



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 28, 2024 – 08:06 AM EDT

PDB ID : 5V4M  
Title : Structure of HLA-DR15 with bound alpha3(135-145) peptide  
Authors : Petersen, J.; Rossjohn, J.  
Deposited on : 2017-03-10  
Resolution : 2.10 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)

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<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

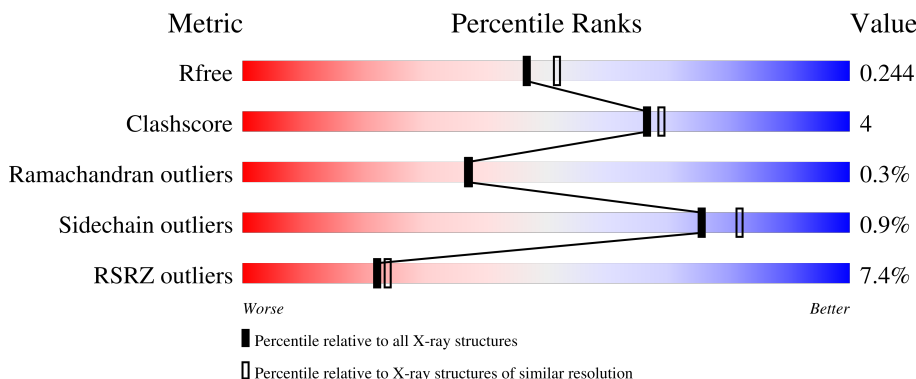
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	189	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>5% • 6%</div> </div> </div>
1	D	189	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>6% 6%</div> </div> </div>
1	G	189	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>10% • 6%</div> </div> </div>
1	J	189	<div> <div>7%</div> <div> <div></div> <div>84%</div> <div>10% 6%</div> </div> </div>
2	C	216	<div> <div>7%</div> <div> <div></div> <div>81%</div> <div>12% 7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	216	
2	I	216	
2	L	216	
3	B	3	
3	H	3	
4	E	2	
4	K	2	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13349 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 HLA-DRA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	178	Total	C	N	O	S	0	0	0
			1464	949	238	272	5			
1	A	178	Total	C	N	O	S	0	0	0
			1464	949	238	272	5			
1	G	178	Total	C	N	O	S	0	1	0
			1470	953	238	274	5			
1	J	178	Total	C	N	O	S	0	0	0
			1464	949	238	272	5			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	182	THR	-	expression tag	UNP P01903
D	183	SER	-	expression tag	UNP P01903
D	184	GLY	-	expression tag	UNP P01903
D	185	ASP	-	expression tag	UNP P01903
D	186	ASP	-	expression tag	UNP P01903
D	187	ASP	-	expression tag	UNP P01903
D	188	ASP	-	expression tag	UNP P01903
D	189	LYS	-	expression tag	UNP P01903
A	182	THR	-	expression tag	UNP P01903
A	183	SER	-	expression tag	UNP P01903
A	184	GLY	-	expression tag	UNP P01903
A	185	ASP	-	expression tag	UNP P01903
A	186	ASP	-	expression tag	UNP P01903
A	187	ASP	-	expression tag	UNP P01903
A	188	ASP	-	expression tag	UNP P01903
A	189	LYS	-	expression tag	UNP P01903
G	182	THR	-	expression tag	UNP P01903
G	183	SER	-	expression tag	UNP P01903
G	184	GLY	-	expression tag	UNP P01903
G	185	ASP	-	expression tag	UNP P01903
G	186	ASP	-	expression tag	UNP P01903

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Chain	Residue	Modelled	Actual	Comment	Reference
G	187	ASP	-	expression tag	UNP P01903
G	188	ASP	-	expression tag	UNP P01903
G	189	LYS	-	expression tag	UNP P01903
J	182	THR	-	expression tag	UNP P01903
J	183	SER	-	expression tag	UNP P01903
J	184	GLY	-	expression tag	UNP P01903
J	185	ASP	-	expression tag	UNP P01903
J	186	ASP	-	expression tag	UNP P01903
J	187	ASP	-	expression tag	UNP P01903
J	188	ASP	-	expression tag	UNP P01903
J	189	LYS	-	expression tag	UNP P01903

- Molecule 2 is a protein called alpha3(135-145)-HLA-DRB1\*15:01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	200	Total	C	N	O	S	0	2	0
			1664	1061	293	304	6			
2	C	200	Total	C	N	O	S	0	2	0
			1666	1062	295	303	6			
2	I	200	Total	C	N	O	S	0	1	0
			1658	1057	292	303	6			
2	L	200	Total	C	N	O	S	0	2	0
			1664	1061	293	304	6			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	233	GLY	-	linker	PDB ?
F	234	SER	-	linker	PDB ?
F	235	GLY	-	linker	PDB ?
F	236	GLY	-	linker	PDB ?
F	237	SER	-	linker	PDB ?
F	238	ILE	-	linker	PDB ?
F	239	GLU	-	linker	PDB ?
F	240	GLY	-	linker	PDB ?
F	241	ARG	-	linker	PDB ?
F	242	GLY	-	linker	PDB ?
F	243	GLY	-	linker	PDB ?
F	244	SER	-	linker	PDB ?
F	245	GLY	-	linker	PDB ?
F	246	ALA	-	linker	PDB ?
C	233	GLY	-	linker	PDB ?

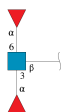
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Chain	Residue	Modelled	Actual	Comment	Reference
C	234	SER	-	linker	PDB ?
C	235	GLY	-	linker	PDB ?
C	236	GLY	-	linker	PDB ?
C	237	SER	-	linker	PDB ?
C	238	ILE	-	linker	PDB ?
C	239	GLU	-	linker	PDB ?
C	240	GLY	-	linker	PDB ?
C	241	ARG	-	linker	PDB ?
C	242	GLY	-	linker	PDB ?
C	243	GLY	-	linker	PDB ?
C	244	SER	-	linker	PDB ?
C	245	GLY	-	linker	PDB ?
C	246	ALA	-	linker	PDB ?
I	233	GLY	-	linker	PDB ?
I	234	SER	-	linker	PDB ?
I	235	GLY	-	linker	PDB ?
I	236	GLY	-	linker	PDB ?
I	237	SER	-	linker	PDB ?
I	238	ILE	-	linker	PDB ?
I	239	GLU	-	linker	PDB ?
I	240	GLY	-	linker	PDB ?
I	241	ARG	-	linker	PDB ?
I	242	GLY	-	linker	PDB ?
I	243	GLY	-	linker	PDB ?
I	244	SER	-	linker	PDB ?
I	245	GLY	-	linker	PDB ?
I	246	ALA	-	linker	PDB ?
L	233	GLY	-	linker	PDB ?
L	234	SER	-	linker	PDB ?
L	235	GLY	-	linker	PDB ?
L	236	GLY	-	linker	PDB ?
L	237	SER	-	linker	PDB ?
L	238	ILE	-	linker	PDB ?
L	239	GLU	-	linker	PDB ?
L	240	GLY	-	linker	PDB ?
L	241	ARG	-	linker	PDB ?
L	242	GLY	-	linker	PDB ?
L	243	GLY	-	linker	PDB ?
L	244	SER	-	linker	PDB ?
L	245	GLY	-	linker	PDB ?
L	246	ALA	-	linker	PDB ?

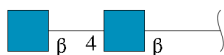
- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[alpha-L-fucopyranose-(1

-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



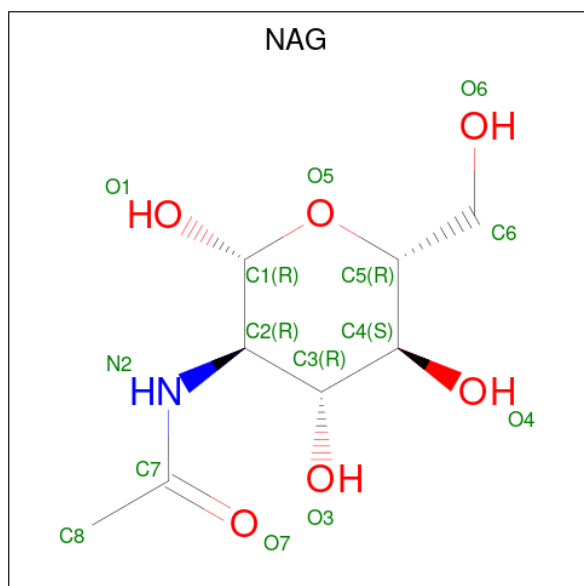
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	3	Total	C	N	O	0	0	0
			34	20	1	13			
3	H	3	Total	C	N	O	0	0	0
			34	20	1	13			

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



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 6 is water.


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	87	Total O 87 87	0	0
6	F	89	Total O 89 89	0	0
6	A	73	Total O 73 73	0	0
6	C	78	Total O 78 78	0	0
6	G	90	Total O 90 90	0	0
6	I	84	Total O 84 84	0	0
6	J	81	Total O 81 81	0	0
6	L	73	Total O 73 73	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: HLA-DRA1

Chain D: 




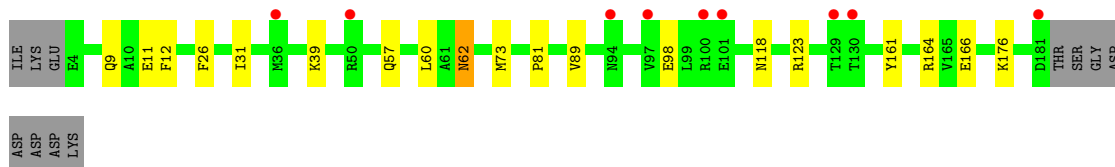
#### • Molecule 1: HLA-DRA1

Chain A: 




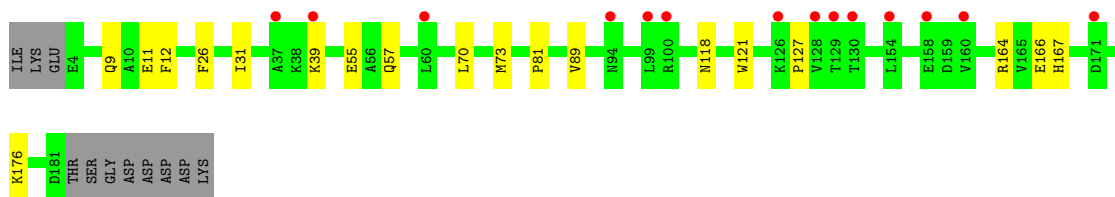
#### • Molecule 1: HLA-DRA1

Chain G: 




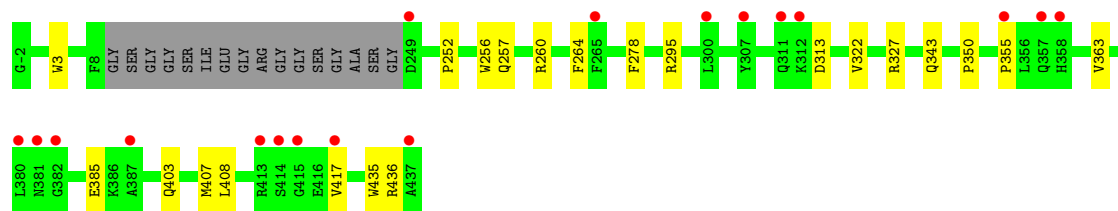
#### • Molecule 1: HLA-DRA1

Chain J: 

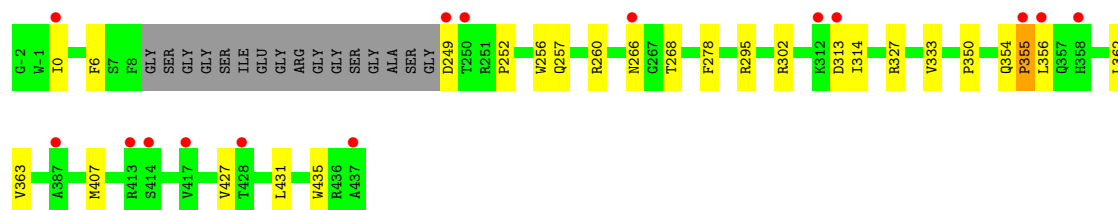
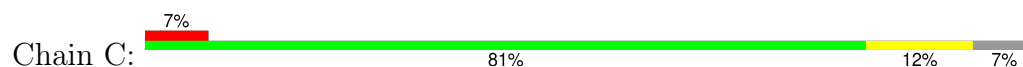


#### • Molecule 2: alpha3(135-145)-HLA-DRB1\*15:01

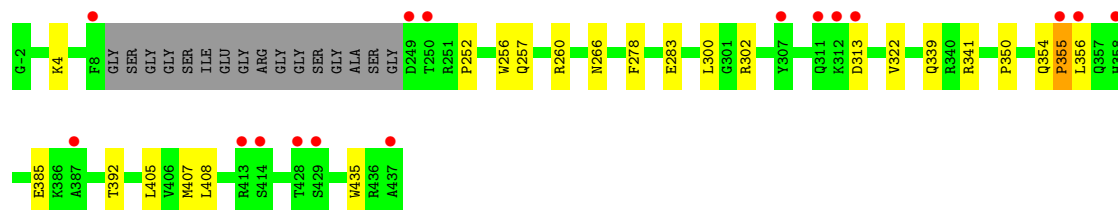
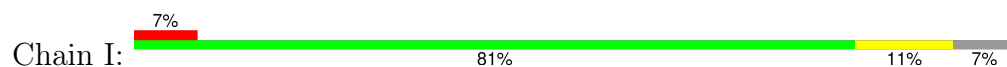
Chain F: 



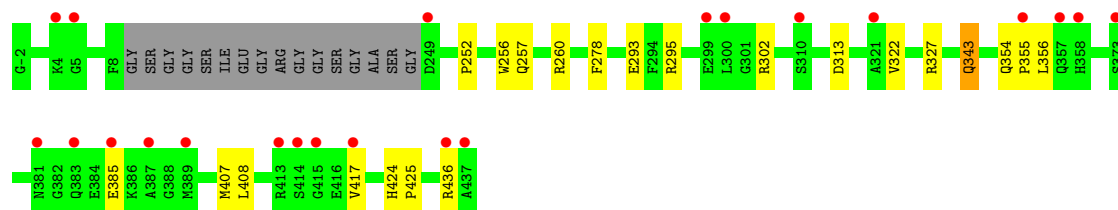
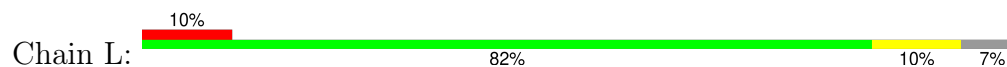
- Molecule 2: alpha3(135-145)-HLA-DRB1\*15:01



- Molecule 2: alpha3(135-145)-HLA-DRB1\*15:01



- Molecule 2: alpha3(135-145)-HLA-DRB1\*15:01



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



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

Chain H:  33% 67%

MAG1  
FUC2  
FUC3

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

Chain E:  50% 50%

MAG1  
MAG2

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

Chain K:  100%

MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.59Å 79.01Å 95.82Å 87.64° 73.29° 89.97°	Depositor
Resolution (Å)	48.32 – 2.10 48.32 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.2 (48.32-2.10) 96.2 (48.32-2.10)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.217 , 0.244 0.218 , 0.244	Depositor DCC
$R_{free}$ test set	3184 reflections (2.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.8	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 42.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.096 for -h,k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13349	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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: FUC, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.28	0/1509	0.49	0/2058
1	D	0.27	0/1509	0.46	0/2058
1	G	0.26	0/1518	0.46	0/2070
1	J	0.27	0/1509	0.46	0/2058
2	C	0.26	0/1721	0.46	0/2337
2	F	0.25	0/1719	0.46	0/2336
2	I	0.26	0/1710	0.45	0/2323
2	L	0.25	0/1719	0.46	0/2336
All	All	0.26	0/12914	0.46	0/17576

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	1464	0	1399	7	0
1	D	1464	0	1399	8	0
1	G	1470	0	1405	14	0
1	J	1464	0	1399	14	0
2	C	1666	0	1589	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1664	0	1584	13	0
2	I	1658	0	1576	18	0
2	L	1664	0	1584	16	0
3	B	34	0	31	0	0
3	H	34	0	31	0	0
4	E	28	0	25	2	0
4	K	28	0	25	0	0
5	A	14	0	13	0	0
5	D	14	0	13	0	0
5	J	28	0	26	1	0
6	A	73	0	0	0	0
6	C	78	0	0	2	0
6	D	87	0	0	0	0
6	F	89	0	0	2	0
6	G	90	0	0	0	0
6	I	84	0	0	2	0
6	J	81	0	0	0	0
6	L	73	0	0	2	0
All	All	13349	0	12099	89	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 4.

The worst 5 of 89 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:C:249:ASP:N	4:E:2:NAG:HO6	1.62	0.95
2:C:363:VAL:HG22	2:C:407:MET:HG3	1.70	0.72
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.72	0.70
1:G:164:ARG:NH2	1:G:166:GLU:OE2	2.29	0.66
1:J:118:ASN:HB2	1:J:166:GLU:HB2	1.77	0.66

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	176/189 (93%)	174 (99%)	2 (1%)	0	100	100
1	D	176/189 (93%)	174 (99%)	2 (1%)	0	100	100
1	G	177/189 (94%)	175 (99%)	2 (1%)	0	100	100
1	J	176/189 (93%)	174 (99%)	2 (1%)	0	100	100
2	C	198/216 (92%)	195 (98%)	2 (1%)	1 (0%)	25	23
2	F	198/216 (92%)	195 (98%)	2 (1%)	1 (0%)	25	23
2	I	197/216 (91%)	194 (98%)	2 (1%)	1 (0%)	25	23
2	L	198/216 (92%)	195 (98%)	2 (1%)	1 (0%)	25	23
All	All	1496/1620 (92%)	1476 (99%)	16 (1%)	4 (0%)	37	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	355	PRO
2	I	355	PRO
2	C	355	PRO
2	L	355	PRO

### 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	163/173 (94%)	161 (99%)	2 (1%)	67	74
1	D	163/173 (94%)	162 (99%)	1 (1%)	84	89
1	G	164/173 (95%)	161 (98%)	3 (2%)	54	61
1	J	163/173 (94%)	163 (100%)	0	100	100
2	C	182/187 (97%)	181 (100%)	1 (0%)	86	91
2	F	182/187 (97%)	179 (98%)	3 (2%)	58	65
2	I	181/187 (97%)	179 (99%)	2 (1%)	70	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	182/187 (97%)	179 (98%)	3 (2%)	58	65
All	All	1380/1440 (96%)	1365 (99%)	15 (1%)	75	77

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	60	LEU
2	L	343[B]	GLN
1	G	62	ASN
2	L	407	MET
2	I	407	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	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 ⓘ

10 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	1,3	14,14,15	0.34	0	17,19,21	0.34	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FUC	B	2	3	10,10,11	0.75	0	14,14,16	0.76	0
3	FUC	B	3	3	10,10,11	0.88	0	14,14,16	0.78	0
4	NAG	E	1	1,4	14,14,15	0.17	0	17,19,21	0.50	0
4	NAG	E	2	4	14,14,15	0.25	0	17,19,21	0.39	0
3	NAG	H	1	1,3	14,14,15	0.62	0	17,19,21	1.58	3 (17%)
3	FUC	H	2	3	10,10,11	0.78	0	14,14,16	0.85	0
3	FUC	H	3	3	10,10,11	1.12	1 (10%)	14,14,16	0.76	0
4	NAG	K	1	1,4	14,14,15	0.19	0	17,19,21	0.50	0
4	NAG	K	2	4	14,14,15	0.21	0	17,19,21	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	B	2	3	-	-	0/1/1/1
3	FUC	B	3	3	-	-	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	FUC	H	2	3	-	-	0/1/1/1
3	FUC	H	3	3	-	-	0/1/1/1
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	3	FUC	C2-C3	2.14	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	C1-O5-C5	4.41	118.10	112.19
3	H	1	NAG	C1-C2-N2	2.04	113.66	110.43
3	H	1	NAG	C4-C3-C2	-2.04	108.03	111.02

There are no chirality outliers.

All (5) torsion outliers are listed below:

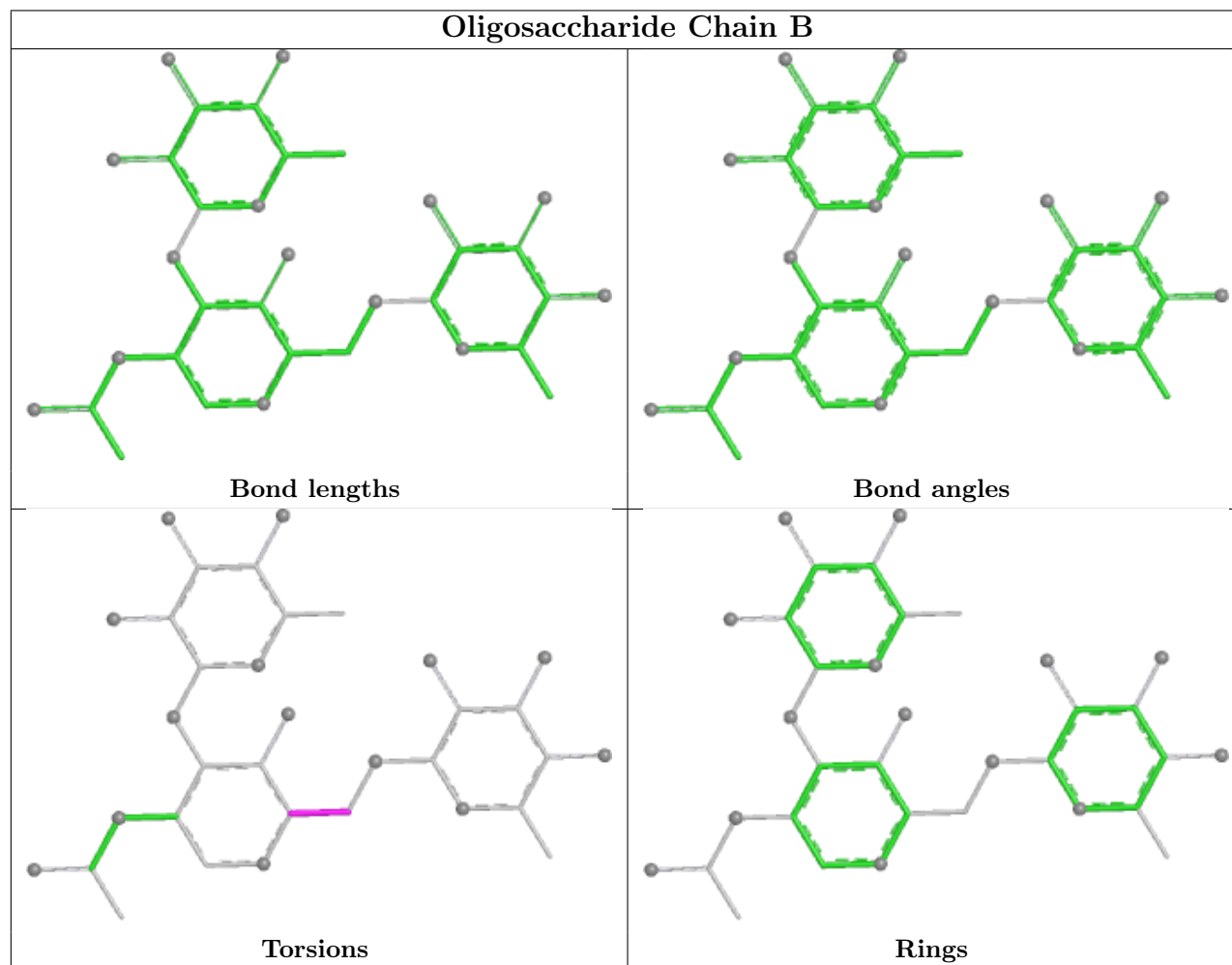
Mol	Chain	Res	Type	Atoms
3	B	1	NAG	O5-C5-C6-O6
3	B	1	NAG	C4-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6

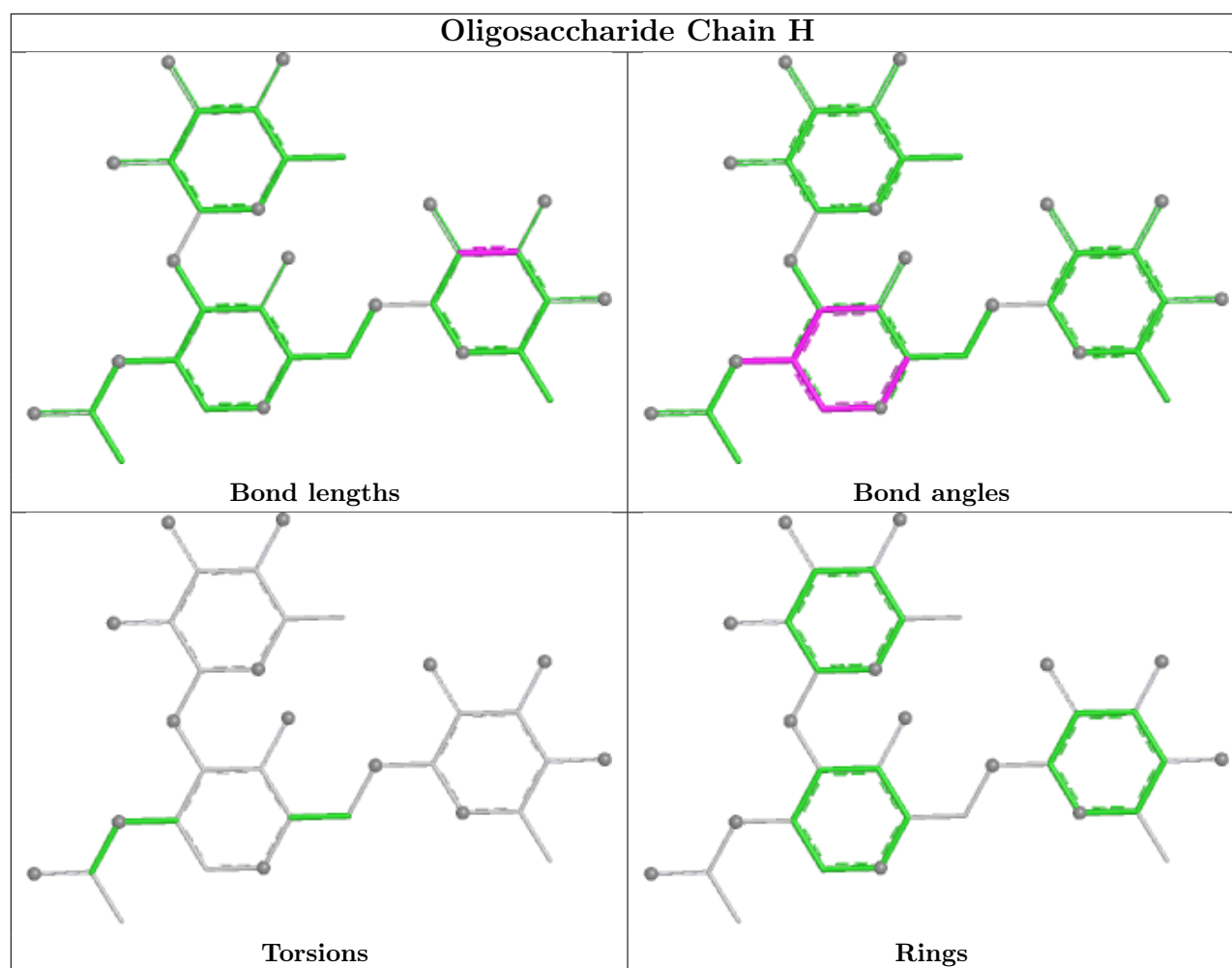
There are no ring outliers.

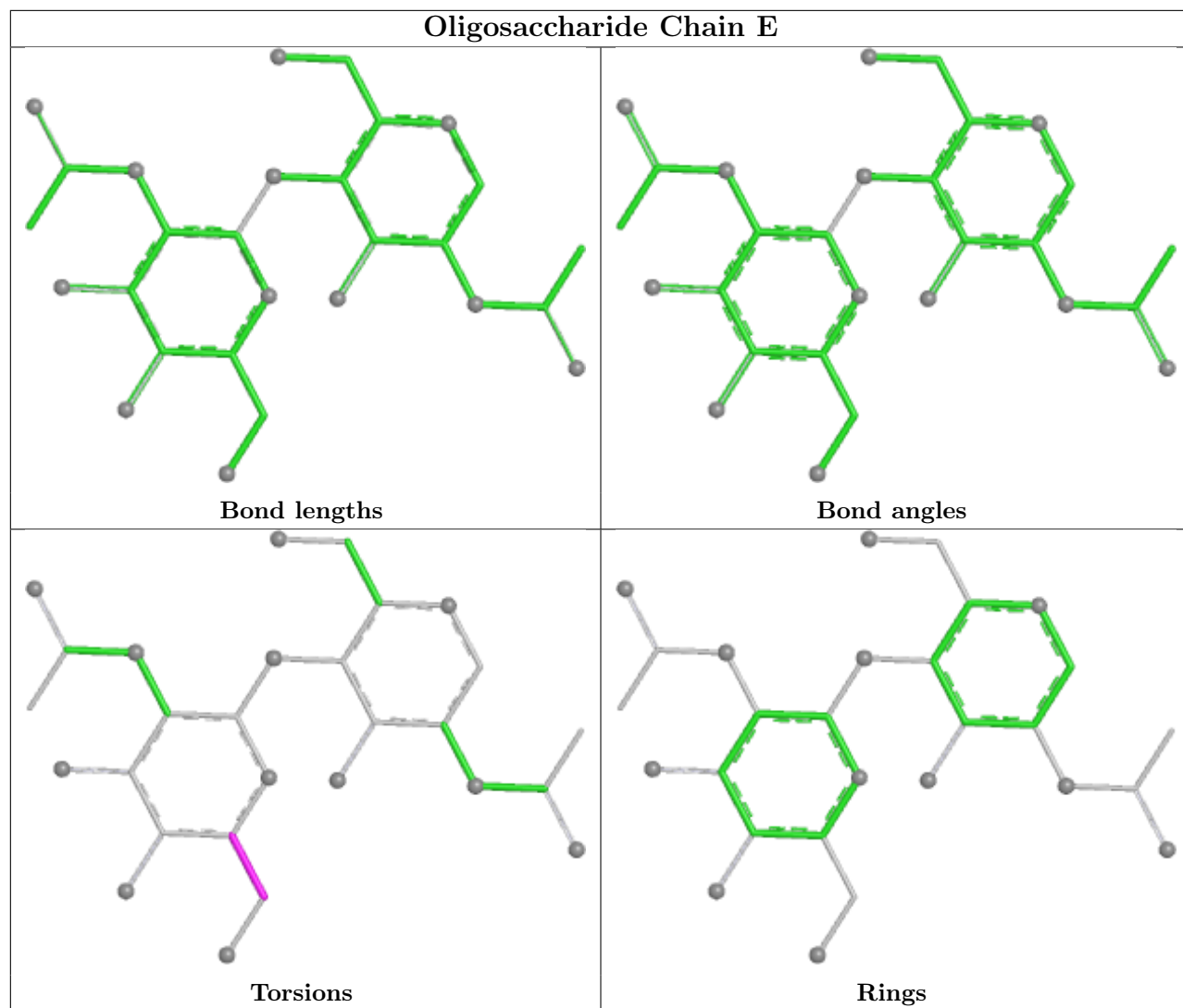
1 monomer is involved in 2 short contacts:

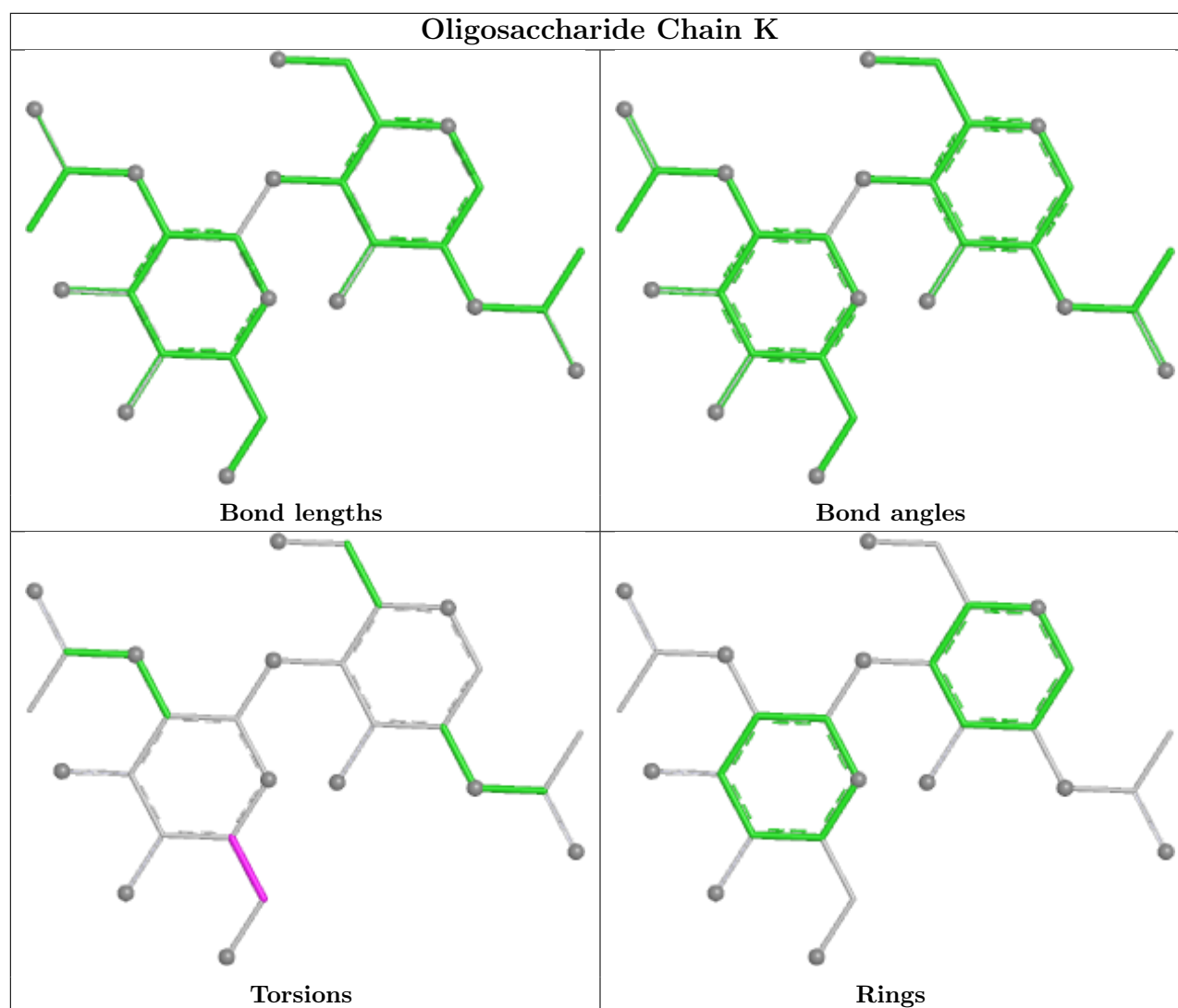
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	NAG	2	0

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









## 5.6 Ligand geometry [i](#)

4 ligands 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	J	202	1	14,14,15	0.60	0	17,19,21	0.47	0
5	NAG	J	201	1	14,14,15	0.53	0	17,19,21	1.24	2 (11%)
5	NAG	A	201	1	14,14,15	0.81	1 (7%)	17,19,21	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	D	204	1	14,14,15	0.20	0	17,19,21	0.59	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
5	NAG	J	202	1	-	2/6/23/26	0/1/1/1
5	NAG	J	201	1	-	3/6/23/26	0/1/1/1
5	NAG	A	201	1	-	2/6/23/26	0/1/1/1
5	NAG	D	204	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	201	NAG	C1-C2	2.07	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	201	NAG	C2-N2-C7	3.53	127.63	122.90
5	J	201	NAG	C1-C2-N2	2.55	114.46	110.43

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	201	NAG	C1-C2-N2-C7
5	J	201	NAG	O5-C5-C6-O6
5	J	201	NAG	C4-C5-C6-O6
5	J	202	NAG	O5-C5-C6-O6
5	D	204	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	202	NAG	1	0

## 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	178/189 (94%)	0.54	8 (4%) 39 41	20, 33, 61, 84	0
1	D	178/189 (94%)	0.38	10 (5%) 31 33	19, 29, 59, 79	0
1	G	178/189 (94%)	0.32	9 (5%) 34 36	14, 29, 53, 80	1 (0%)
1	J	178/189 (94%)	0.58	14 (7%) 20 22	21, 34, 57, 79	0
2	C	200/216 (92%)	0.68	15 (7%) 22 23	16, 32, 63, 91	2 (1%)
2	F	200/216 (92%)	0.58	18 (9%) 17 18	13, 31, 63, 71	2 (1%)
2	I	200/216 (92%)	0.58	16 (8%) 20 21	18, 31, 58, 73	1 (0%)
2	L	200/216 (92%)	0.72	22 (11%) 12 12	14, 33, 61, 81	2 (1%)
All	All	1512/1620 (93%)	0.55	112 (7%) 22 24	13, 32, 60, 91	8 (0%)

The worst 5 of 112 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	387	ALA	6.7
2	L	437	ALA	6.2
2	F	387	ALA	5.7
2	I	387	ALA	5.1
2	L	387	ALA	4.9

### 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
5	NAG	A	201	14/15	0.56	0.17	71,77,81,82	0
5	NAG	J	201	14/15	0.57	0.18	74,84,87,89	0
5	NAG	D	204	14/15	0.74	0.17	60,63,69,70	0
5	NAG	J	202	14/15	0.75	0.19	64,70,81,81	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.