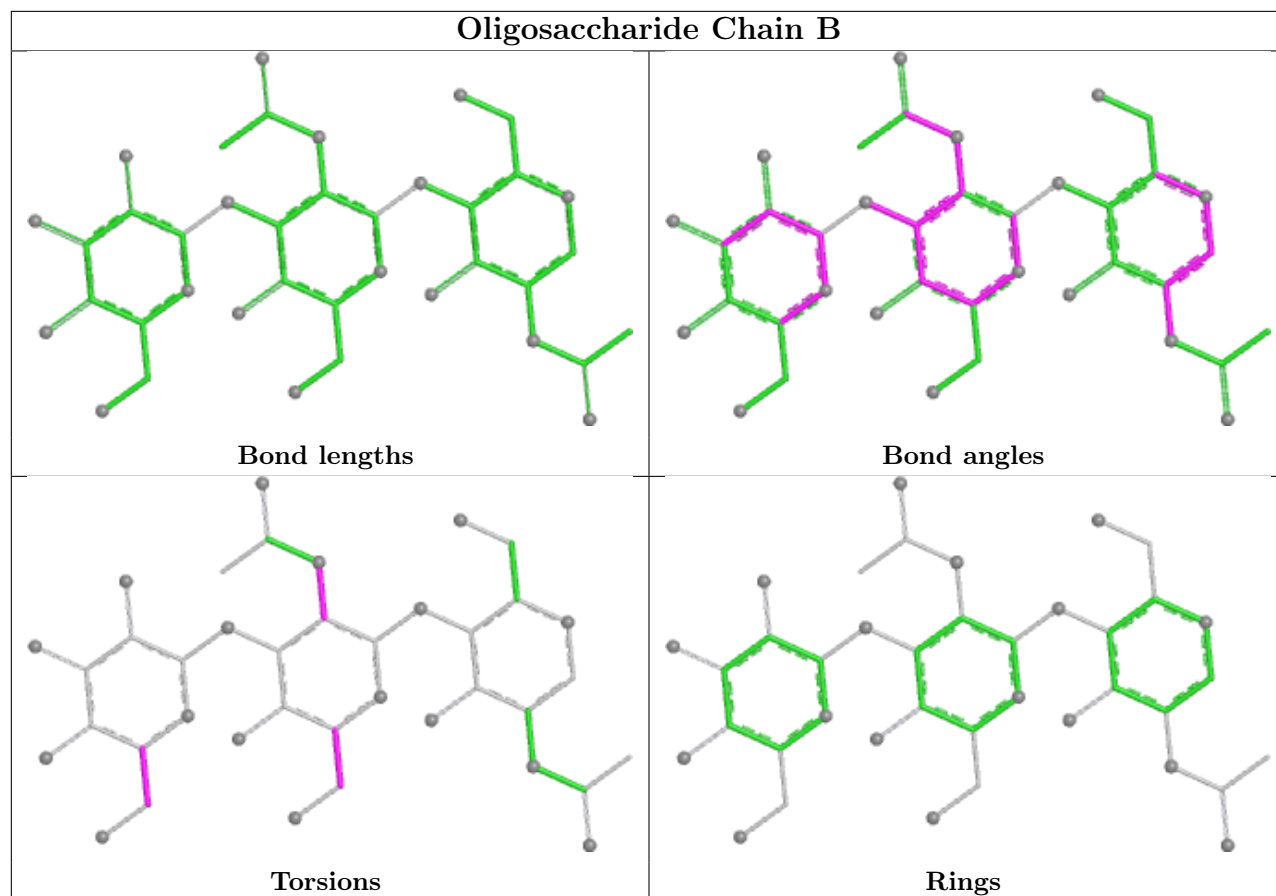
Mol	Chain	Res	Type	Atoms
5	D	1	NAG	C1-C2-N2-C7
6	G	7	NAG	O5-C5-C6-O6
6	G	4	MAN	O5-C5-C6-O6
3	B	2	NAG	O5-C5-C6-O6
6	G	1	NAG	O5-C5-C6-O6
6	F	4	MAN	O5-C5-C6-O6
6	G	7	NAG	C4-C5-C6-O6
6	F	4	MAN	C4-C5-C6-O6
6	G	4	MAN	C4-C5-C6-O6
6	F	5	NAG	C4-C5-C6-O6
6	G	1	NAG	C4-C5-C6-O6
3	B	2	NAG	C4-C5-C6-O6
6	G	2	NAG	O5-C5-C6-O6
6	F	5	NAG	C8-C7-N2-C2
6	F	5	NAG	O7-C7-N2-C2
6	G	5	NAG	C8-C7-N2-C2
6	G	5	NAG	O7-C7-N2-C2
6	F	5	NAG	O5-C5-C6-O6
6	G	2	NAG	C4-C5-C6-O6
3	B	3	MAN	O5-C5-C6-O6
5	D	1	NAG	C3-C2-N2-C7
3	B	2	NAG	C1-C2-N2-C7
5	D	2	NAG	C1-C2-N2-C7
3	B	2	NAG	C3-C2-N2-C7
5	D	2	NAG	C3-C2-N2-C7

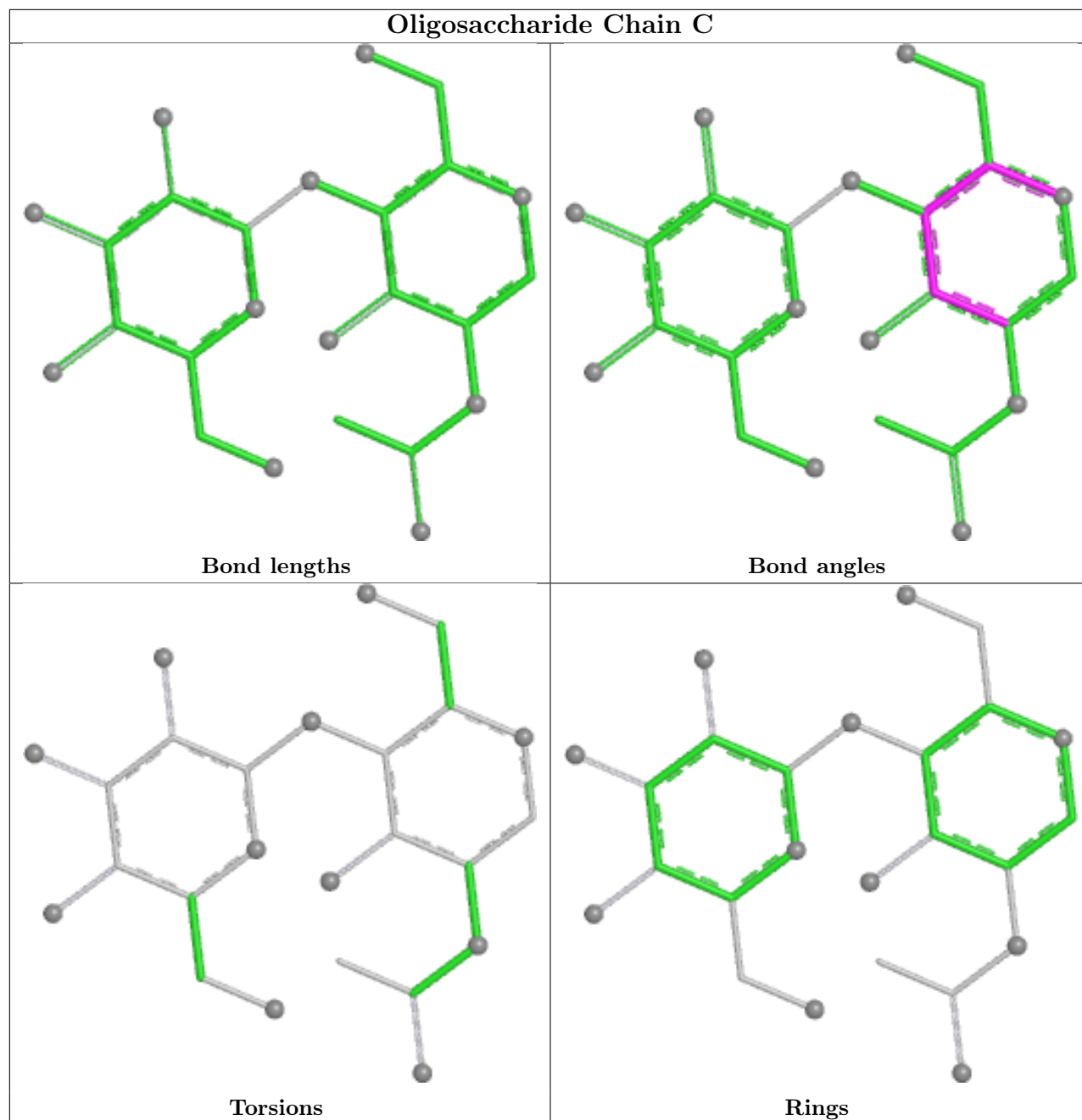
There are no ring outliers.

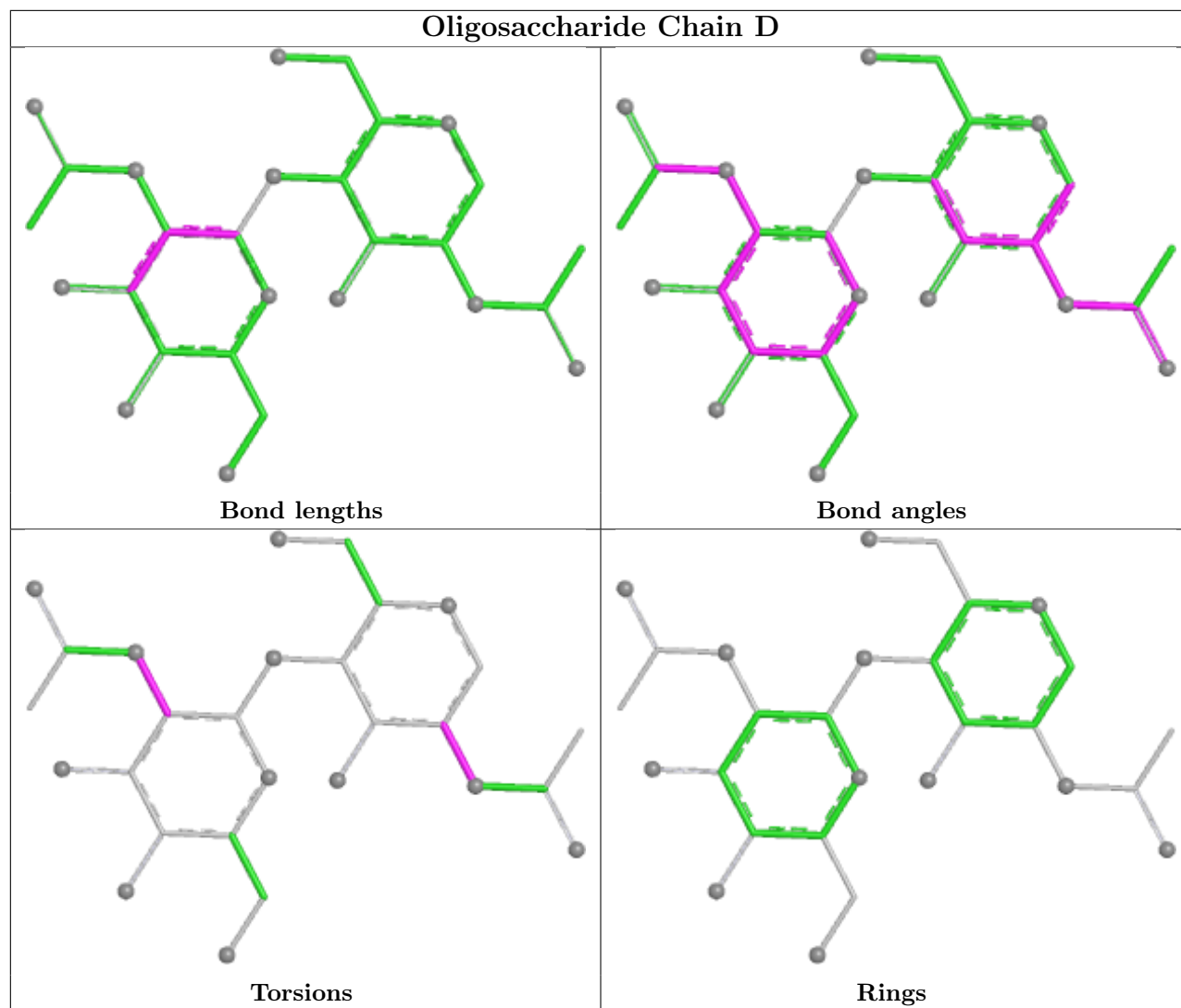
2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	1	NAG	1	0
6	G	8	FUL	1	0

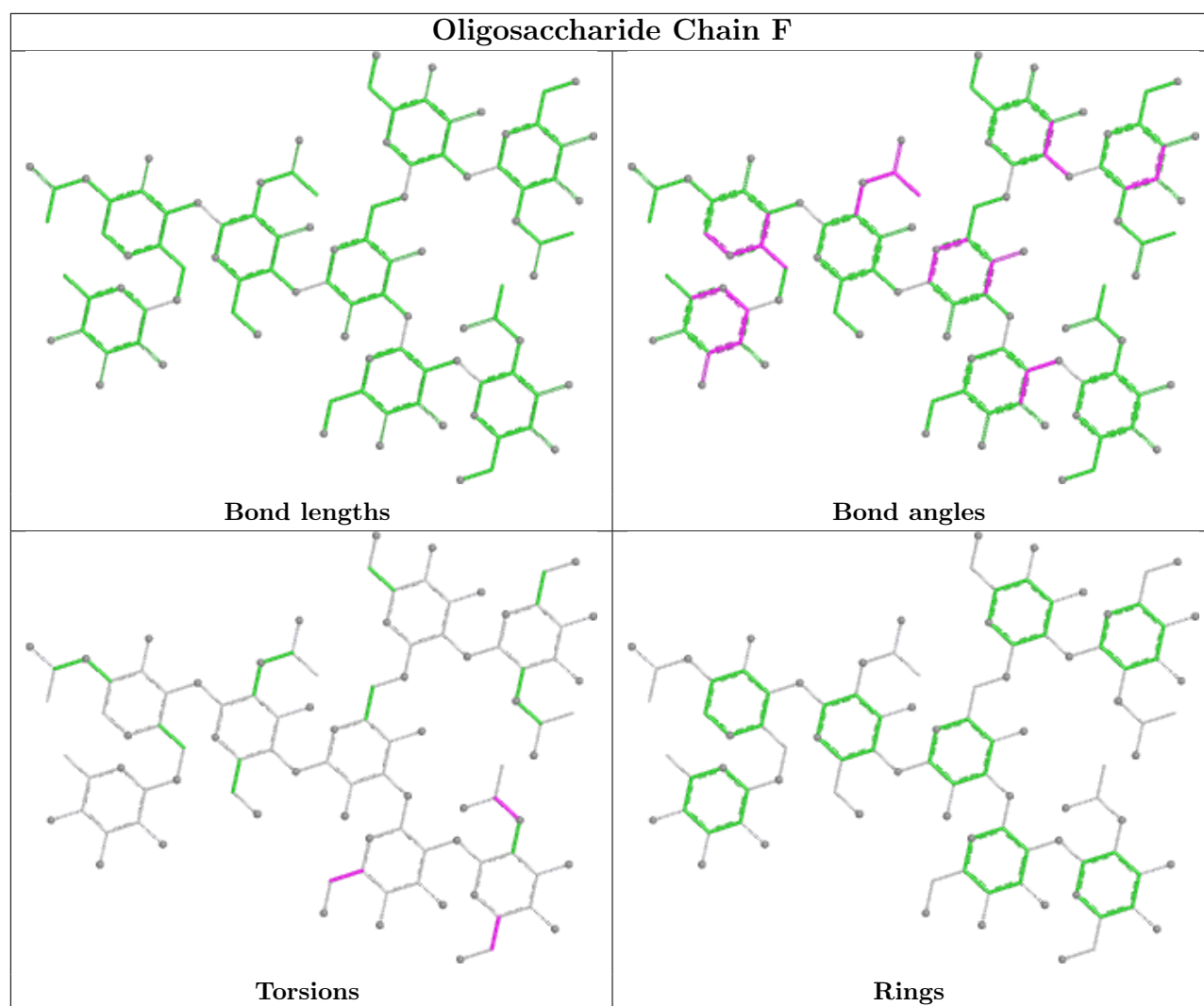
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

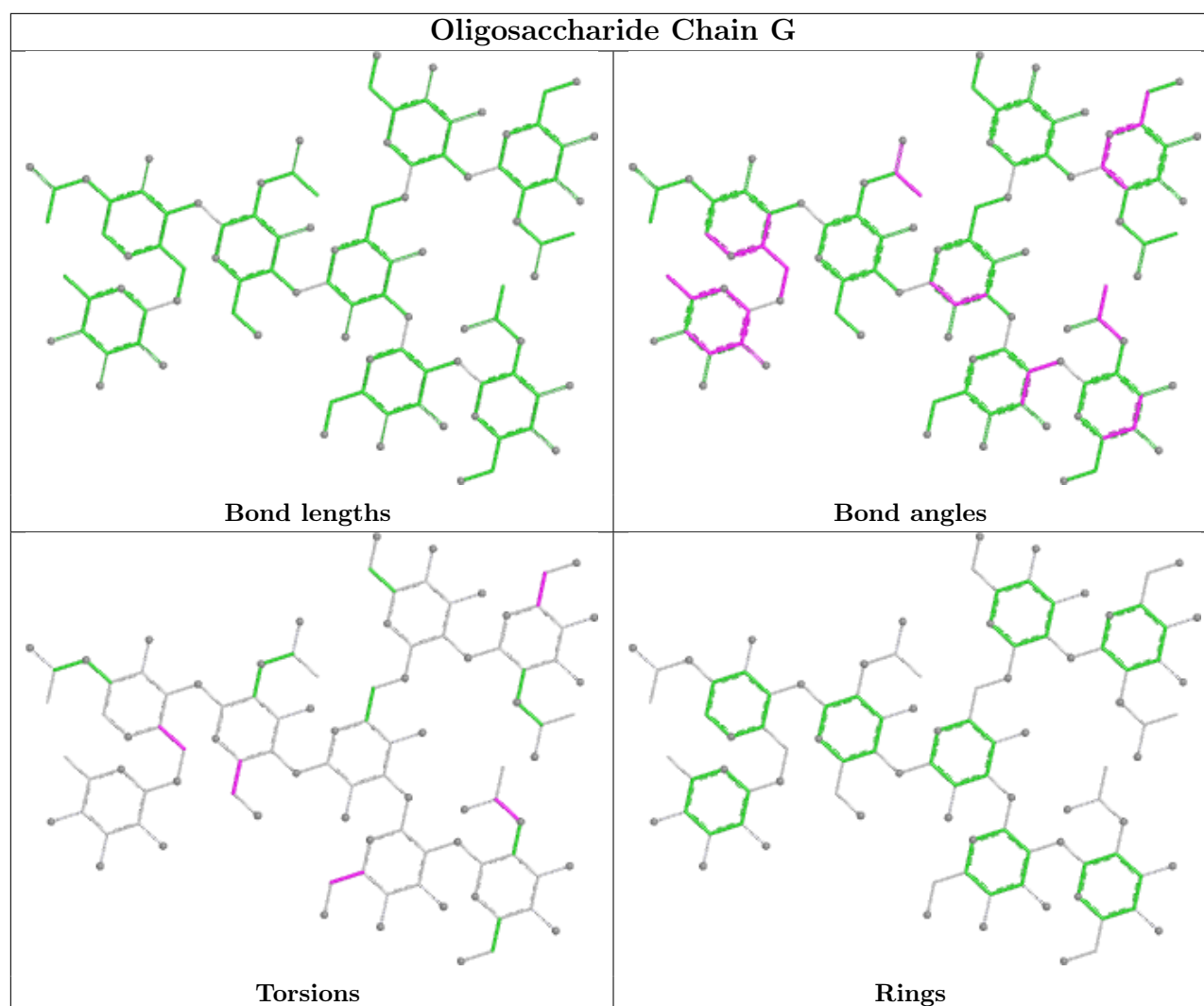












## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\# Z  > 2$
7	NAG	A	305	1	14,14,15	1.33	1 (7%)	17,19,21	1.77	4 (23%)
7	NAG	A	304	1	14,14,15	0.60	0	17,19,21	1.69	5 (29%)

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
7	NAG	A	305	1	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	A	304	1	-	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)
7	A	305	NAG	C1-C2	3.73	1.57	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	305	NAG	C4-C3-C2	4.67	117.86	111.02
7	A	305	NAG	O5-C1-C2	3.62	116.89	111.29
7	A	304	NAG	C1-C2-N2	3.17	115.42	110.43
7	A	304	NAG	O5-C1-C2	-3.03	106.60	111.29
7	A	304	NAG	C4-C3-C2	2.99	115.40	111.02
7	A	304	NAG	C1-O5-C5	2.44	115.45	112.19
7	A	305	NAG	C3-C4-C5	2.39	114.57	110.23
7	A	305	NAG	C2-N2-C7	2.30	125.98	122.90
7	A	304	NAG	C3-C4-C5	2.05	113.94	110.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	305	NAG	C1

There are no torsion outliers.

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 ⓘ

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	242/267 (90%)	0.18	9 (3%)	45 43	20, 38, 58, 72	0
2	E	215/227 (94%)	-0.25	1 (0%)	87 86	25, 34, 48, 60	0
2	J	209/227 (92%)	-0.25	1 (0%)	87 86	24, 35, 50, 73	0
All	All	666/721 (92%)	-0.09	11 (1%)	69 66	20, 35, 55, 73	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	LEU	4.3
1	A	218	LEU	3.4
1	A	91	GLY	3.3
2	J	444	SER	2.8
2	E	232	PRO	2.7
1	A	44	GLU	2.5
1	A	200	SER	2.3
1	A	55	GLN	2.2
1	A	57	PHE	2.2
1	A	68	PRO	2.0
1	A	42	HIS	2.0

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

MODRES-RSR INFOmissingINFO

### 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(Å <sup>2</sup> )	Q<0.9
7	NAG	A	305	14/15	0.53	0.23	85,108,125,126	0
7	NAG	A	304	14/15	0.58	0.20	104,121,131,131	0
8	ZN	J	509	1/1	0.97	0.15	47,47,47,47	0
8	ZN	A	310	1/1	0.98	0.10	67,67,67,67	0
8	ZN	E	509	1/1	0.99	0.12	49,49,49,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.