



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 5, 2025 – 04:14 pm BST

PDB ID : 9GHJ / pdb\_00009ghj  
Title : Junin virus GP1-GP2 heterodimer in complex with Fab of JUN1  
Authors : Bowden, T.A.; Paesen, G.C.  
Deposited on : 2024-08-15  
Resolution : 2.09 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 : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
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) : 2.43.1

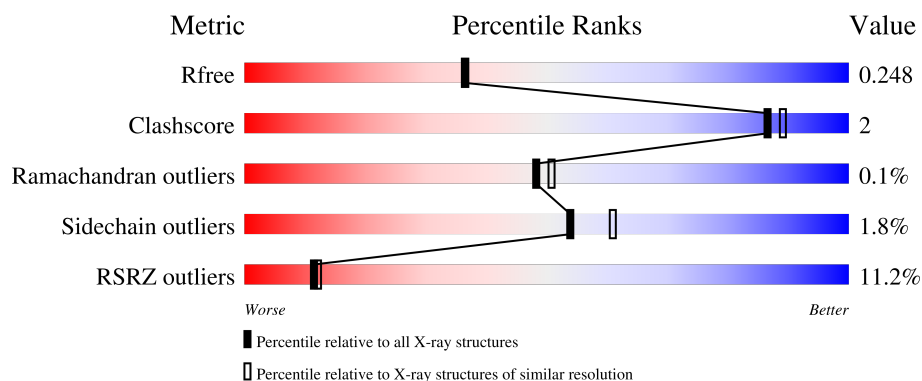
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.09 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.




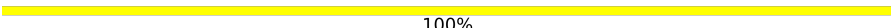


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	193	<div> <div>6%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>6%</div> </div> </div>
2	B	203	<div> <div>10%</div> <div> <div></div> <div>66%</div> <div>•</div> <div>30%</div> </div> </div>
3	H	242	<div> <div>7%</div> <div> <div></div> <div>87%</div> <div>5%</div> <div>8%</div> </div> </div>
4	L	217	<div> <div>17%</div> <div> <div></div> <div>92%</div> <div>6%</div> <div>•</div> </div> </div>
5	C	4	<div> <div></div> <div> <div>25%</div> <div>75%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
6	D	3	 67% 33%
7	E	4	 100%
8	F	2	 50% 50%
8	G	2	 50% 50%

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12252 atoms, of which 5889 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 Pre-glycoprotein polyprotein GP complex.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	181	2857	938	1396	249	262	12	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	CYS	LEU	engineered mutation	UNP C1K9J9
A	249	ARG	SER	engineered mutation	UNP C1K9J9
A	250	ARG	LEU	engineered mutation	UNP C1K9J9
A	251	ARG	LYS	engineered mutation	UNP C1K9J9

- Molecule 2 is a protein called Glycoprotein G2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	143	2313	754	1139	193	214	13	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	321	PRO	GLU	engineered mutation	UNP P26313
B	329	CYS	MET	engineered mutation	UNP P26313
B	417	SER	-	expression tag	UNP P26313
B	418	GLY	-	expression tag	UNP P26313
B	419	ASP	-	expression tag	UNP P26313
B	420	ASP	-	expression tag	UNP P26313
B	421	ASP	-	expression tag	UNP P26313
B	422	ASP	-	expression tag	UNP P26313
B	423	LYS	-	expression tag	UNP P26313
B	424	GLY	-	expression tag	UNP P26313
B	425	SER	-	expression tag	UNP P26313
B	426	GLY	-	expression tag	UNP P26313

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Chain	Residue	Modelled	Actual	Comment	Reference
B	427	TRP	-	expression tag	UNP P26313
B	428	SER	-	expression tag	UNP P26313
B	429	HIS	-	expression tag	UNP P26313
B	430	PRO	-	expression tag	UNP P26313
B	431	GLN	-	expression tag	UNP P26313
B	432	PHE	-	expression tag	UNP P26313
B	433	GLU	-	expression tag	UNP P26313
B	434	LYS	-	expression tag	UNP P26313
B	435	GLY	-	expression tag	UNP P26313
B	436	GLY	-	expression tag	UNP P26313
B	437	GLY	-	expression tag	UNP P26313
B	438	SER	-	expression tag	UNP P26313
B	439	GLY	-	expression tag	UNP P26313
B	440	GLY	-	expression tag	UNP P26313
B	441	GLY	-	expression tag	UNP P26313
B	442	SER	-	expression tag	UNP P26313
B	443	GLY	-	expression tag	UNP P26313
B	444	GLY	-	expression tag	UNP P26313
B	445	SER	-	expression tag	UNP P26313
B	446	ALA	-	expression tag	UNP P26313
B	447	TRP	-	expression tag	UNP P26313
B	448	SER	-	expression tag	UNP P26313
B	449	HIS	-	expression tag	UNP P26313
B	450	PRO	-	expression tag	UNP P26313
B	451	GLN	-	expression tag	UNP P26313
B	452	PHE	-	expression tag	UNP P26313
B	453	GLU	-	expression tag	UNP P26313
B	454	LYS	-	expression tag	UNP P26313

- Molecule 3 is a protein called JUN1 heavy chain.

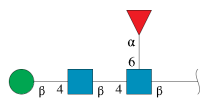
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	H	223	Total	C	H	N	O	S	0	0	0
			3372	1080	1666	286	332	8			

- Molecule 4 is a protein called JUN1 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	L	212	Total	C	H	N	O	S	0	0	0
			3222	1025	1581	276	333	7			

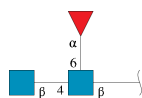
- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	4	Total	C	H	N	O	0	0	0
			92	28	43	2	19			

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



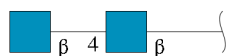
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	D	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 7 is an oligosaccharide called 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.



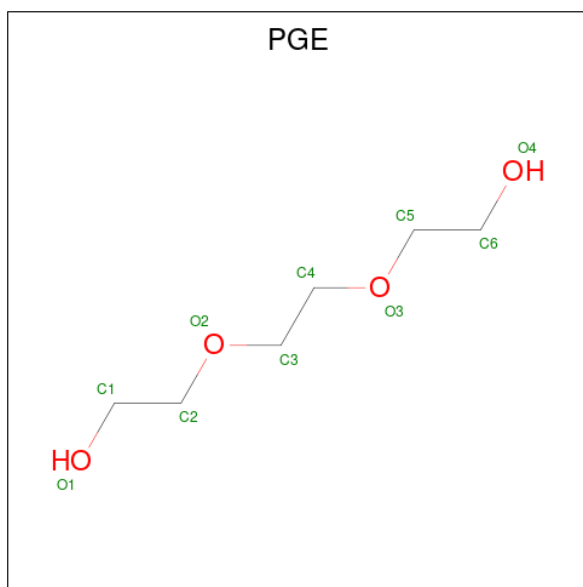
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- 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	H	N	O	0	0	0
			53	16	25	2	10			
8	G	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	0	0
			24	6	14	4		

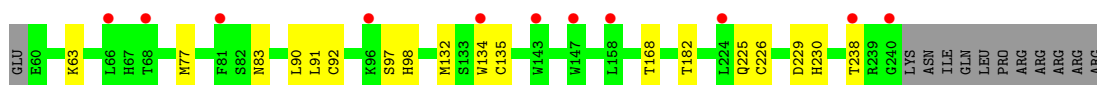
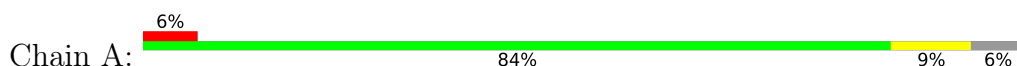
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	51	Total O 51 51	0	0
10	B	33	Total O 33 33	0	0
10	H	48	Total O 48 48	0	0
10	L	46	Total O 46 46	0	0

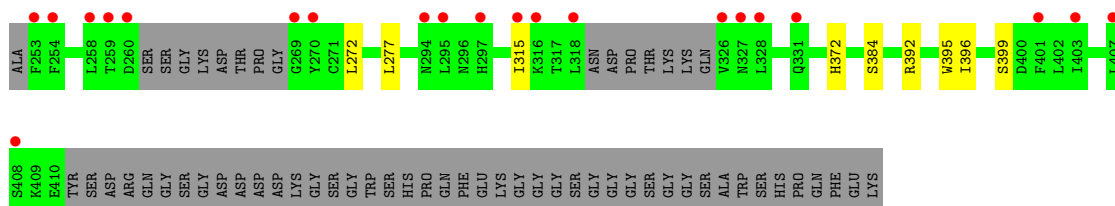
### 3 Residue-property plots [i](#)

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 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.

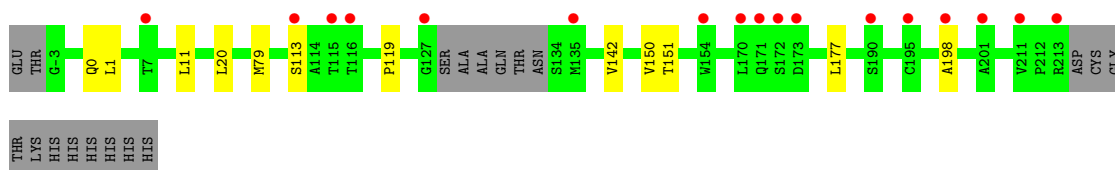
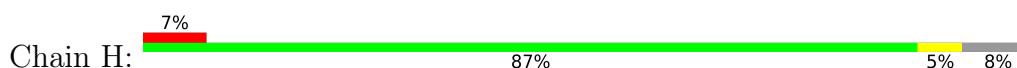
- Molecule 1: Pre-glycoprotein polyprotein GP complex



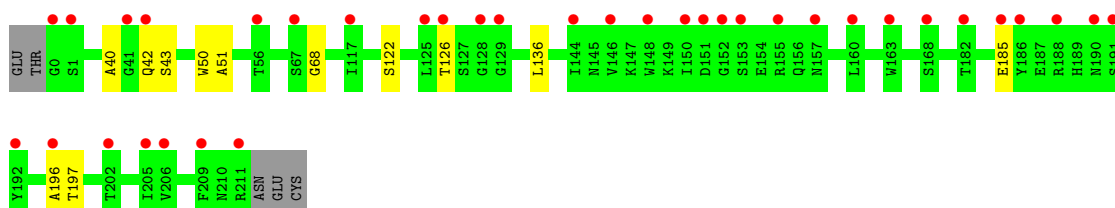
- Molecule 2: Glycoprotein G2



- Molecule 3: JUN1 heavy chain



- Molecule 4: JUN1 light chain





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

Chain C:  25% 75%

NAG1  
NAG2  
BMA3  
FUC4

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

Chain D:  67% 33%

NAG1  
NAG2  
FUC3

- Molecule 7: 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:  100%

NAG1  
NAG2  
BMA3  
MAN4

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

Chain F:  50% 50%

NAG1  
NAG2

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

Chain G:  50% 50%

NAG1  
NAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	225.79Å 71.97Å 80.23Å 90.00° 95.89° 90.00°	Depositor
Resolution (Å)	79.81 – 2.09 79.81 – 2.09	Depositor EDS
% Data completeness (in resolution range)	98.8 (79.81-2.09) 98.8 (79.81-2.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.02 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, $R_{free}$	0.212 , 0.247 0.213 , 0.248	Depositor DCC
$R_{free}$ test set	3731 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.6	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.44 , 51.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12252	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.11	0/1507	0.31	0/2047
2	B	0.09	0/1200	0.27	0/1619
3	H	0.11	0/1749	0.31	0/2384
4	L	0.11	0/1677	0.29	0/2278
All	All	0.11	0/6133	0.30	0/8328

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	1461	1396	1395	10	0
2	B	1174	1139	1136	6	0
3	H	1706	1666	1667	5	0
4	L	1641	1581	1583	4	0
5	C	49	43	43	0	0
6	D	38	0	34	3	0
7	E	50	0	43	1	0
8	F	28	25	25	1	0
8	G	28	25	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	10	14	14	0	0
10	A	51	0	0	0	0
10	B	33	0	0	0	0
10	H	48	0	0	0	0
10	L	46	0	0	0	0
All	All	6363	5889	5965	24	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 2.

All (24) 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:182:THR:HG21	7:E:2:NAG:H82	1.66	0.75
1:A:229:ASP:HA	8:F:1:NAG:H81	1.83	0.59
1:A:168:THR:HG21	6:D:1:NAG:H62	1.86	0.57
2:B:372:HIS:CD2	8:G:1:NAG:H82	2.40	0.56
4:L:122:SER:O	4:L:126:THR:HG23	2.05	0.56
2:B:272:LEU:HD13	2:B:277:LEU:HD21	1.88	0.56
4:L:40:ALA:O	4:L:42:GLN:NE2	2.37	0.54
1:A:134:TRP:CH2	6:D:1:NAG:H3	2.45	0.52
3:H:177:LEU:C	3:H:177:LEU:HD12	2.37	0.50
2:B:396:ILE:O	2:B:399:SER:OG	2.29	0.49
1:A:83:ASN:O	2:B:315:ILE:HD11	2.13	0.48
3:H:151:THR:CG2	3:H:198:ALA:HB3	2.42	0.48
1:A:90:LEU:C	1:A:91:LEU:HD12	2.40	0.47
3:H:0:GLN:C	3:H:1:LEU:HD12	2.40	0.47
1:A:97:SER:OG	1:A:98:HIS:ND1	2.43	0.46
2:B:392:ARG:HA	2:B:395:TRP:NE1	2.31	0.45
3:H:119:PRO:HB2	3:H:142:VAL:HG13	1.98	0.45
4:L:136:LEU:CD2	4:L:196:ALA:HB2	2.47	0.44
3:H:20:LEU:HG	3:H:79:MET:HE2	2.00	0.43
1:A:77:MET:SD	1:A:230:HIS:ND1	2.91	0.43
2:B:392:ARG:HA	2:B:395:TRP:CE2	2.55	0.42
4:L:50:TRP:O	4:L:51:ALA:HB3	2.20	0.41
1:A:132:MET:HA	1:A:135:CYS:SG	2.61	0.41
1:A:134:TRP:CZ2	6:D:1:NAG:H3	2.56	0.41

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	179/193 (93%)	173 (97%)	6 (3%)	0	100	100
2	B	137/203 (68%)	135 (98%)	2 (2%)	0	100	100
3	H	219/242 (90%)	214 (98%)	5 (2%)	0	100	100
4	L	210/217 (97%)	204 (97%)	5 (2%)	1 (0%)	25	23
All	All	745/855 (87%)	726 (97%)	18 (2%)	1 (0%)	48	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	L	68	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	164/176 (93%)	159 (97%)	5 (3%)	36	40
2	B	133/177 (75%)	132 (99%)	1 (1%)	79	84
3	H	193/209 (92%)	190 (98%)	3 (2%)	58	65
4	L	187/192 (97%)	184 (98%)	3 (2%)	58	65
All	All	677/754 (90%)	665 (98%)	12 (2%)	54	61

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LYS
1	A	92	CYS
1	A	225	GLN
1	A	226	CYS
1	A	238	THR
2	B	384	SER
3	H	11	LEU
3	H	113	SER
3	H	150	VAL
4	L	43	SER
4	L	185	GLU
4	L	197	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	382	ASN
3	H	0	GLN
4	L	137	ASN

### 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 ⓘ

15 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	5,1	14,14,15	0.72	0	17,19,21	0.96	0
5	NAG	C	2	5	14,14,15	0.70	0	17,19,21	1.14	1 (5%)
5	BMA	C	3	5	11,11,12	0.87	0	15,15,17	3.12	7 (46%)
5	FUC	C	4	5	10,10,11	0.88	0	14,14,16	1.29	1 (7%)
6	NAG	D	1	6,1	14,14,15	0.75	0	17,19,21	1.07	2 (11%)
6	NAG	D	2	6	14,14,15	0.71	0	17,19,21	0.79	0
6	FUC	D	3	6	10,10,11	0.83	0	14,14,16	0.94	0
7	NAG	E	1	7,1	14,14,15	0.75	0	17,19,21	1.03	1 (5%)
7	NAG	E	2	7	14,14,15	0.70	0	17,19,21	0.83	0
7	BMA	E	3	7	11,11,12	0.84	0	15,15,17	2.30	3 (20%)
7	MAN	E	4	7	11,11,12	0.66	0	15,15,17	1.43	1 (6%)
8	NAG	F	1	8,2	14,14,15	0.70	0	17,19,21	1.20	2 (11%)
8	NAG	F	2	8	14,14,15	0.73	0	17,19,21	1.40	2 (11%)
8	NAG	G	1	8,2	14,14,15	0.74	0	17,19,21	1.01	1 (5%)
8	NAG	G	2	8	14,14,15	0.74	0	17,19,21	1.03	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	5,1	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1
5	BMA	C	3	5	-	1/2/19/22	0/1/1/1
5	FUC	C	4	5	-	-	0/1/1/1
6	NAG	D	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	D	2	6	-	1/6/23/26	0/1/1/1
6	FUC	D	3	6	-	-	0/1/1/1
7	NAG	E	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	E	2	7	-	0/6/23/26	0/1/1/1
7	BMA	E	3	7	-	1/2/19/22	0/1/1/1
7	MAN	E	4	7	-	2/2/19/22	0/1/1/1
8	NAG	F	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	F	2	8	-	2/6/23/26	0/1/1/1
8	NAG	G	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	G	2	8	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	3	BMA	C1-O5-C5	8.60	123.84	112.19
7	E	3	BMA	C1-O5-C5	7.07	121.77	112.19
7	E	4	MAN	C1-O5-C5	4.39	118.14	112.19
5	C	3	BMA	C2-C3-C4	4.21	118.18	110.89
5	C	3	BMA	C3-C4-C5	4.03	117.42	110.24
5	C	3	BMA	C1-C2-C3	3.67	114.18	109.67
8	F	2	NAG	C2-N2-C7	3.66	128.12	122.90
5	C	2	NAG	O5-C1-C2	-3.19	106.26	111.29
8	F	1	NAG	O5-C1-C2	-3.05	106.48	111.29
8	G	2	NAG	O5-C1-C2	-2.95	106.63	111.29
8	F	2	NAG	O5-C1-C2	-2.90	106.70	111.29
5	C	3	BMA	O4-C4-C3	-2.76	103.96	110.35
7	E	3	BMA	C3-C4-C5	2.76	115.16	110.24
5	C	3	BMA	O3-C3-C2	-2.73	104.77	109.99
5	C	4	FUC	C1-C2-C3	2.54	112.79	109.67
7	E	1	NAG	O4-C4-C3	-2.33	104.96	110.35
8	G	1	NAG	O4-C4-C3	-2.28	105.08	110.35
6	D	1	NAG	O4-C4-C3	-2.27	105.11	110.35
8	F	1	NAG	C1-O5-C5	2.22	115.20	112.19
6	D	1	NAG	C1-O5-C5	2.21	115.19	112.19
7	E	3	BMA	O4-C4-C3	-2.10	105.49	110.35
5	C	3	BMA	O5-C5-C4	2.10	115.94	110.83

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	E	4	MAN	C4-C5-C6-O6
8	F	2	NAG	C8-C7-N2-C2
8	F	2	NAG	O7-C7-N2-C2
7	E	4	MAN	O5-C5-C6-O6
6	D	2	NAG	O5-C5-C6-O6
5	C	3	BMA	C4-C5-C6-O6
7	E	3	BMA	O5-C5-C6-O6
7	E	1	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 6 short contacts:

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

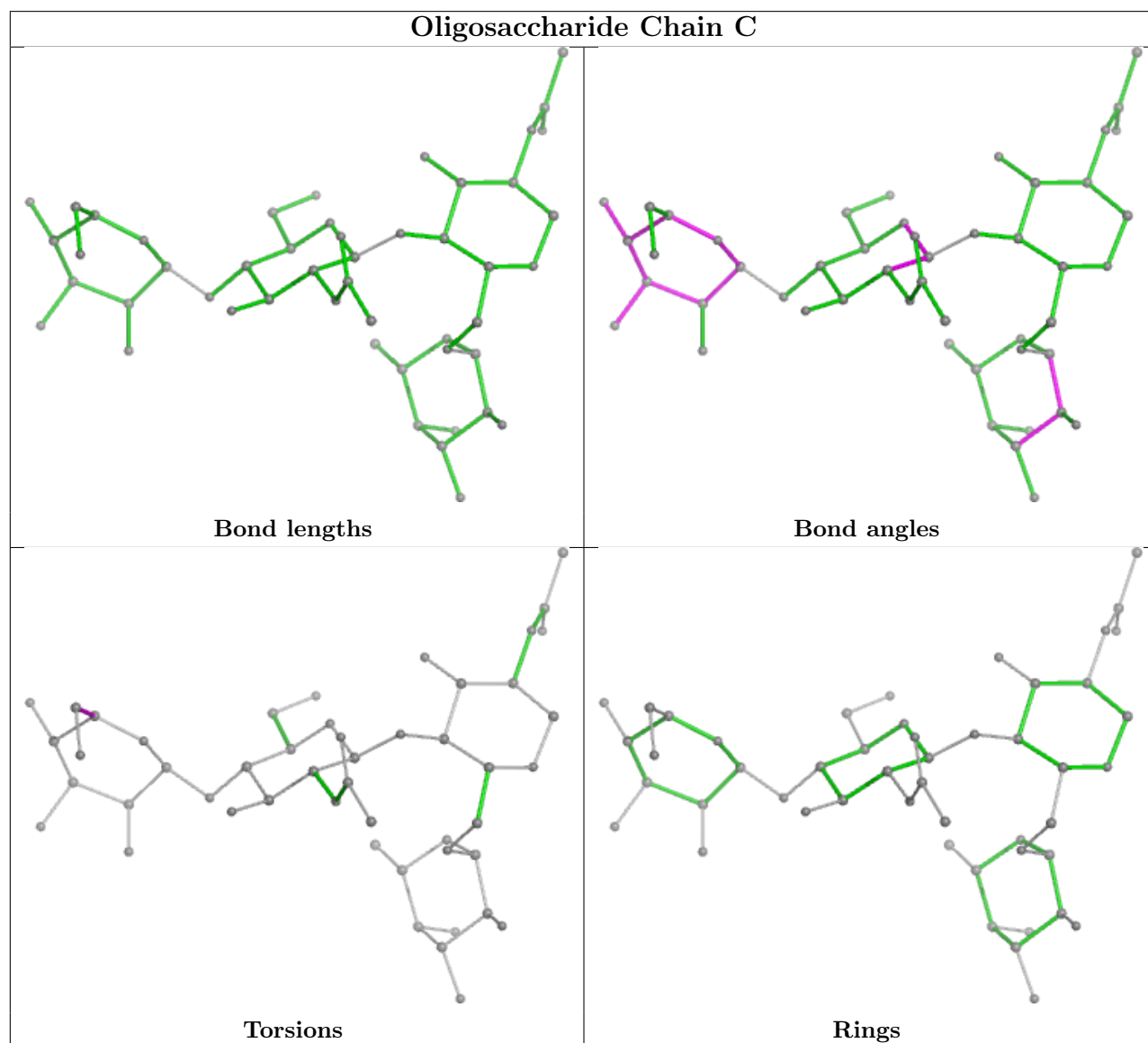
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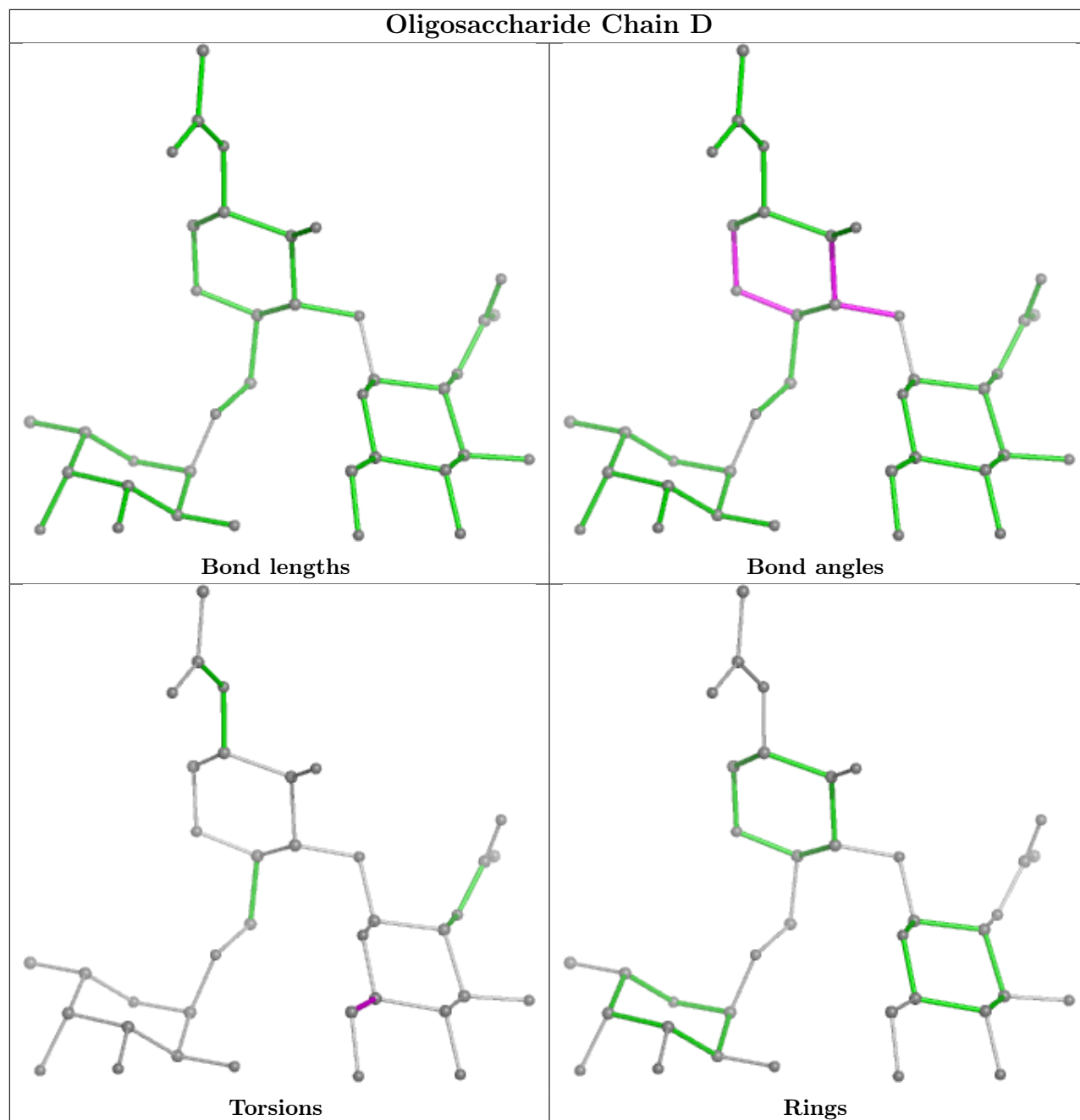


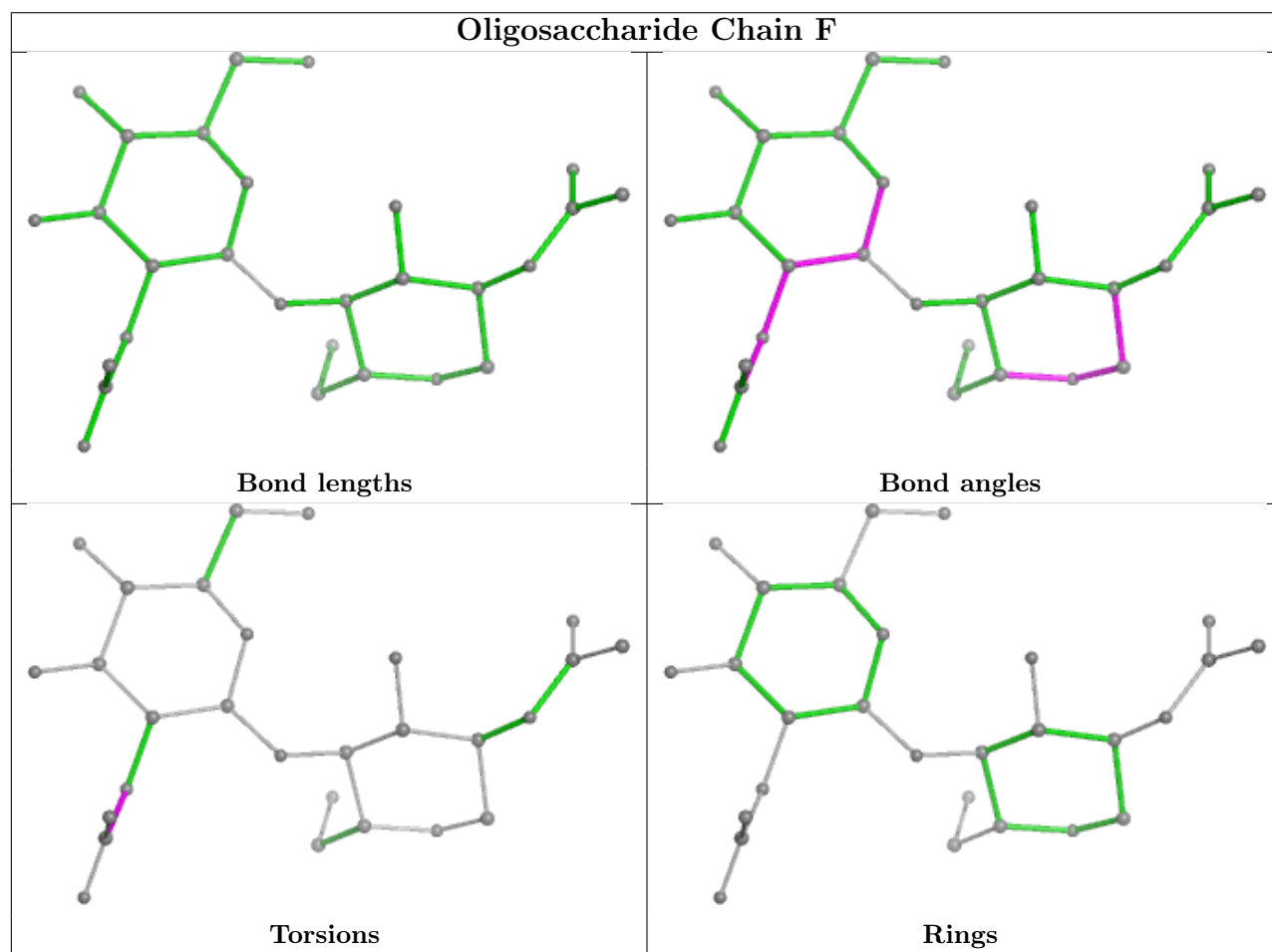
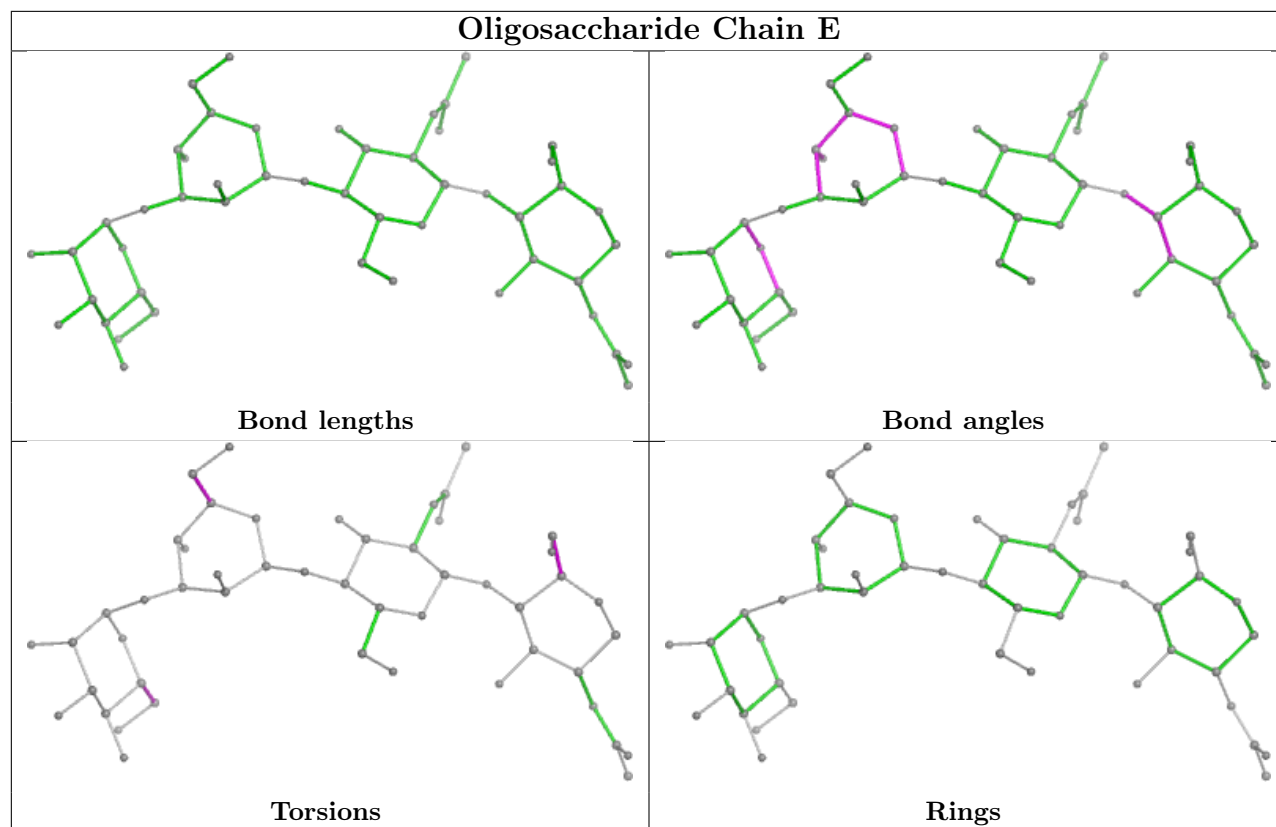
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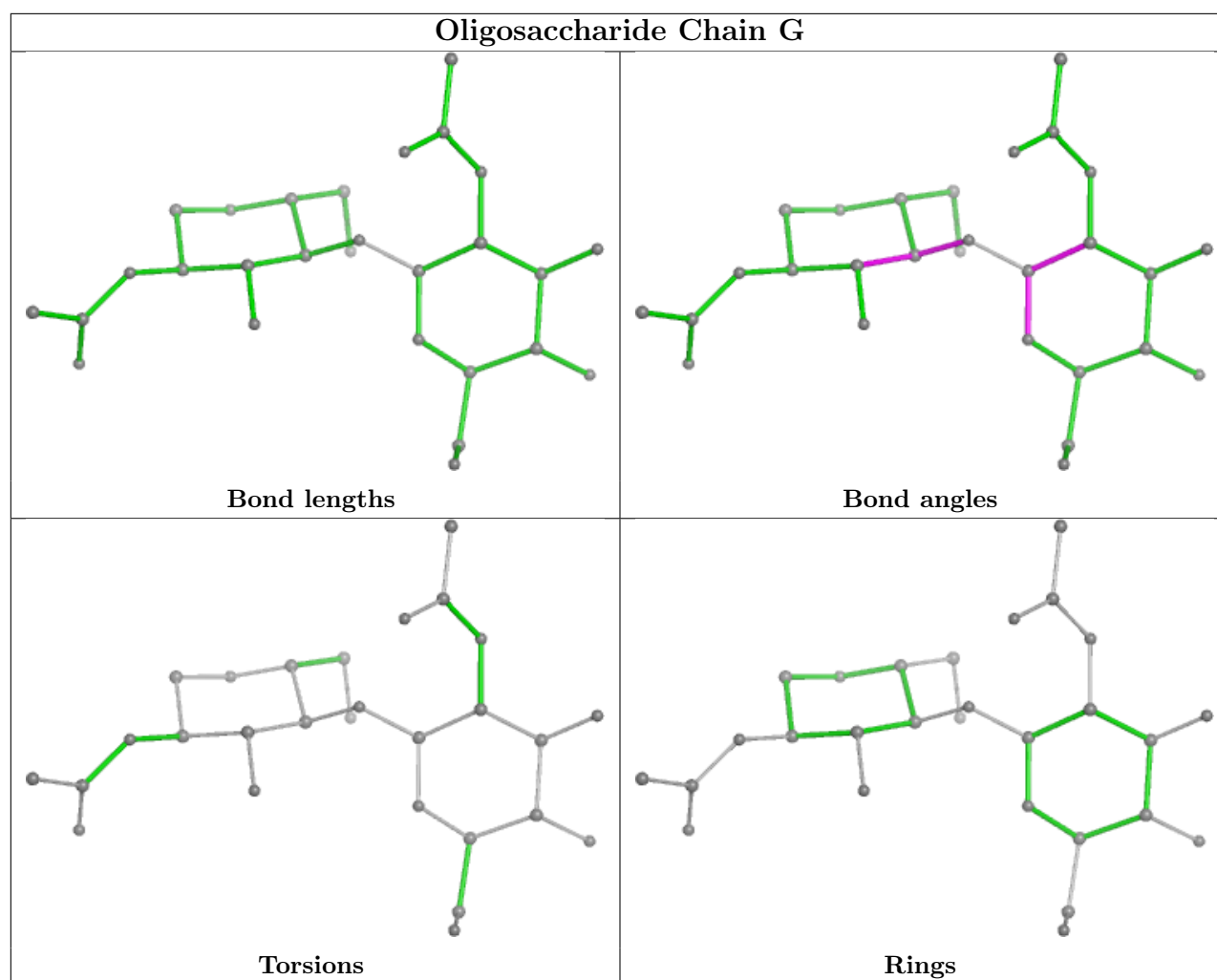
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	1	NAG	1	0
6	D	1	NAG	3	0
7	E	2	NAG	1	0

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









## 5.6 Ligand geometry [i](#)

1 ligand 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	$\# Z  > 2$
9	PGE	A	301	-	9,9,9	0.30	0	8,8,8	0.55	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
9	PGE	A	301	-	-	5/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	301	PGE	O3-C5-C6-O4
9	A	301	PGE	O1-C1-C2-O2
9	A	301	PGE	O2-C3-C4-O3
9	A	301	PGE	C6-C5-O3-C4
9	A	301	PGE	C4-C3-O2-C2

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	181/193 (93%)	0.26	11 (6%) 28 30	35, 52, 78, 95	0
2	B	143/203 (70%)	0.84	21 (14%) 7 7	41, 59, 95, 145	0
3	H	223/242 (92%)	0.68	17 (7%) 21 23	38, 64, 90, 118	0
4	L	212/217 (97%)	0.92	36 (16%) 5 5	36, 66, 106, 122	0
All	All	759/855 (88%)	0.68	85 (11%) 11 12	35, 60, 99, 145	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	295	LEU	5.0
2	B	253	PHE	4.3
2	B	326	VAL	4.3
2	B	401	PHE	4.1
2	B	269	GLY	4.1
4	L	168	SER	4.1
2	B	316	LYS	3.9
4	L	1	SER	3.9
4	L	0	GLY	3.9
2	B	259	THR	3.9
4	L	209	PHE	3.9
4	L	191	SER	3.8
2	B	328	LEU	3.6
2	B	318	LEU	3.5
2	B	254	PHE	3.4
2	B	297	HIS	3.4
4	L	157	ASN	3.3
3	H	172	SER	3.3
2	B	294	ASN	3.2
2	B	408	SER	3.1
1	A	66	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
4	L	153	SER	3.1
4	L	163	TRP	3.0
4	L	186	TYR	3.0
1	A	147	TRP	2.9
1	A	240	GLY	2.9
4	L	202	THR	2.9
1	A	68	THR	2.8
1	A	134	TRP	2.8
4	L	148	TRP	2.8
4	L	56	THR	2.8
4	L	160	LEU	2.8
1	A	143	TRP	2.8
3	H	211	VAL	2.8
4	L	182	THR	2.7
1	A	224	LEU	2.7
4	L	150	ILE	2.7
4	L	41	GLY	2.6
4	L	126	THR	2.6
4	L	67	SER	2.6
4	L	146	VAL	2.6
3	H	115	THR	2.5
2	B	315	ILE	2.5
2	B	270	TYR	2.5
4	L	151	ASP	2.5
4	L	205	ILE	2.5
4	L	129	GLY	2.5
3	H	201	ALA	2.5
3	H	170	LEU	2.4
3	H	127	GLY	2.4
3	H	116	THR	2.4
4	L	192	TYR	2.4
4	L	42	GLN	2.4
1	A	158	LEU	2.4
3	H	171	GLN	2.4
2	B	407	LEU	2.3
2	B	327	ASN	2.3
1	A	96	LYS	2.3
3	H	213	ARG	2.3
2	B	331	GLN	2.3
4	L	144	ILE	2.3
4	L	190	ASN	2.3
4	L	125	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	258	LEU	2.3
4	L	185	GLU	2.2
4	L	128	GLY	2.2
3	H	113	SER	2.2
4	L	206	VAL	2.2
3	H	154	TRP	2.2
1	A	238	THR	2.2
4	L	196	ALA	2.2
4	L	211	ARG	2.2
3	H	7	THR	2.1
2	B	260	ASP	2.1
4	L	155	ARG	2.1
4	L	188	ARG	2.1
3	H	195	CYS	2.1
4	L	117	ILE	2.1
3	H	198	ALA	2.1
3	H	135	MET	2.1
4	L	152	GLY	2.1
2	B	403	ILE	2.1
3	H	190	SER	2.0
1	A	81	PHE	2.0
3	H	173	ASP	2.0

## 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(Å <sup>2</sup> )	Q<0.9
9	PGE	A	301	10/10	0.93	0.14	51,67,87,94	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.