



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 19, 2024 – 11:36 AM EDT

PDB ID : 4OWL  
Title : Crystal Structure of the Vibrio vulnificus Hemolysin/Cytolysin Beta-Trefoil Lectin with N-Acetyl-D-Lactosamine Bound  
Authors : Kaus, K.; Olson, R.  
Deposited on : 2014-02-02  
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)

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

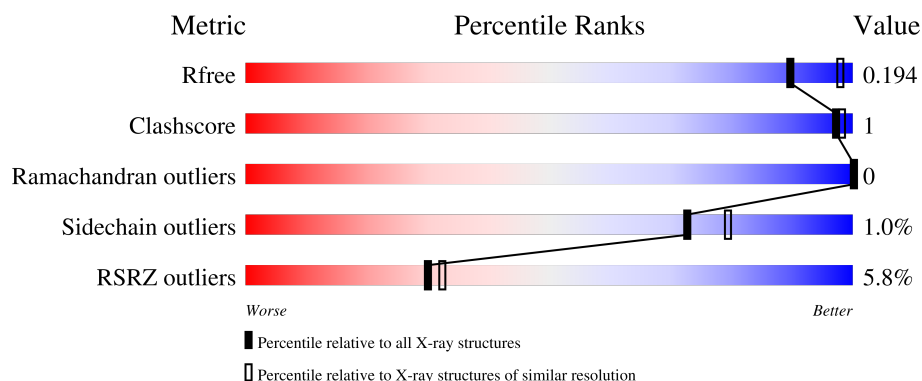
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	138	<div> <div>10%</div> <div>93%</div> <div>• •</div> </div>
1	B	138	<div> <div>9%</div> <div>93%</div> <div>• 5%</div> </div>
1	C	138	<div> <div>5%</div> <div>92%</div> <div>• 5%</div> </div>
1	D	138	<div> <div>4%</div> <div>96%</div> <div>• • •</div> </div>
1	E	138	<div> <div>90%</div> <div>6%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	138	<div><div></div><div>3%</div><div>91%</div><div>5%</div></div>
1	G	138	<div><div></div><div>8%</div><div>94%</div><div>5%</div></div>
2	H	2	<div><div></div><div>100%</div></div>
2	I	2	<div><div></div><div>50%</div><div>50%</div></div>
2	J	2	<div><div></div><div>100%</div></div>
2	K	2	<div><div></div><div>100%</div></div>
2	L	2	<div><div></div><div>50%</div><div>50%</div></div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14288 atoms, of which 6571 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 Cytolysin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	132	Total	C	H	N	O	S	0	0	0
			1811	599	844	175	189	4			
1	B	131	Total	C	H	N	O	S	0	0	0
			1854	603	877	178	191	5			
1	C	131	Total	C	H	N	O	S	0	0	0
			1913	613	919	183	193	5			
1	D	137	Total	C	H	N	O	S	0	0	0
			2050	657	983	196	209	5			
1	E	132	Total	C	H	N	O	S	0	0	0
			2009	636	974	191	203	5			
1	F	131	Total	C	H	N	O	S	0	0	0
			1938	616	934	186	197	5			
1	G	131	Total	C	H	N	O	S	0	0	0
			1837	599	864	179	190	5			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	334	GLY	-	expression tag	UNP P19247
A	335	SER	-	expression tag	UNP P19247
A	336	ALA	-	expression tag	UNP P19247
A	337	MET	-	expression tag	UNP P19247
B	334	GLY	-	expression tag	UNP P19247
B	335	SER	-	expression tag	UNP P19247
B	336	ALA	-	expression tag	UNP P19247
B	337	MET	-	expression tag	UNP P19247
C	334	GLY	-	expression tag	UNP P19247
C	335	SER	-	expression tag	UNP P19247
C	336	ALA	-	expression tag	UNP P19247
C	337	MET	-	expression tag	UNP P19247
D	334	GLY	-	expression tag	UNP P19247
D	335	SER	-	expression tag	UNP P19247
D	336	ALA	-	expression tag	UNP P19247

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Chain	Residue	Modelled	Actual	Comment	Reference
D	337	MET	-	expression tag	UNP P19247
E	334	GLY	-	expression tag	UNP P19247
E	335	SER	-	expression tag	UNP P19247
E	336	ALA	-	expression tag	UNP P19247
E	337	MET	-	expression tag	UNP P19247
F	334	GLY	-	expression tag	UNP P19247
F	335	SER	-	expression tag	UNP P19247
F	336	ALA	-	expression tag	UNP P19247
F	337	MET	-	expression tag	UNP P19247
G	334	GLY	-	expression tag	UNP P19247
G	335	SER	-	expression tag	UNP P19247
G	336	ALA	-	expression tag	UNP P19247
G	337	MET	-	expression tag	UNP P19247

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



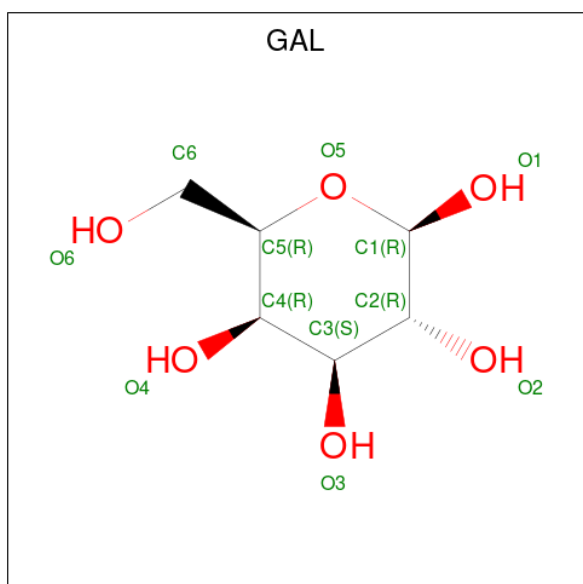
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	2	Total	C	H	N	O	0	0	0
			51	14	25	1	11			
2	I	2	Total	C	H	N	O	0	0	0
			51	14	25	1	11			
2	J	2	Total	C	H	N	O	0	0	0
			51	14	25	1	11			
2	K	2	Total	C	H	N	O	0	0	0
			51	14	25	1	11			
2	L	2	Total	C	H	N	O	0	0	0
			51	14	25	1	11			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		
3	E	1	Total	C	H	O	0	0
			14	3	8	3		
3	F	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is beta-D-galactopyranose (three-letter code: GAL) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	C	H	O	0	0
			22	6	11	5		

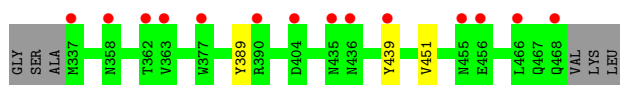
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	B	16	Total	O	0	0
			16	16		
5	C	62	Total	O	0	0
			62	62		
5	D	142	Total	O	0	0
			142	142		
5	E	157	Total	O	0	0
			157	157		
5	F	117	Total	O	0	0
			117	117		
5	G	24	Total	O	0	0
			24	24		

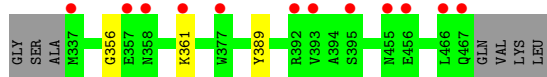
### 3 Residue-property plots [i](#)

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.

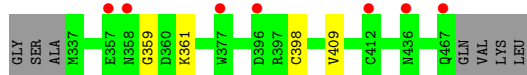
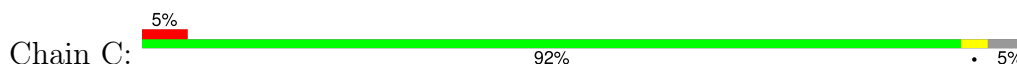
- Molecule 1: Cytolysin



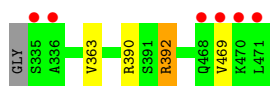
- Molecule 1: Cytolysin



- Molecule 1: Cytolysin



- Molecule 1: Cytolysin

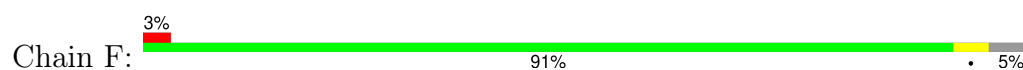


- Molecule 1: Cytolysin

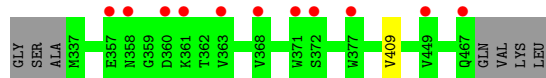


- Molecule 1: Cytolysin





- Molecule 1: Cytolysin



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



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



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



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	326.90Å 79.84Å 55.61Å 90.00° 95.71° 90.00°	Depositor
Resolution (Å)	40.16 – 2.10 40.16 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.16-2.10) 99.8 (40.16-2.10)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.94 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, $R_{free}$	0.162 , 0.188 0.168 , 0.194	Depositor DCC
$R_{free}$ test set	4152 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.2	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 54.5	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	0.96	EDS
Total number of atoms	14288	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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, GAL, GOL

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	0.37	0/985	0.52	0/1345
1	B	0.39	0/995	0.53	0/1360
1	C	0.55	0/1012	0.62	0/1378
1	D	0.88	0/1087	0.81	1/1478 (0.1%)
1	E	0.88	2/1055 (0.2%)	0.83	2/1435 (0.1%)
1	F	0.74	0/1022	0.74	1/1390 (0.1%)
1	G	0.40	0/991	0.54	0/1352
All	All	0.65	2/7147 (0.0%)	0.67	4/9738 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	387	GLU	CG-CD	5.83	1.60	1.51
1	E	456	GLU	CG-CD	5.33	1.59	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	398	CYS	CA-CB-SG	-7.86	99.86	114.00
1	D	390	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	E	397	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	F	388	ARG	NE-CZ-NH1	5.55	123.08	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	967	844	864	1	0
1	B	977	877	886	1	0
1	C	994	919	927	3	0
1	D	1067	983	1003	1	0
1	E	1035	974	975	3	0
1	F	1004	934	935	2	0
1	G	973	864	877	0	0
2	H	26	25	24	0	0
2	I	26	25	24	1	0
2	J	26	25	24	0	0
2	K	26	25	24	1	0
2	L	26	25	24	0	0
3	A	6	8	8	0	0
3	C	6	8	8	0	0
3	D	6	8	8	0	0
3	E	6	8	8	0	0
3	F	6	8	8	0	0
4	G	11	11	10	0	0
5	A	11	0	0	0	0
5	B	16	0	0	0	0
5	C	62	0	0	1	0
5	D	142	0	0	0	0
5	E	157	0	0	1	1
5	F	117	0	0	1	0
5	G	24	0	0	0	0
All	All	7717	6571	6637	11	1

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 1.

The worst 5 of 11 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:D:392:ARG:HH11	1:D:469:VAL:HG11	1.62	0.63
1:C:361:LYS:O	5:C:653:HOH:O	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:356:GLY:O	5:F:703:HOH:O	2.19	0.50
1:C:359:GLY:HA3	2:I:1:NAG:H83	1.94	0.50
1:E:359:GLY:HA3	2:K:1:NAG:H83	1.96	0.47

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:619:HOH:O	5:E:623:HOH:O[4_758]	2.09	0.11

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	130/138 (94%)	124 (95%)	6 (5%)	0	100	100
1	B	129/138 (94%)	121 (94%)	8 (6%)	0	100	100
1	C	129/138 (94%)	125 (97%)	4 (3%)	0	100	100
1	D	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
1	E	130/138 (94%)	126 (97%)	4 (3%)	0	100	100
1	F	129/138 (94%)	126 (98%)	3 (2%)	0	100	100
1	G	129/138 (94%)	121 (94%)	8 (6%)	0	100	100
All	All	911/966 (94%)	874 (96%)	37 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	92/116 (79%)	91 (99%)	1 (1%)	70	77
1	B	97/116 (84%)	96 (99%)	1 (1%)	73	79
1	C	102/116 (88%)	102 (100%)	0	100	100
1	D	112/116 (97%)	110 (98%)	2 (2%)	54	61
1	E	110/116 (95%)	110 (100%)	0	100	100
1	F	104/116 (90%)	102 (98%)	2 (2%)	52	59
1	G	95/116 (82%)	94 (99%)	1 (1%)	70	77
All	All	712/812 (88%)	705 (99%)	7 (1%)	73	79

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	392	ARG
1	F	389	TYR
1	G	409	VAL
1	F	395	SER
1	D	363	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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
2	NAG	H	1	2	15,15,15	0.38	0	21,21,21	0.41	0
2	GAL	H	2	2	11,11,12	0.75	0	15,15,17	0.94	0
2	NAG	I	1	2	15,15,15	0.31	0	21,21,21	0.38	0
2	GAL	I	2	2	11,11,12	0.82	0	15,15,17	0.75	0
2	NAG	J	1	2	15,15,15	0.68	1 (6%)	21,21,21	0.60	0
2	GAL	J	2	2	11,11,12	1.29	0	15,15,17	1.16	2 (13%)
2	NAG	K	1	2	15,15,15	0.29	0	21,21,21	0.61	0
2	GAL	K	2	2	11,11,12	1.29	1 (9%)	15,15,17	1.10	1 (6%)
2	NAG	L	1	2	15,15,15	0.45	0	21,21,21	0.59	0
2	GAL	L	2	2	11,11,12	1.90	3 (27%)	15,15,17	0.84	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
2	NAG	H	1	2	-	0/6/26/26	0/1/1/1
2	GAL	H	2	2	-	2/2/19/22	0/1/1/1
2	NAG	I	1	2	-	0/6/26/26	0/1/1/1
2	GAL	I	2	2	-	0/2/19/22	0/1/1/1
2	NAG	J	1	2	-	0/6/26/26	0/1/1/1
2	GAL	J	2	2	-	0/2/19/22	0/1/1/1
2	NAG	K	1	2	-	0/6/26/26	0/1/1/1
2	GAL	K	2	2	-	0/2/19/22	0/1/1/1
2	NAG	L	1	2	-	0/6/26/26	0/1/1/1
2	GAL	L	2	2	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	2	GAL	C2-C3	-4.63	1.45	1.52
2	L	2	GAL	O3-C3	2.37	1.48	1.43
2	K	2	GAL	C4-C3	2.20	1.58	1.52
2	L	2	GAL	O2-C2	-2.09	1.38	1.43
2	J	1	NAG	C1-C2	-2.04	1.50	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	2	GAL	O2-C2-C3	-2.59	104.79	110.15
2	J	2	GAL	O5-C5-C6	-2.45	102.90	107.66
2	K	2	GAL	C1-C2-C3	2.15	112.78	109.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	2	GAL	C4-C5-C6-O6
2	H	2	GAL	O5-C5-C6-O6

There are no ring outliers.

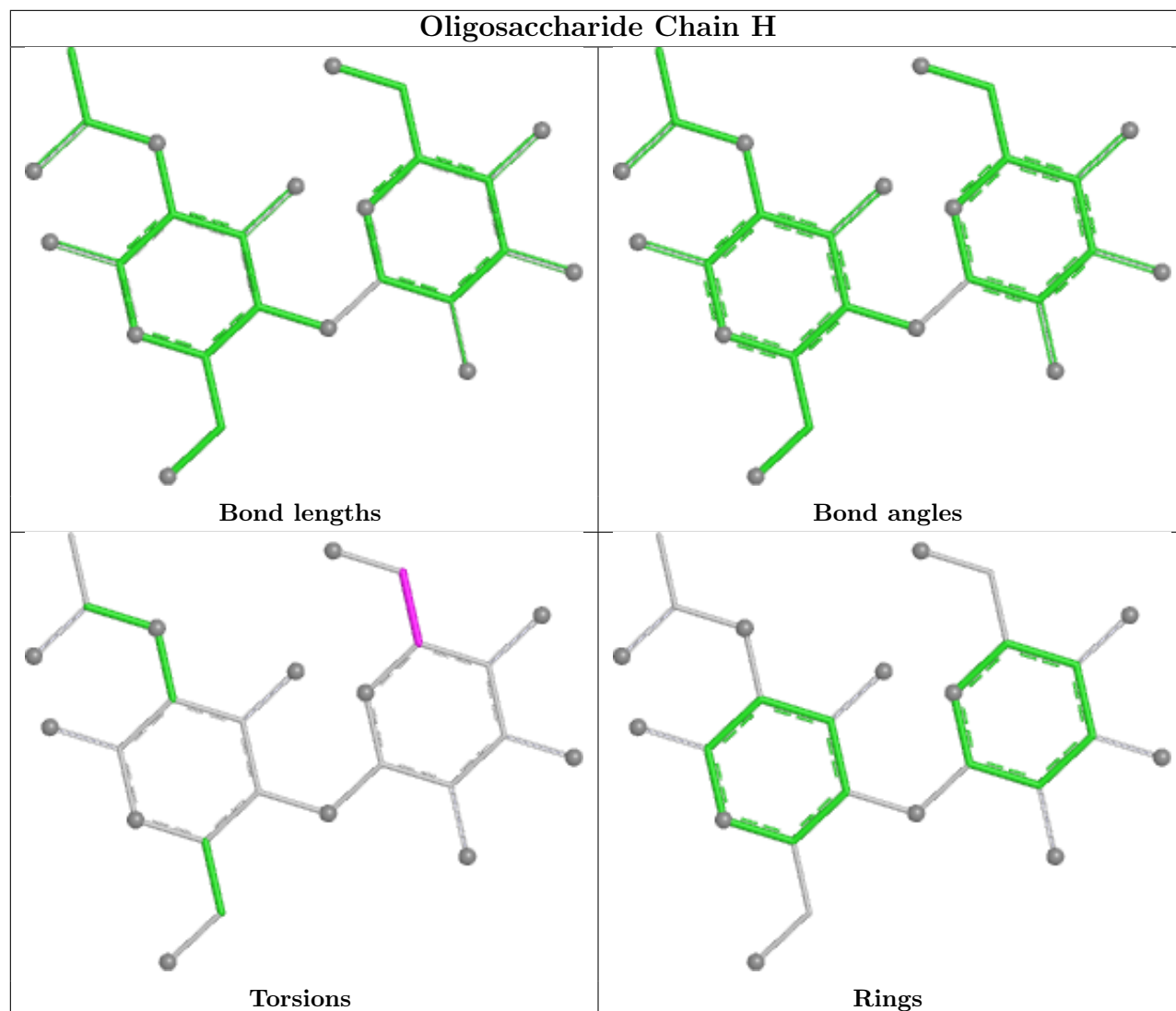
2 monomers are involved in 2 short contacts:

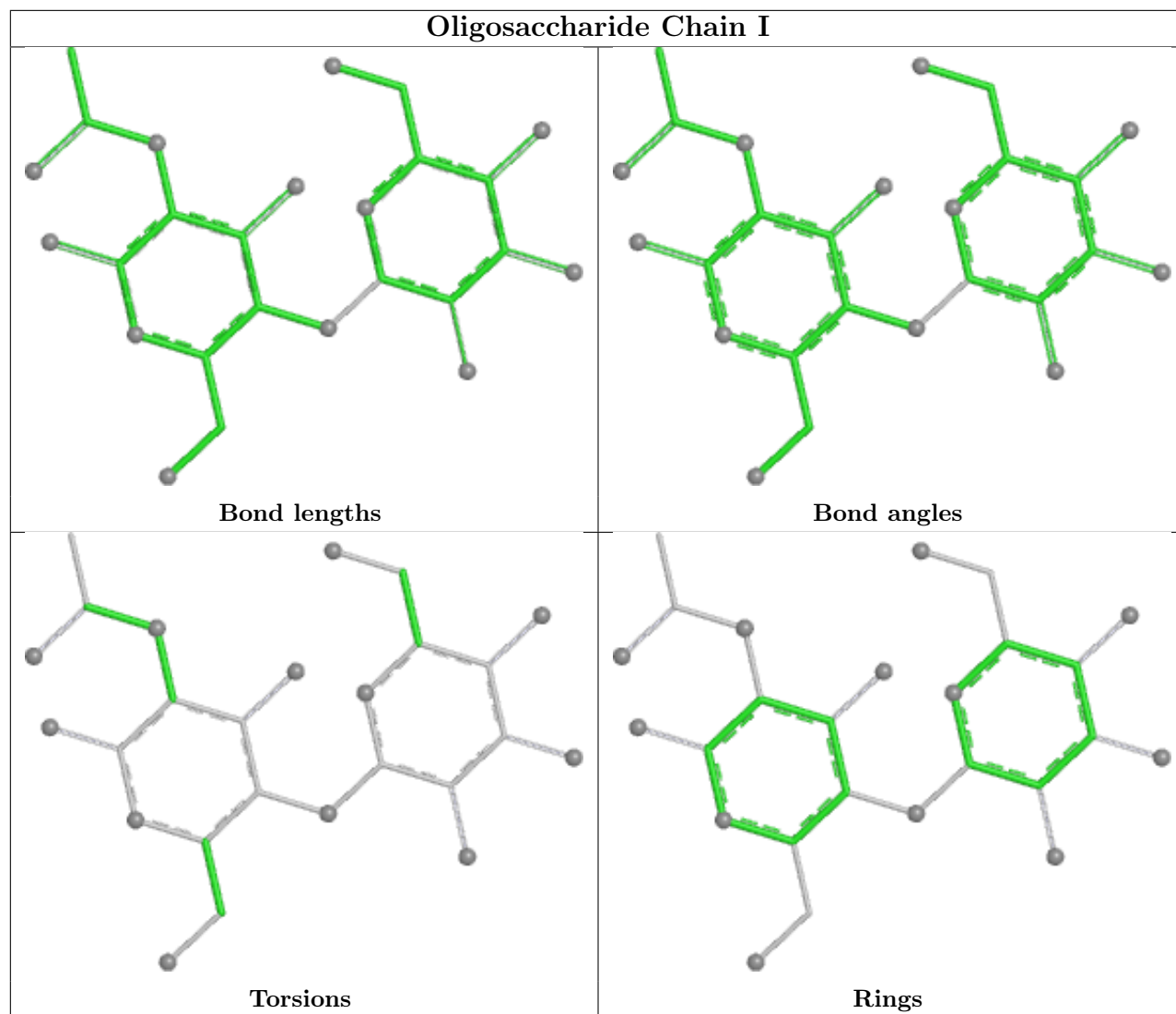
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1	NAG	1	0
2	I	1	NAG	1	0

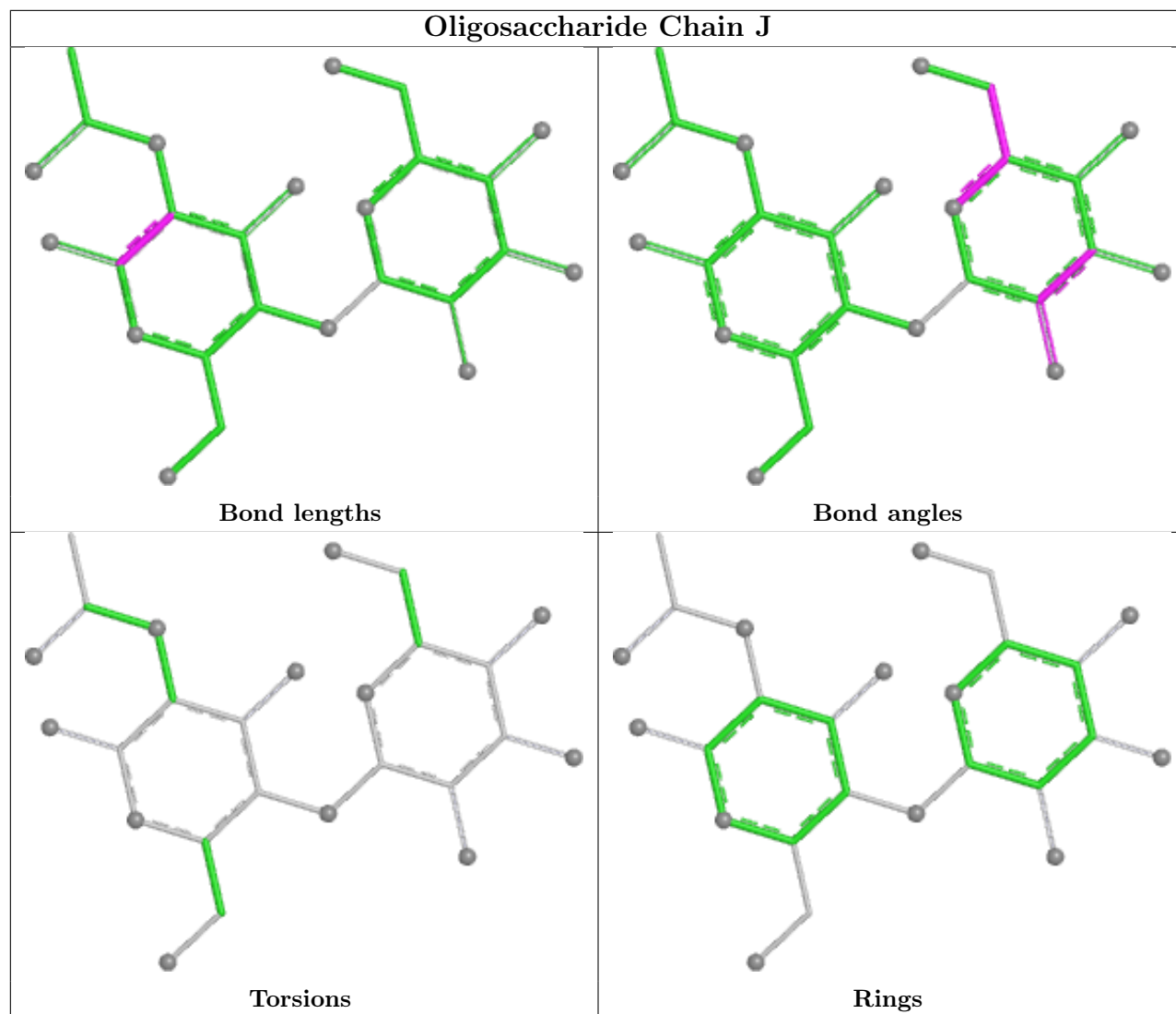
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



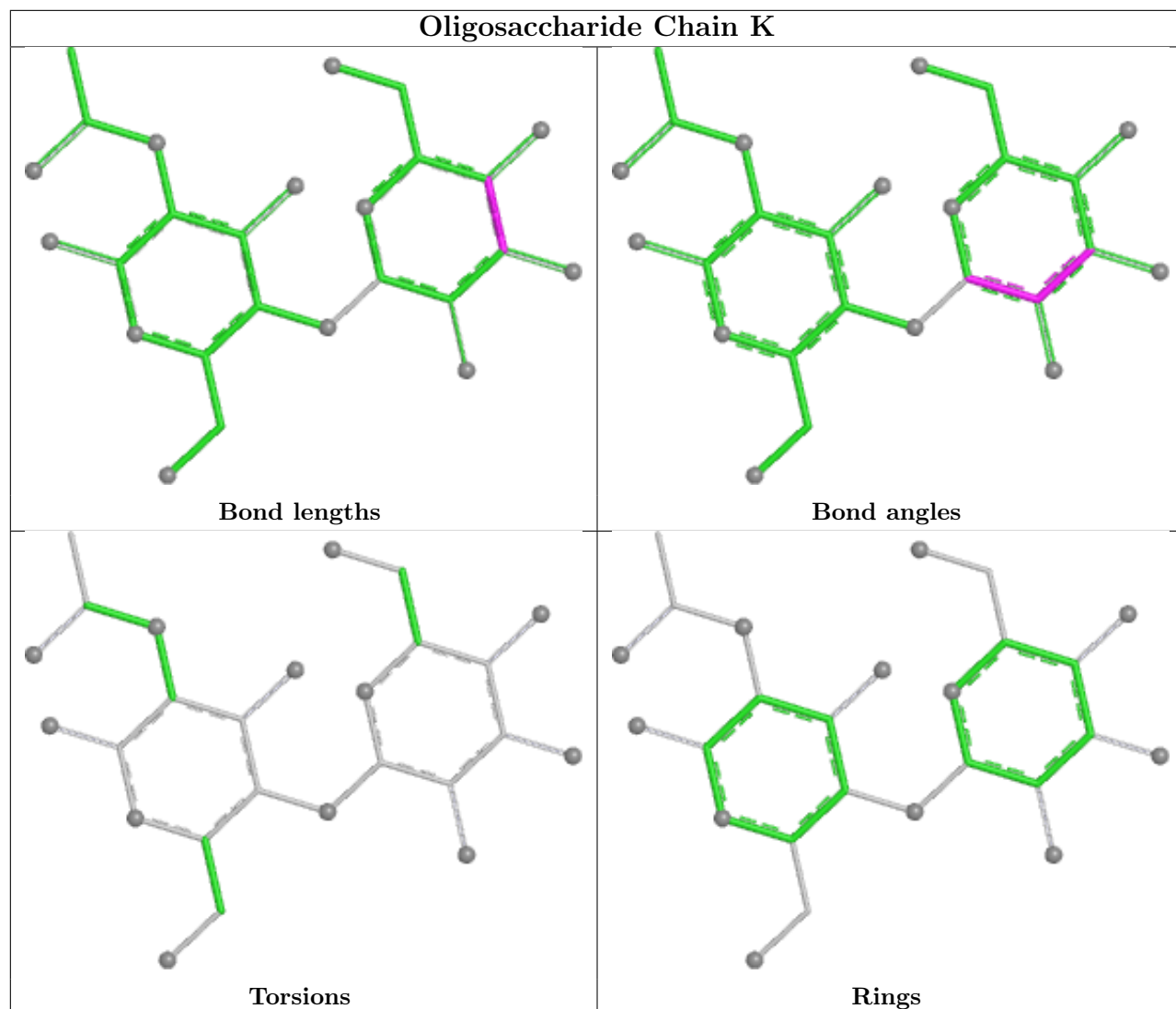
## Oligosaccharide Chain H

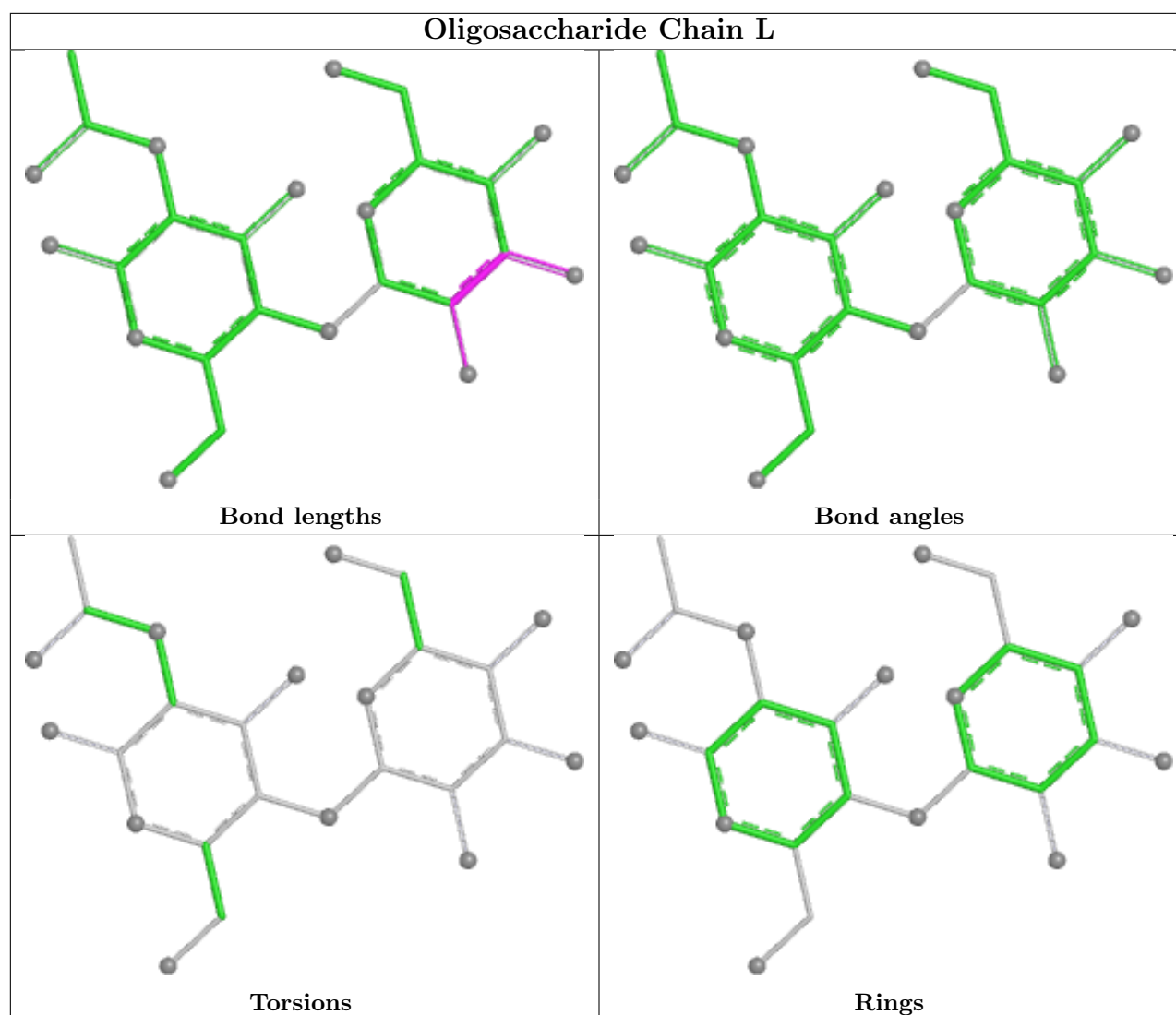






## Oligosaccharide Chain K





## 5.6 Ligand geometry [i](#)

6 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	$\# Z  > 2$
3	GOL	F	503	-	5,5,5	0.37	0	5,5,5	0.37	0
4	GAL	G	501	-	11,11,12	0.96	0	15,15,17	1.16	1 (6%)
3	GOL	D	503	-	5,5,5	0.50	0	5,5,5	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	C	503	-	5,5,5	0.38	0	5,5,5	0.32	0
3	GOL	E	503	-	5,5,5	0.39	0	5,5,5	0.25	0
3	GOL	A	501	-	5,5,5	0.33	0	5,5,5	0.39	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	GOL	F	503	-	-	0/4/4/4	-
4	GAL	G	501	-	-	2/2/19/22	0/1/1/1
3	GOL	D	503	-	-	0/4/4/4	-
3	GOL	C	503	-	-	0/4/4/4	-
3	GOL	E	503	-	-	2/4/4/4	-
3	GOL	A	501	-	-	1/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	501	GAL	C1-O5-C5	2.79	115.93	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	501	GAL	C4-C5-C6-O6
4	G	501	GAL	O5-C5-C6-O6
3	E	503	GOL	O1-C1-C2-C3
3	E	503	GOL	O1-C1-C2-O2
3	A	501	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

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	132/138 (95%)	0.78	14 (10%) 13 13	62, 81, 108, 121	0
1	B	131/138 (94%)	0.63	12 (9%) 16 17	59, 78, 103, 121	0
1	C	131/138 (94%)	0.30	7 (5%) 33 35	31, 59, 90, 110	0
1	D	137/138 (99%)	-0.50	6 (4%) 39 42	21, 31, 63, 88	0
1	E	132/138 (95%)	-0.64	0 100 100	18, 29, 49, 73	0
1	F	131/138 (94%)	-0.43	4 (3%) 51 53	23, 39, 59, 69	0
1	G	131/138 (94%)	0.73	11 (8%) 18 20	46, 80, 101, 133	0
All	All	925/966 (95%)	0.12	54 (5%) 30 32	18, 59, 98, 133	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	363	VAL	5.8
1	G	377	TRP	5.8
1	A	337	MET	5.4
1	G	357	GLU	4.8
1	G	467	GLN	4.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

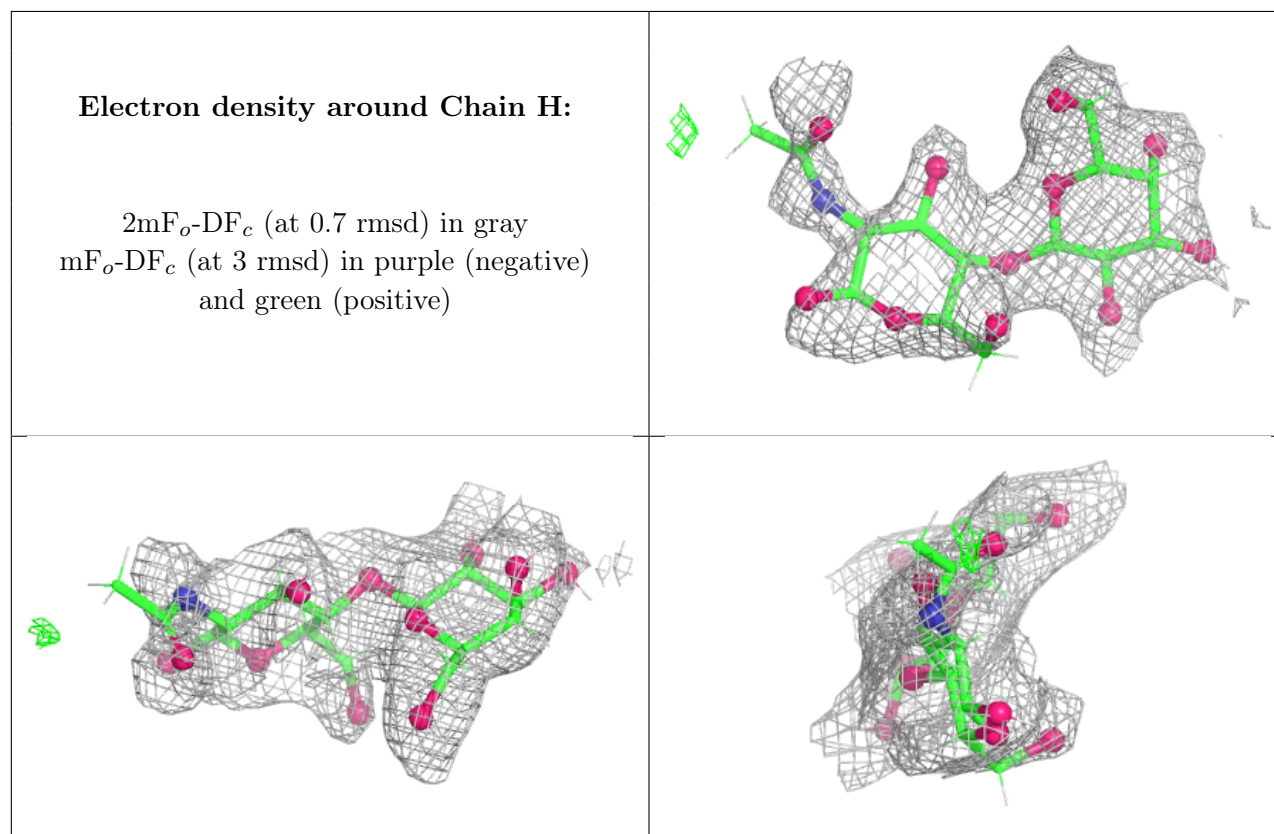
### 6.3 Carbohydrates [i](#)

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



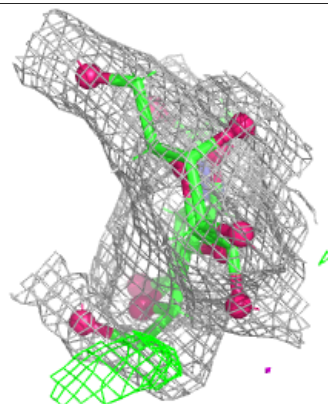
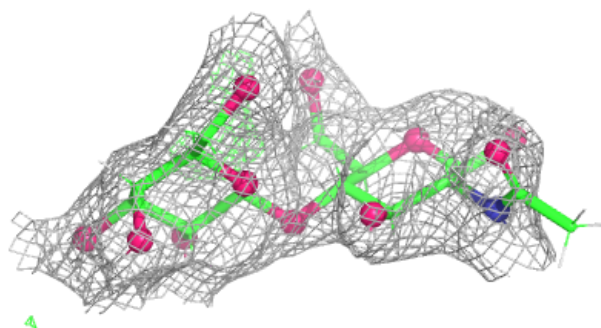
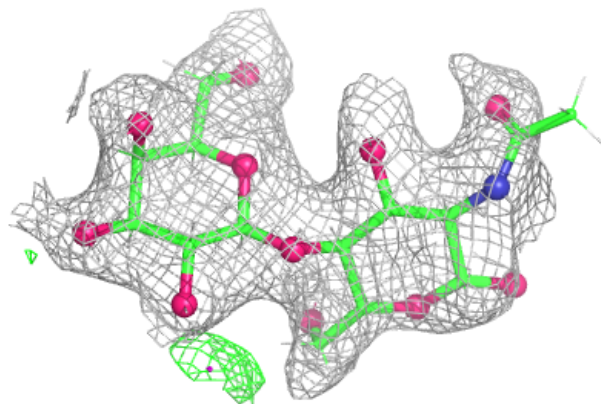
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	H	1	15/15	0.76	0.12	97,112,137,137	0
2	NAG	I	1	15/15	0.76	0.14	85,106,130,130	0
2	NAG	K	1	15/15	0.83	0.14	50,72,88,88	0
2	NAG	J	1	15/15	0.89	0.10	42,55,66,72	0
2	GAL	H	2	11/12	0.91	0.08	79,88,102,106	0
2	NAG	L	1	15/15	0.91	0.11	55,72,88,89	0
2	GAL	I	2	11/12	0.93	0.09	60,71,82,86	0
2	GAL	L	2	11/12	0.96	0.07	38,46,53,56	0
2	GAL	J	2	11/12	0.97	0.07	26,33,39,43	0
2	GAL	K	2	11/12	0.98	0.05	25,32,38,44	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

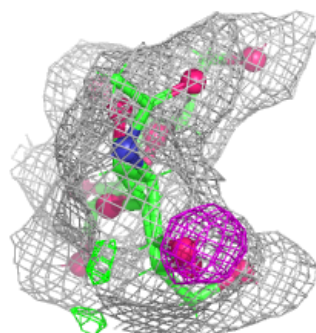
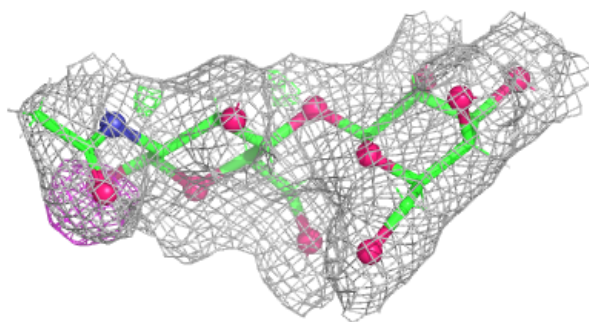
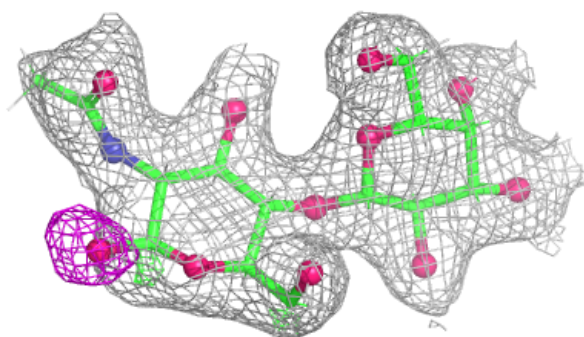


**Electron density around Chain I:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

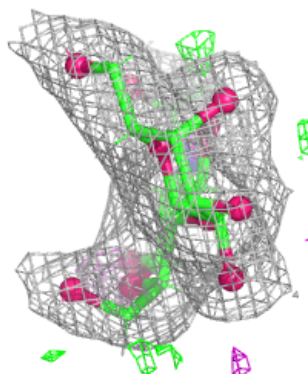
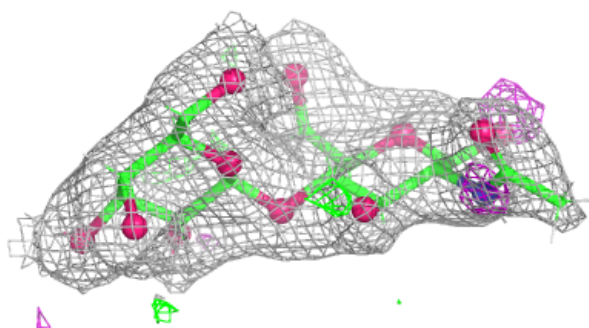
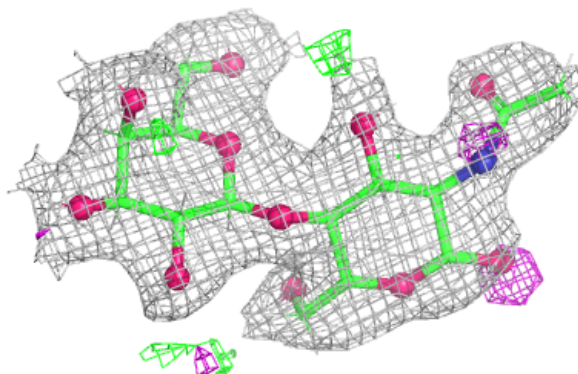
**Electron density around Chain J:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

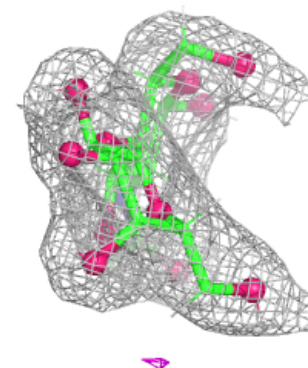
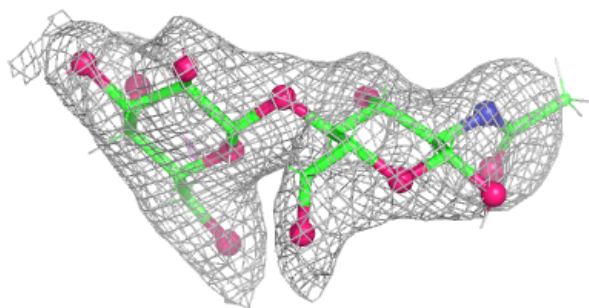
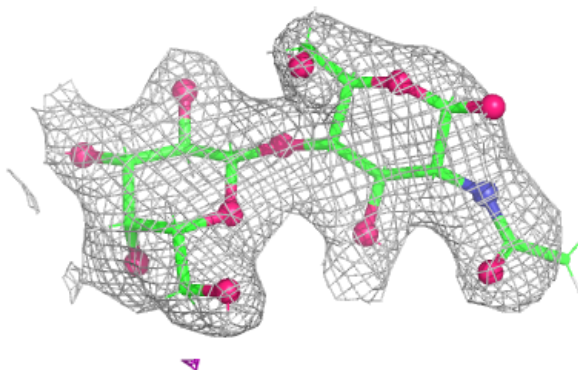


**Electron density around Chain K:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain L:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 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
4	GAL	G	501	11/12	0.75	0.17	92,103,120,123	0
3	GOL	F	503	6/6	0.79	0.18	73,88,90,91	0
3	GOL	E	503	6/6	0.79	0.17	62,74,77,77	0
3	GOL	A	501	6/6	0.81	0.16	78,93,97,100	0
3	GOL	C	503	6/6	0.85	0.18	79,95,99,102	0
3	GOL	D	503	6/6	0.86	0.12	53,64,69,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.