



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2025 – 10:43 PM EDT

PDB ID : 9MFG / pdb\_00009mfg  
Title : Complex of IL23 receptor and VHH  
Authors : Kiefer, J.R.; Wallweber, H.A.; Koerber, J.T.; Ota, N.; Davies, C.  
Deposited on : 2024-12-09  
Resolution : 2.85 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 : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

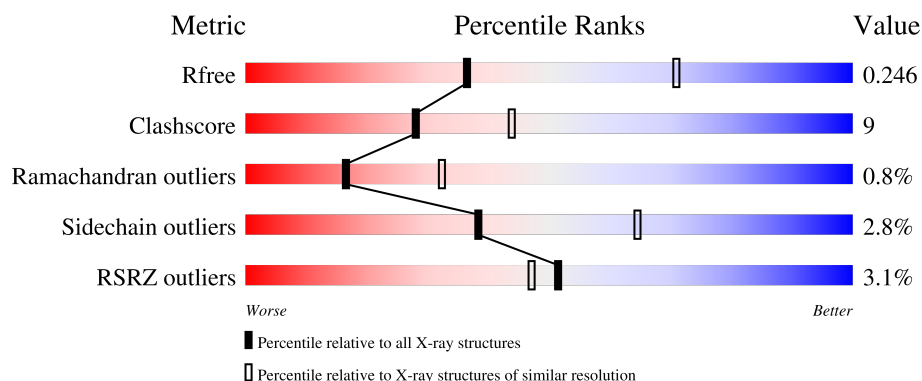
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	1268 (2.88-2.84)
Clashscore	180529	1351 (2.88-2.84)
Ramachandran outliers	177936	1318 (2.88-2.84)
Sidechain outliers	177891	1319 (2.88-2.84)
RSRZ outliers	164620	1269 (2.88-2.84)

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	304	<div> <div>3%</div> <div>80% 13% 7%</div> </div>
1	B	304	<div> <div>6%</div> <div>74% 21% . .</div> </div>
1	C	304	<div> <div>7%</div> <div>83% 14% .</div> </div>
1	D	304	<div> <div>2%</div> <div>82% 12% . .</div> </div>
2	E	120	<div> <div>87% 13%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	120	
2	G	120	
2	H	120	
3	I	3	
3	T	3	
4	J	2	
4	N	2	
4	Q	2	
4	R	2	
4	U	2	
5	K	4	
5	O	4	
6	L	4	
6	P	4	
6	S	4	
7	M	3	

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
8	NAG	B	401	-	-	X	-

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 25903 atoms, of which 12393 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 Interleukin-23 receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	284	Total	C	H	N	O	S	0	0	0
			4320	1432	2081	366	425	16			
1	B	298	Total	C	H	N	O	S	0	0	0
			4553	1504	2197	385	451	16			
1	C	295	Total	C	H	N	O	S	0	0	0
			4322	1435	2065	376	430	16			
1	D	291	Total	C	H	N	O	S	0	0	0
			4433	1470	2142	373	432	16			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	GLY	-	expression tag	UNP Q5VWK5
A	24	SER	-	expression tag	UNP Q5VWK5
A	318	GLY	-	expression tag	UNP Q5VWK5
A	319	ASN	-	expression tag	UNP Q5VWK5
A	320	SER	-	expression tag	UNP Q5VWK5
A	321	HIS	-	expression tag	UNP Q5VWK5
A	322	HIS	-	expression tag	UNP Q5VWK5
A	323	HIS	-	expression tag	UNP Q5VWK5
A	324	HIS	-	expression tag	UNP Q5VWK5
A	325	HIS	-	expression tag	UNP Q5VWK5
A	326	HIS	-	expression tag	UNP Q5VWK5
B	23	GLY	-	expression tag	UNP Q5VWK5
B	24	SER	-	expression tag	UNP Q5VWK5
B	318	GLY	-	expression tag	UNP Q5VWK5
B	319	ASN	-	expression tag	UNP Q5VWK5
B	320	SER	-	expression tag	UNP Q5VWK5
B	321	HIS	-	expression tag	UNP Q5VWK5
B	322	HIS	-	expression tag	UNP Q5VWK5
B	323	HIS	-	expression tag	UNP Q5VWK5
B	324	HIS	-	expression tag	UNP Q5VWK5
B	325	HIS	-	expression tag	UNP Q5VWK5

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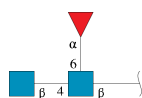
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Chain	Residue	Modelled	Actual	Comment	Reference
B	326	HIS	-	expression tag	UNP Q5VWK5
C	23	GLY	-	expression tag	UNP Q5VWK5
C	24	SER	-	expression tag	UNP Q5VWK5
C	318	GLY	-	expression tag	UNP Q5VWK5
C	319	ASN	-	expression tag	UNP Q5VWK5
C	320	SER	-	expression tag	UNP Q5VWK5
C	321	HIS	-	expression tag	UNP Q5VWK5
C	322	HIS	-	expression tag	UNP Q5VWK5
C	323	HIS	-	expression tag	UNP Q5VWK5
C	324	HIS	-	expression tag	UNP Q5VWK5
C	325	HIS	-	expression tag	UNP Q5VWK5
C	326	HIS	-	expression tag	UNP Q5VWK5
D	23	GLY	-	expression tag	UNP Q5VWK5
D	24	SER	-	expression tag	UNP Q5VWK5
D	318	GLY	-	expression tag	UNP Q5VWK5
D	319	ASN	-	expression tag	UNP Q5VWK5
D	320	SER	-	expression tag	UNP Q5VWK5
D	321	HIS	-	expression tag	UNP Q5VWK5
D	322	HIS	-	expression tag	UNP Q5VWK5
D	323	HIS	-	expression tag	UNP Q5VWK5
D	324	HIS	-	expression tag	UNP Q5VWK5
D	325	HIS	-	expression tag	UNP Q5VWK5
D	326	HIS	-	expression tag	UNP Q5VWK5

- Molecule 2 is a protein called VHH.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	120	Total	C	H	N	O	S	0	2	0
			1769	577	849	157	181	5			
2	F	120	Total	C	H	N	O	S	0	2	0
			1769	577	849	157	181	5			
2	G	120	Total	C	H	N	O	S	0	2	0
			1769	577	849	157	181	5			
2	H	120	Total	C	H	N	O	S	0	2	0
			1769	577	849	157	181	5			

- Molecule 3 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.



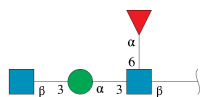
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	3	Total	C	H	N	O	0	0	0
			72	22	34	2	14			
3	T	3	Total	C	H	N	O	0	0	0
			72	22	34	2	14			

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



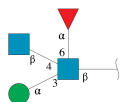
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
4	N	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
4	Q	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
4	R	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
4	U	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

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



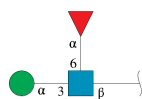
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	4	Total	C	H	N	O	0	0	0
			92	28	43	2	19			
5	O	4	Total	C	H	N	O	0	0	0
			92	28	43	2	19			

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



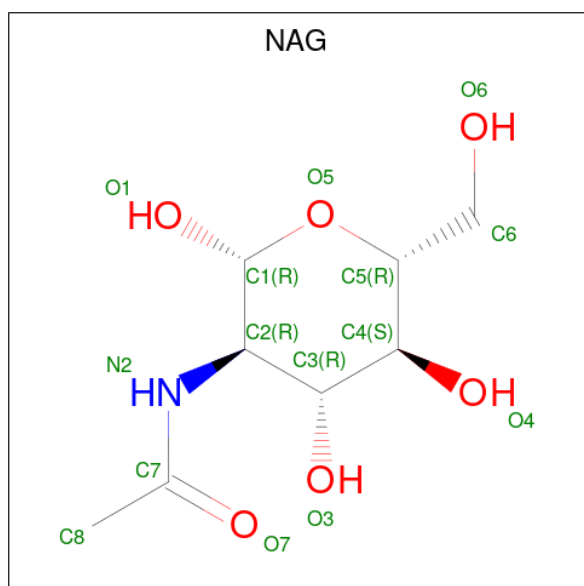
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	4	Total	C	H	N	O	0	0	0
			92	28	43	2	19			
6	P	4	Total	C	H	N	O	0	0	0
			92	28	43	2	19			
6	S	4	Total	C	H	N	O	0	0	0
			92	28	43	2	19			

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



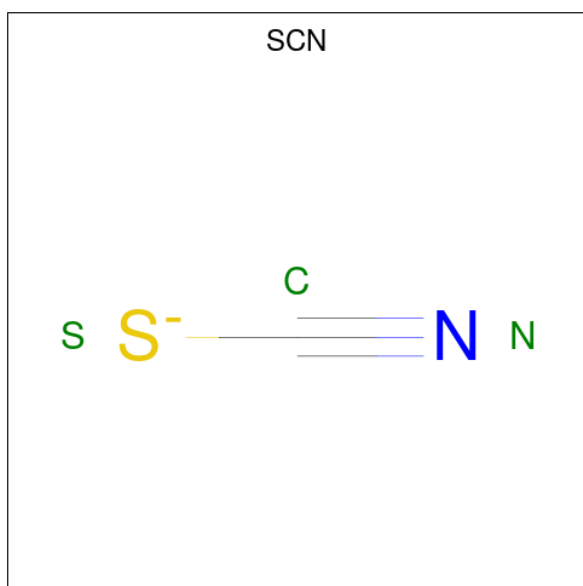
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	M	3	Total	C	H	N	O	0	0	0
			66	20	31	1	14			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
8	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
8	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
8	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
8	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 9 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	S	0	0
			3	1	1	1		
9	D	1	Total	C	N	S	0	0
			3	1	1	1		
9	D	1	Total	C	N	S	0	0
			3	1	1	1		
9	D	1	Total	C	N	S	0	0
			3	1	1	1		
9	G	1	Total	C	N	S	0	0
			3	1	1	1		

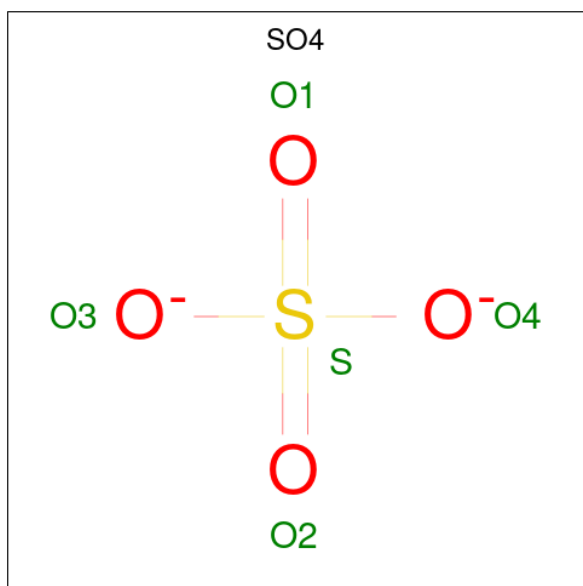
- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).





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

- Molecule 11 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	E	1	Total	O	S	0	0
			5	4	1		
11	F	1	Total	O	S	0	0
			5	4	1		

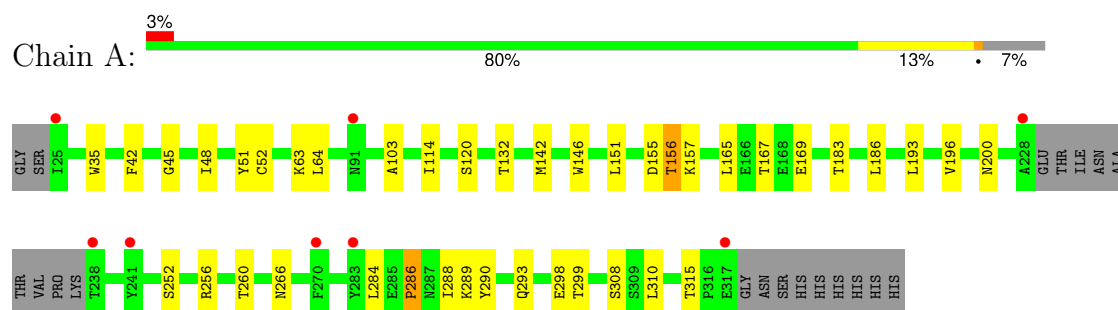
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	13	Total 13	O 13	0	0
12	B	16	Total 16	O 16	0	0
12	C	16	Total 16	O 16	0	0
12	D	12	Total 12	O 12	0	0
12	E	11	Total 11	O 11	0	0
12	F	11	Total 11	O 11	0	0
12	G	3	Total 3	O 3	0	0
12	H	8	Total 8	O 8	0	0

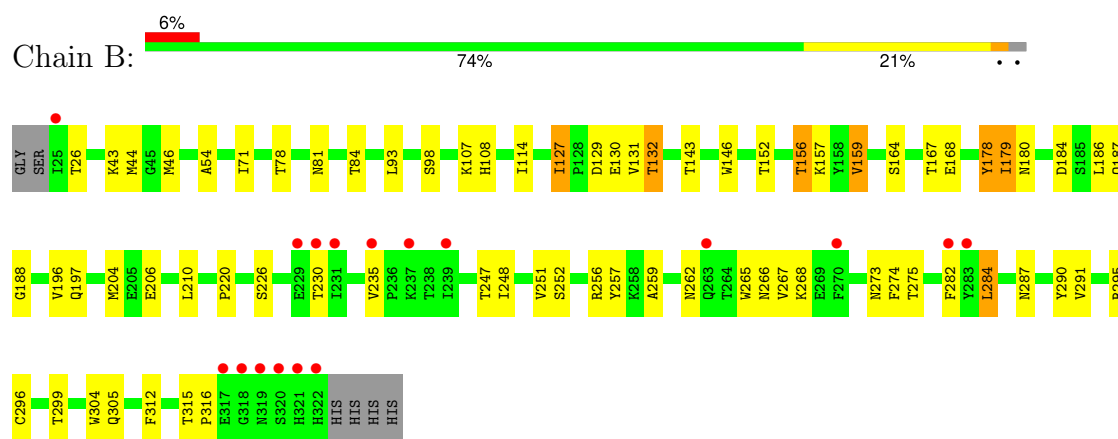
### 3 Residue-property plots [i](#)

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.

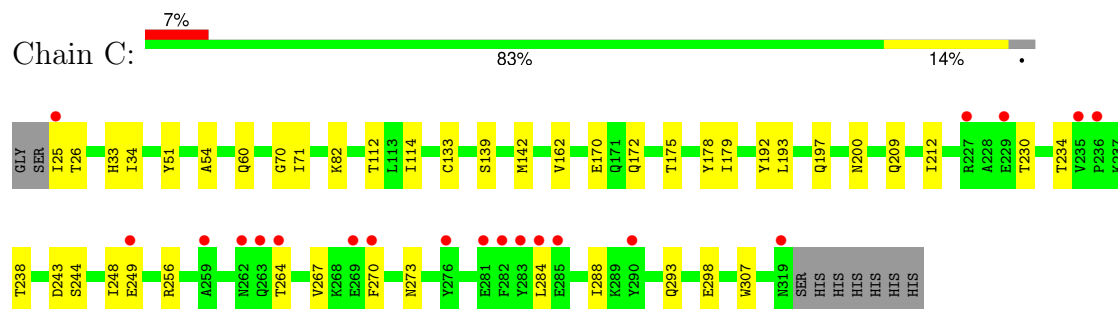
#### • Molecule 1: Interleukin-23 receptor



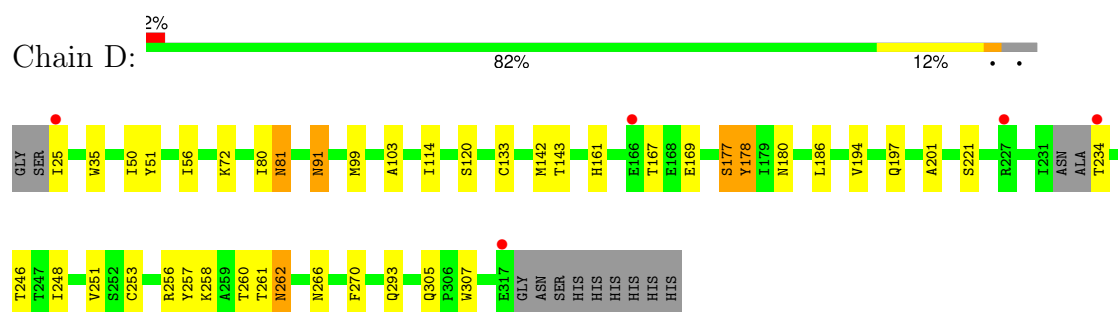
#### • Molecule 1: Interleukin-23 receptor



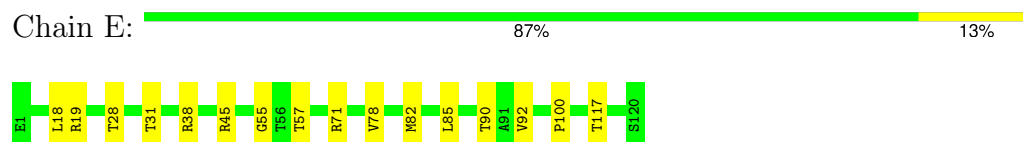
#### • Molecule 1: Interleukin-23 receptor



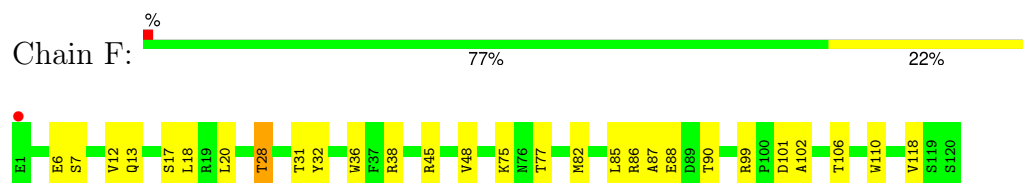
#### • Molecule 1: Interleukin-23 receptor



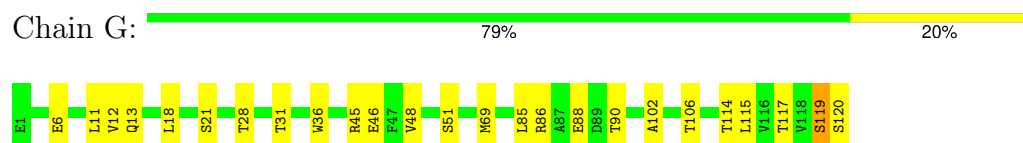
- Molecule 2: VHH



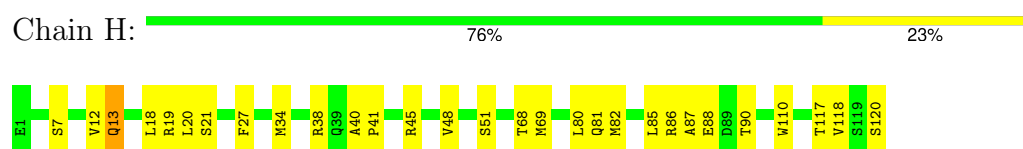
- Molecule 2: VHH



- Molecule 2: VHH



- Molecule 2: VHH



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



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





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

Chain J:

100%



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

Chain N:

50%

50%



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

Chain Q:

100%



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

Chain R:

50%

50%



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

Chain U:

100%



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

Chain K:

25%

75%

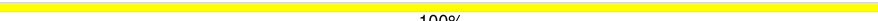


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  25% 50% 25%

NAG1  
MAN2  
FUC4

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

Chain L:  100%

NAG1  
MAN2  
FUC4

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

Chain P:  100%

NAG1  
MAN2  
FUC4

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

Chain S:  25% 50% 25%

NAG1  
MAN2  
FUC4

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

Chain M:  67% 33%

NAG1  
MAN2  
FUC3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.31Å 403.47Å 84.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.97 – 2.85 34.97 – 2.85	Depositor EDS
% Data completeness (in resolution range)	87.2 (34.97-2.85) 87.2 (34.97-2.85)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 2.85Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.204 , 0.246 0.204 , 0.246	Depositor DCC
$R_{free}$ test set	4151 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.8	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 60.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	25903	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: MAN, GOL, SCN, SO4, NAG, FUC

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	0.19	0/2298	0.36	0/3137
1	B	0.19	0/2419	0.37	0/3304
1	C	0.17	0/2314	0.36	0/3166
1	D	0.19	0/2352	0.38	0/3213
2	E	0.18	0/952	0.35	0/1293
2	F	0.18	0/952	0.37	0/1293
2	G	0.20	0/952	0.38	0/1293
2	H	0.21	0/952	0.36	0/1293
All	All	0.19	0/13191	0.37	0/17992

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	2239	2081	2081	30	0
1	B	2356	2197	2197	54	0
1	C	2257	2065	2065	35	0
1	D	2291	2142	2142	30	0
2	E	920	849	842	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	920	849	842	20	0
2	G	920	849	842	23	0
2	H	920	849	842	21	0
3	I	38	34	34	2	0
3	T	38	34	34	0	0
4	J	28	25	25	0	0
4	N	28	25	25	3	0
4	Q	28	25	25	2	0
4	R	28	25	25	1	0
4	U	28	25	25	0	0
5	K	49	43	43	3	0
5	O	49	43	43	1	0
6	L	49	43	43	0	0
6	P	49	43	43	0	0
6	S	49	43	43	3	0
7	M	35	31	31	0	0
8	A	28	26	26	0	0
8	B	14	13	13	7	0
8	C	14	13	13	1	0
8	D	14	13	13	1	0
9	A	3	0	0	1	0
9	D	9	0	0	0	0
9	G	3	0	0	0	0
10	E	6	8	8	0	0
11	E	5	0	0	0	0
11	F	5	0	0	0	0
12	A	13	0	0	0	0
12	B	16	0	0	0	0
12	C	16	0	0	0	0
12	D	12	0	0	1	0
12	E	11	0	0	0	0
12	F	11	0	0	0	0
12	G	3	0	0	0	0
12	H	8	0	0	1	0
All	All	13510	12393	12365	227	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 9.

The worst 5 of 227 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:G:12:VAL:HG11	2:G:85:LEU:HD13	1.44	1.00
2:H:12:VAL:HG21	2:H:18:LEU:HD22	1.54	0.87
1:A:167:THR:OG1	1:A:169:GLU:OE2	1.98	0.81
2:G:12:VAL:HG11	2:G:85:LEU:CD1	2.13	0.78
1:A:284:LEU:HD11	1:A:315:THR:HG21	1.66	0.78

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	280/304 (92%)	254 (91%)	25 (9%)	1 (0%)	30	49
1	B	296/304 (97%)	267 (90%)	27 (9%)	2 (1%)	19	36
1	C	293/304 (96%)	263 (90%)	26 (9%)	4 (1%)	9	20
1	D	287/304 (94%)	266 (93%)	18 (6%)	3 (1%)	13	26
2	E	120/120 (100%)	108 (90%)	11 (9%)	1 (1%)	16	32
2	F	120/120 (100%)	111 (92%)	8 (7%)	1 (1%)	16	32
2	G	120/120 (100%)	108 (90%)	11 (9%)	1 (1%)	16	32
2	H	120/120 (100%)	112 (93%)	8 (7%)	0	100	100
All	All	1636/1696 (96%)	1489 (91%)	134 (8%)	13 (1%)	16	32

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	288	ILE
1	D	178	TYR
1	A	286	PRO
1	C	249	GLU
1	D	177	SER

### 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	239/276 (87%)	234 (98%)	5 (2%)	48	72
1	B	254/276 (92%)	242 (95%)	12 (5%)	22	44
1	C	233/276 (84%)	231 (99%)	2 (1%)	75	88
1	D	245/276 (89%)	239 (98%)	6 (2%)	44	69
2	E	93/95 (98%)	91 (98%)	2 (2%)	47	71
2	F	93/95 (98%)	90 (97%)	3 (3%)	34	60
2	G	93/95 (98%)	88 (95%)	5 (5%)	18	37
2	H	93/95 (98%)	86 (92%)	7 (8%)	11	24
All	All	1343/1484 (90%)	1301 (97%)	42 (3%)	38	61

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	45[B]	ARG
2	H	7	SER
2	F	101	ASP
2	G	45[B]	ARG
2	H	21	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	209	GLN
2	E	76	ASN
2	H	76	ASN
2	F	76	ASN
1	C	29	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 ⓘ

39 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	I	1	1,3	14,14,15	0.67	0	17,19,21	1.11	1 (5%)
3	NAG	I	2	3	14,14,15	0.70	0	17,19,21	0.82	0
3	FUC	I	3	3	10,10,11	0.81	0	14,14,16	1.01	0
4	NAG	J	1	1,4	14,14,15	0.63	0	17,19,21	1.41	2 (11%)
4	NAG	J	2	4	14,14,15	0.70	0	17,19,21	1.08	1 (5%)
5	NAG	K	1	1,5	14,14,15	0.78	0	17,19,21	1.15	1 (5%)
5	MAN	K	2	5	11,11,12	0.74	0	15,15,17	1.85	4 (26%)
5	NAG	K	3	5	14,14,15	0.68	0	17,19,21	1.66	3 (17%)
5	FUC	K	4	5	10,10,11	0.67	0	14,14,16	1.09	1 (7%)
6	NAG	L	1	1,6	14,14,15	0.69	0	17,19,21	1.38	3 (17%)
6	MAN	L	2	6	11,11,12	0.81	1 (9%)	15,15,17	1.07	0
6	NAG	L	3	6	14,14,15	0.64	0	17,19,21	1.36	3 (17%)
6	FUC	L	4	6	10,10,11	0.60	0	14,14,16	1.78	3 (21%)
7	NAG	M	1	1,7	14,14,15	0.64	0	17,19,21	0.87	0
7	MAN	M	2	7	11,11,12	0.67	0	15,15,17	2.54	3 (20%)
7	FUC	M	3	7	10,10,11	0.85	0	14,14,16	1.20	0
4	NAG	N	1	1,4	14,14,15	0.71	0	17,19,21	1.31	3 (17%)
4	NAG	N	2	4	14,14,15	0.66	0	17,19,21	0.75	0
5	NAG	O	1	1,5	14,14,15	0.67	0	17,19,21	0.94	0
5	MAN	O	2	5	11,11,12	0.89	1 (9%)	15,15,17	1.73	5 (33%)
5	NAG	O	3	5	14,14,15	0.68	0	17,19,21	1.42	2 (11%)
5	FUC	O	4	5	10,10,11	0.67	0	14,14,16	1.20	1 (7%)
6	NAG	P	1	1,6	14,14,15	0.63	0	17,19,21	1.68	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	MAN	P	2	6	11,11,12	0.64	0	15,15,17	1.70	4 (26%)
6	NAG	P	3	6	14,14,15	0.66	0	17,19,21	0.92	1 (5%)
6	FUC	P	4	6	10,10,11	0.78	0	14,14,16	1.19	1 (7%)
4	NAG	Q	1	1,4	14,14,15	0.78	0	17,19,21	1.35	2 (11%)
4	NAG	Q	2	4	14,14,15	0.77	0	17,19,21	1.65	3 (17%)
4	NAG	R	1	1,4	14,14,15	0.59	0	17,19,21	0.94	1 (5%)
4	NAG	R	2	4	14,14,15	0.69	0	17,19,21	0.85	0
6	NAG	S	1	1,6	14,14,15	0.65	0	17,19,21	2.28	3 (17%)
6	MAN	S	2	6	11,11,12	0.72	0	15,15,17	1.18	1 (6%)
6	NAG	S	3	6	14,14,15	0.83	1 (7%)	17,19,21	1.48	2 (11%)
6	FUC	S	4	6	10,10,11	0.73	0	14,14,16	1.11	0
3	NAG	T	1	1,3	14,14,15	0.85	0	17,19,21	1.95	3 (17%)
3	NAG	T	2	3	14,14,15	0.65	0	17,19,21	0.98	0
3	FUC	T	3	3	10,10,11	0.86	0	14,14,16	0.97	1 (7%)
4	NAG	U	1	1,4	14,14,15	0.66	0	17,19,21	1.11	2 (11%)
4	NAG	U	2	4	14,14,15	0.69	0	17,19,21	0.95	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
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1
3	FUC	I	3	3	-	-	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
5	NAG	K	1	1,5	-	0/6/23/26	0/1/1/1
5	MAN	K	2	5	-	1/2/19/22	0/1/1/1
5	NAG	K	3	5	-	0/6/23/26	0/1/1/1
5	FUC	K	4	5	-	-	0/1/1/1
6	NAG	L	1	1,6	-	2/6/23/26	0/1/1/1
6	MAN	L	2	6	-	2/2/19/22	0/1/1/1
6	NAG	L	3	6	-	0/6/23/26	0/1/1/1
6	FUC	L	4	6	-	-	0/1/1/1
7	NAG	M	1	1,7	-	2/6/23/26	0/1/1/1
7	MAN	M	2	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FUC	M	3	7	-	-	0/1/1/1
4	NAG	N	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
5	NAG	O	1	1,5	-	0/6/23/26	0/1/1/1
5	MAN	O	2	5	-	2/2/19/22	0/1/1/1
5	NAG	O	3	5	-	0/6/23/26	0/1/1/1
5	FUC	O	4	5	-	-	0/1/1/1
6	NAG	P	1	1,6	-	0/6/23/26	0/1/1/1
6	MAN	P	2	6	-	0/2/19/22	0/1/1/1
6	NAG	P	3	6	-	0/6/23/26	0/1/1/1
6	FUC	P	4	6	-	-	0/1/1/1
4	NAG	Q	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
6	NAG	S	1	1,6	-	2/6/23/26	0/1/1/1
6	MAN	S	2	6	-	2/2/19/22	0/1/1/1
6	NAG	S	3	6	-	4/6/23/26	0/1/1/1
6	FUC	S	4	6	-	-	0/1/1/1
3	NAG	T	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	FUC	T	3	3	-	-	0/1/1/1
4	NAG	U	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	S	3	NAG	C1-C2	2.52	1.55	1.52
5	O	2	MAN	O5-C1	-2.15	1.40	1.43
6	L	2	MAN	O5-C1	-2.03	1.40	1.43

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	2	MAN	C1-O5-C5	7.90	122.78	112.19
6	S	1	NAG	C1-O5-C5	6.98	121.55	112.19
3	T	1	NAG	C1-O5-C5	-6.03	104.11	112.19
6	P	1	NAG	C1-O5-C5	5.18	119.14	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	4	FUC	C1-C2-C3	5.03	116.96	109.64

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

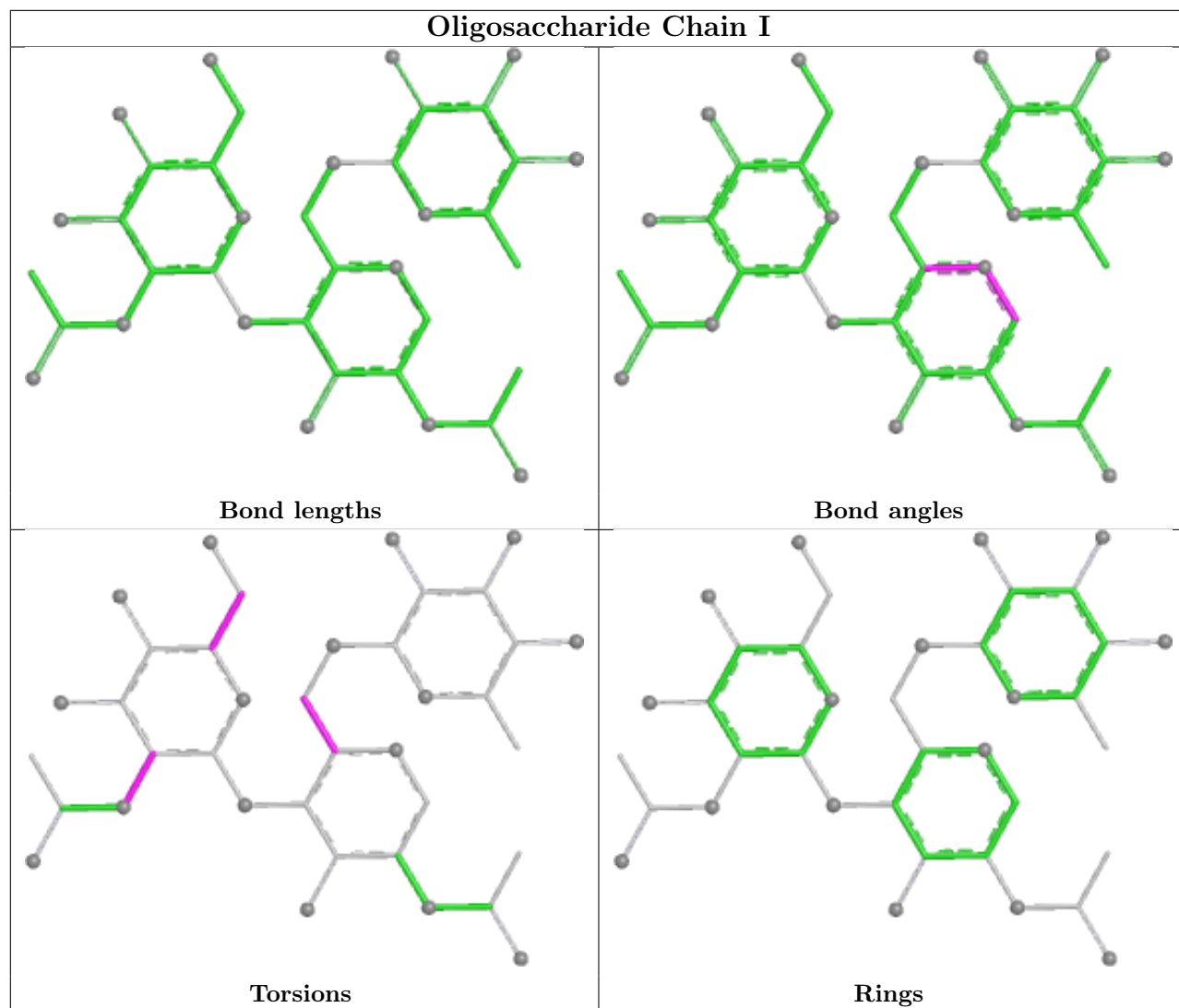
Mol	Chain	Res	Type	Atoms
3	I	2	NAG	C1-C2-N2-C7
4	N	2	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
6	S	2	MAN	O5-C5-C6-O6

There are no ring outliers.

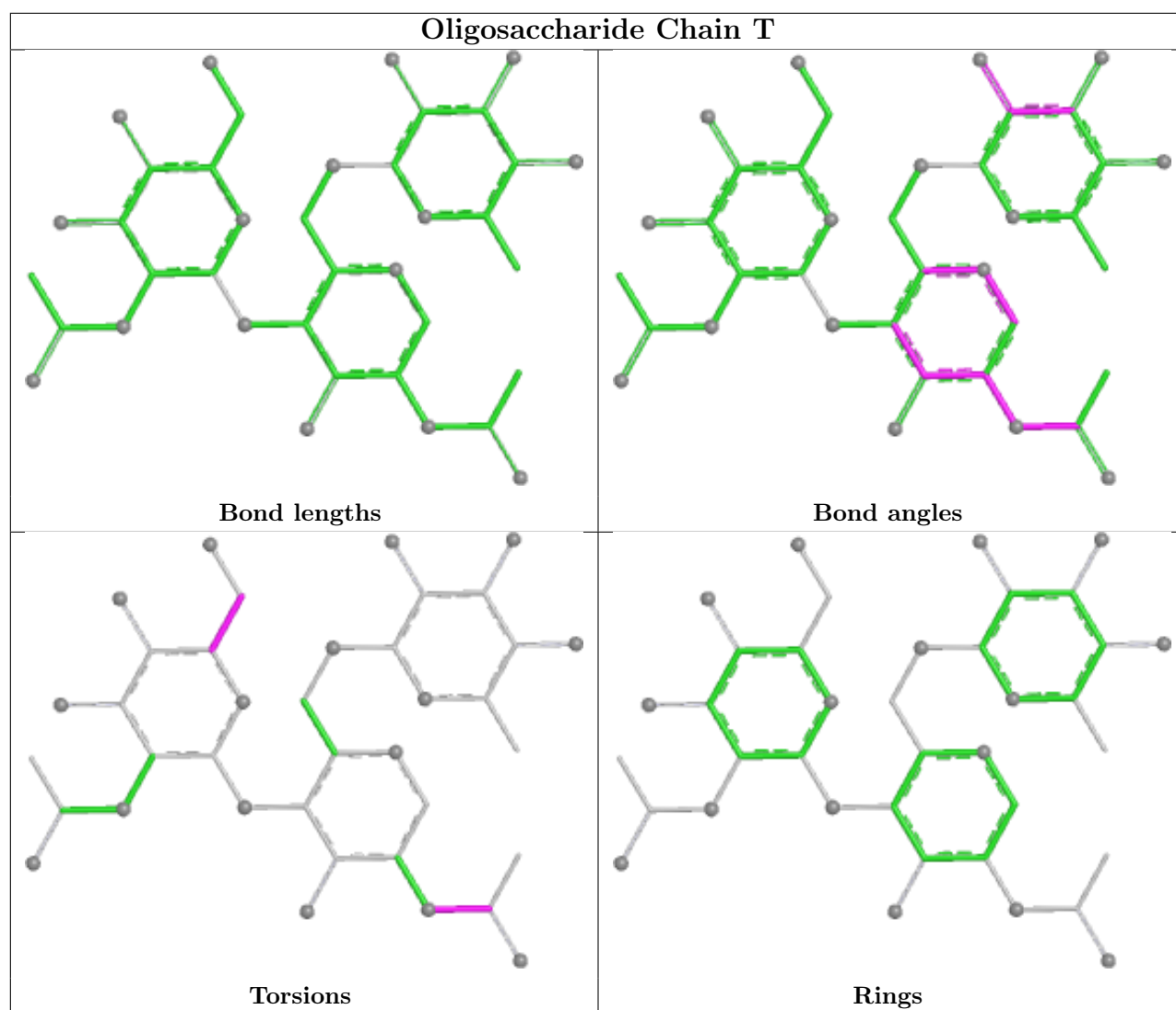
11 monomers are involved in 15 short contacts:

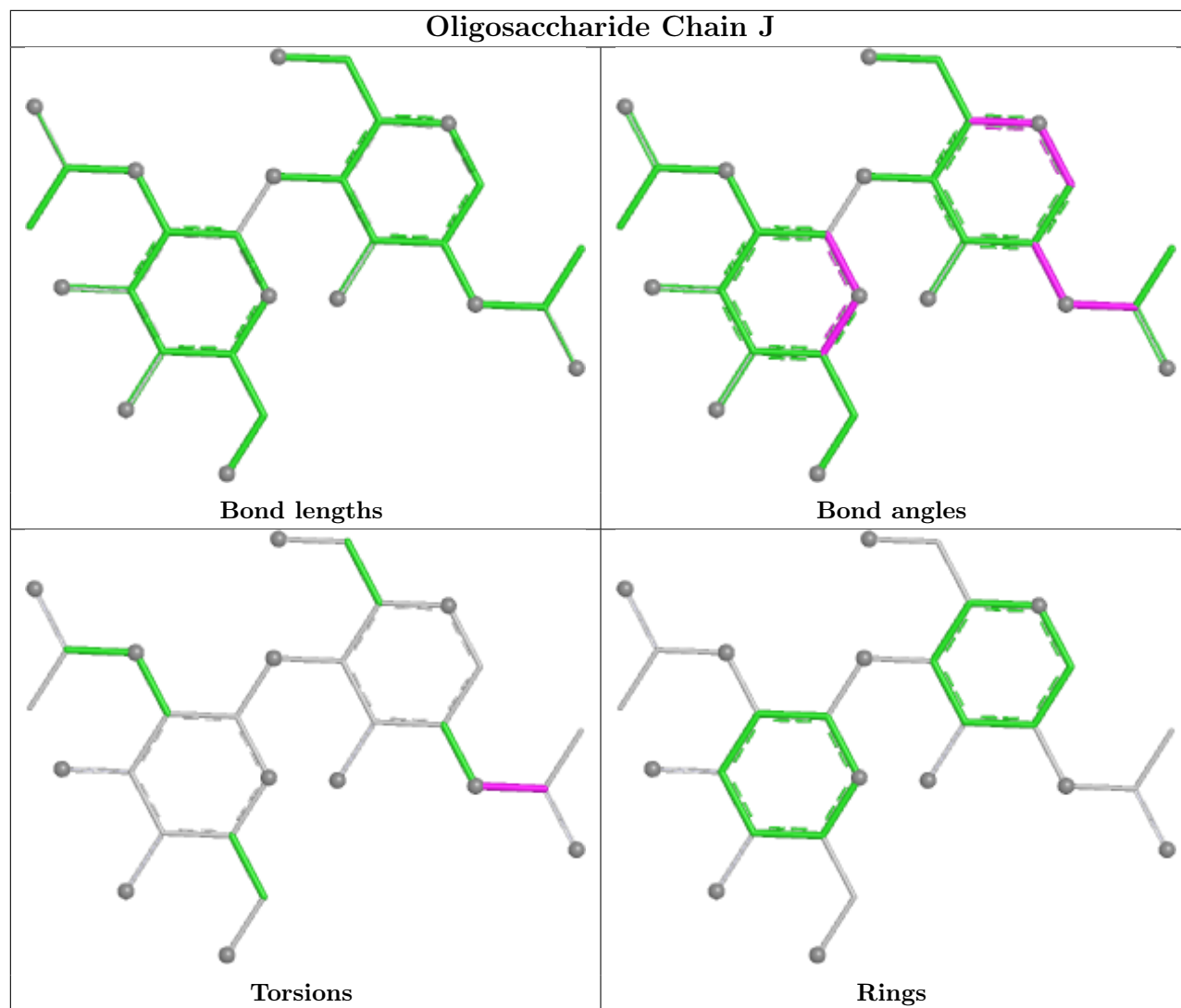
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Q	2	NAG	2	0
4	R	1	NAG	1	0
3	I	1	NAG	2	0
5	O	4	FUC	1	0
6	S	3	NAG	3	0
3	I	2	NAG	1	0
4	N	1	NAG	3	0
5	K	2	MAN	1	0
4	Q	1	NAG	1	0
5	K	3	NAG	2	0
5	K	1	NAG	3	0

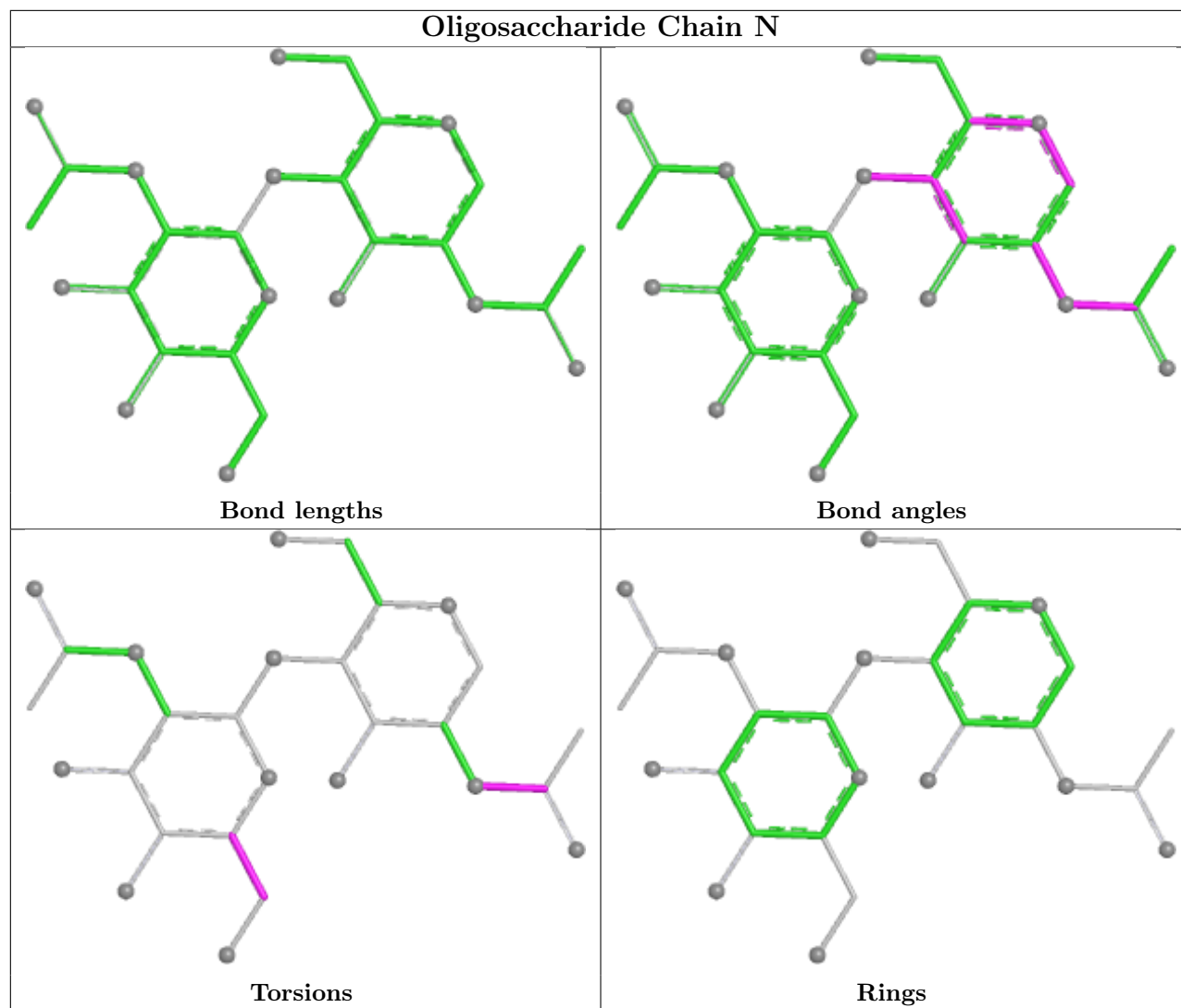
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

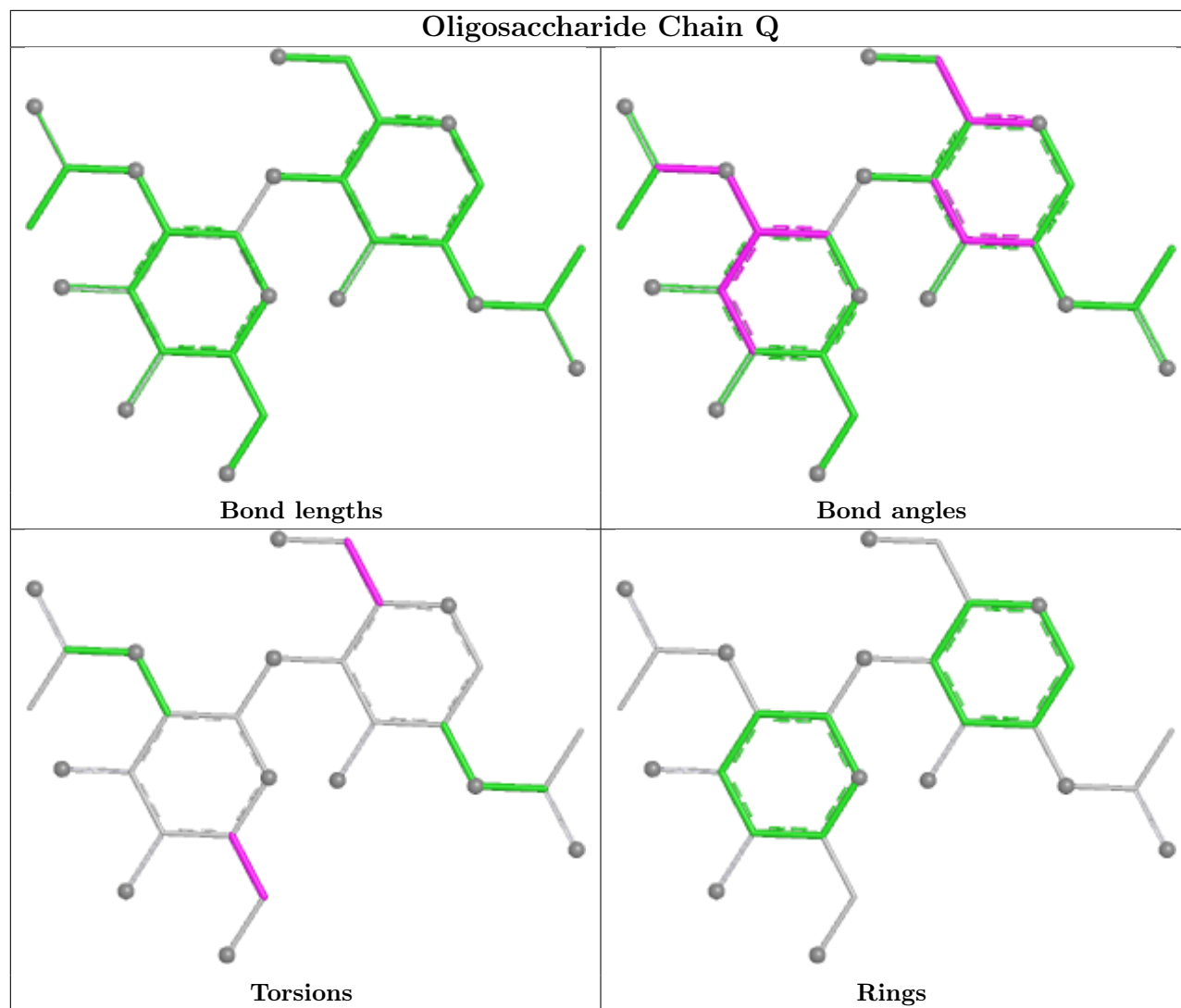


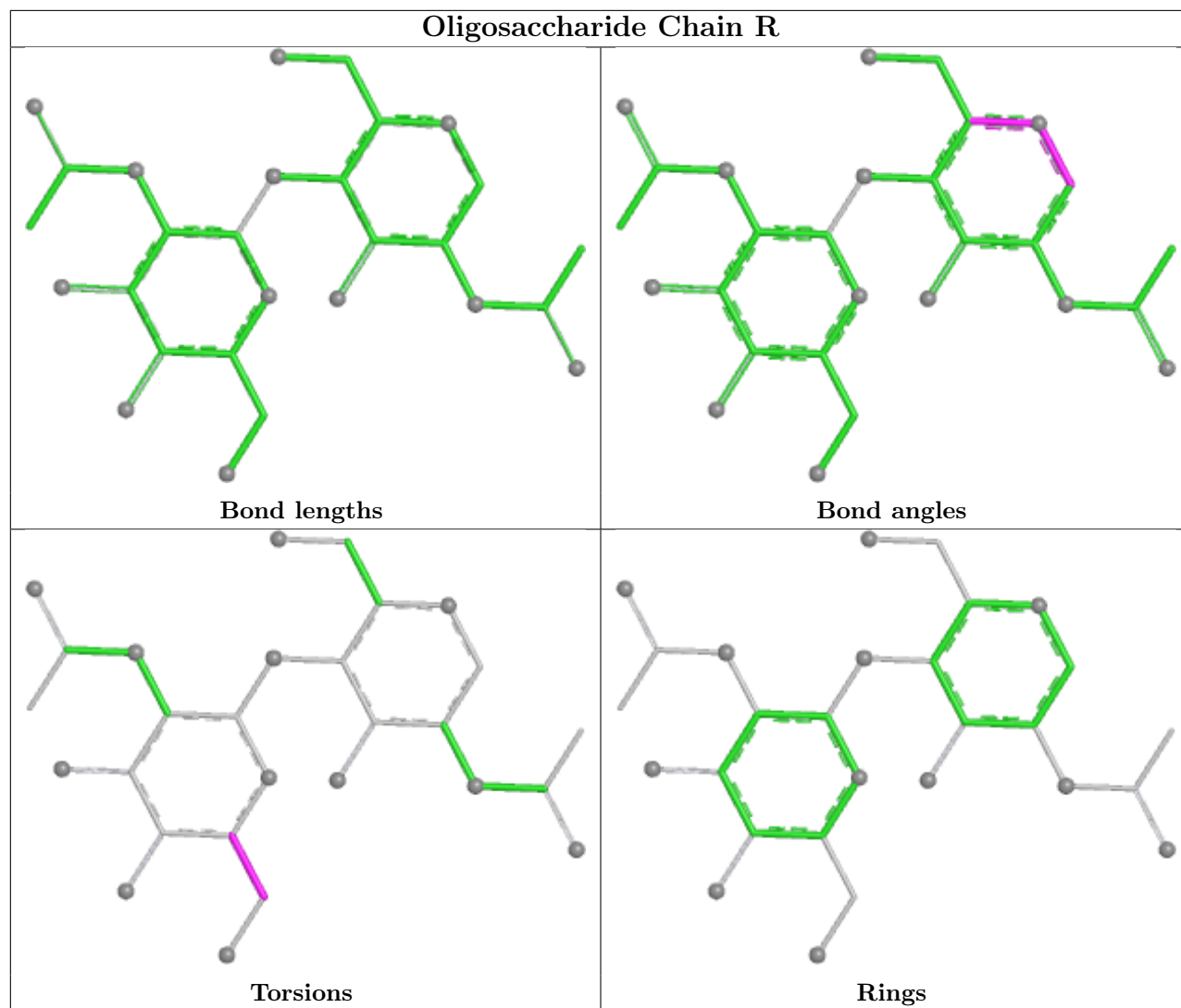


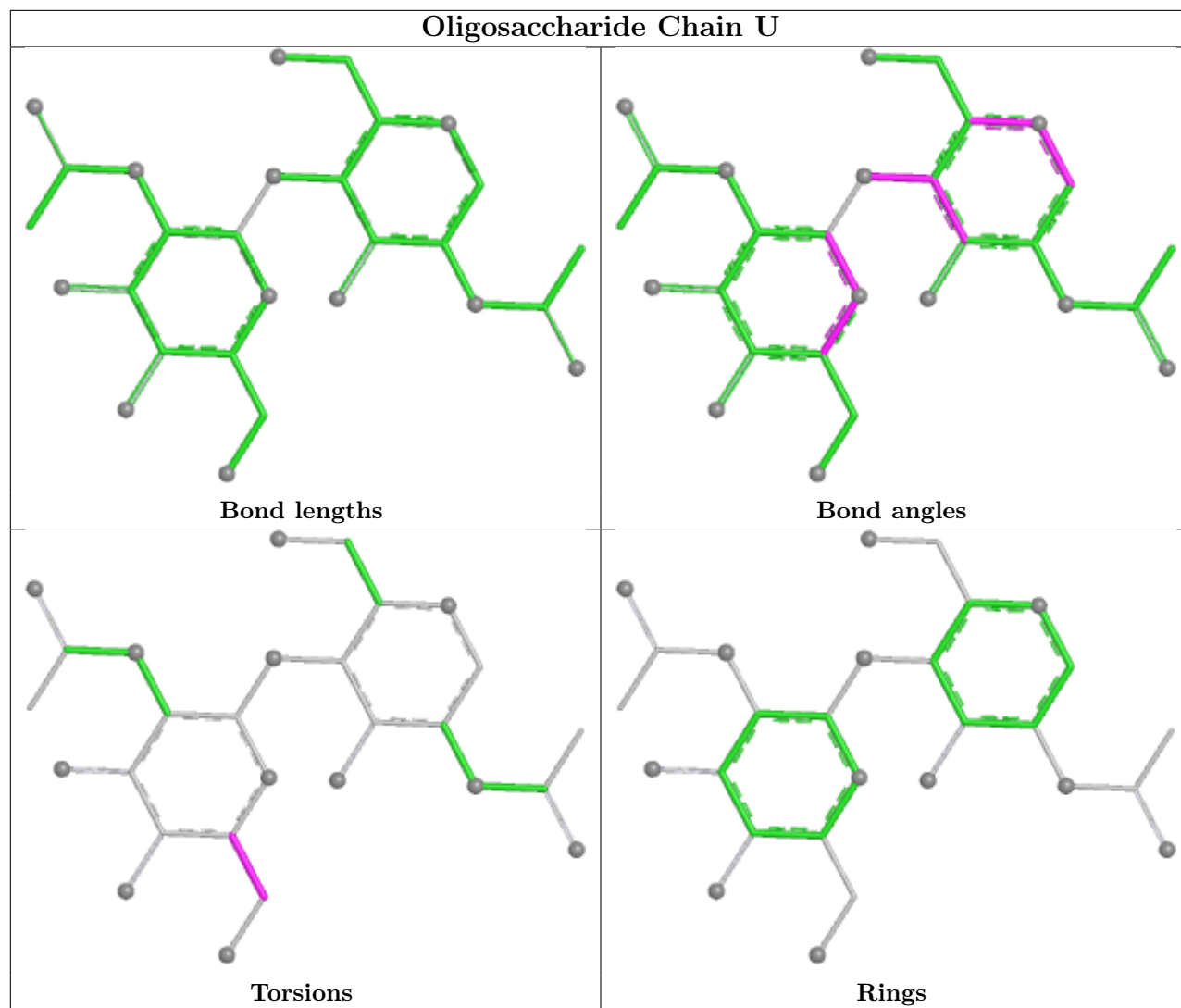




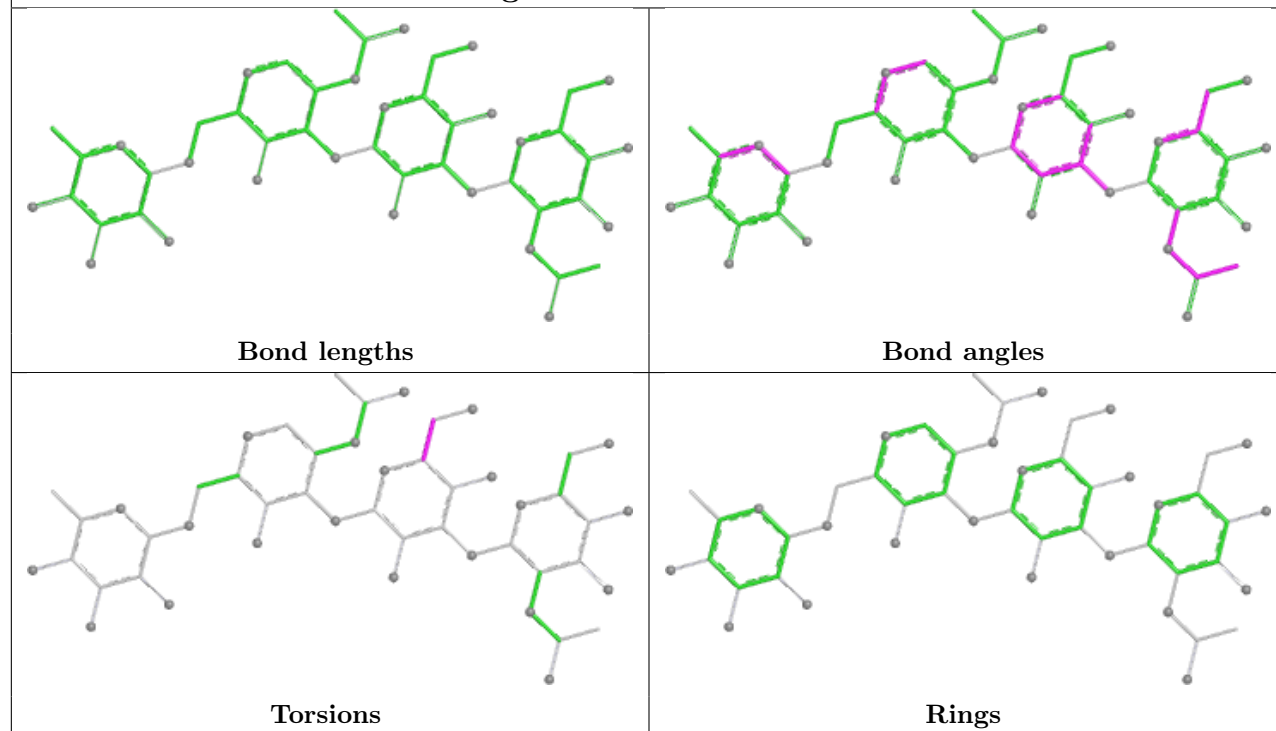




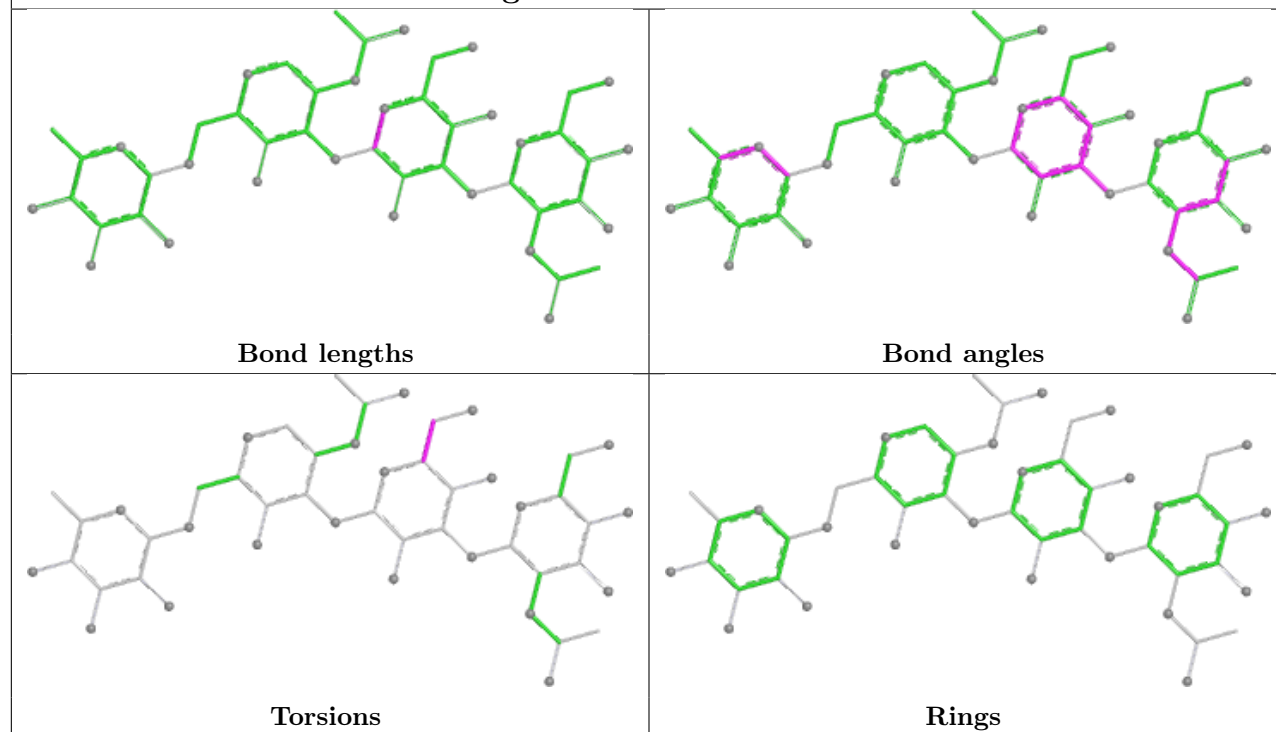


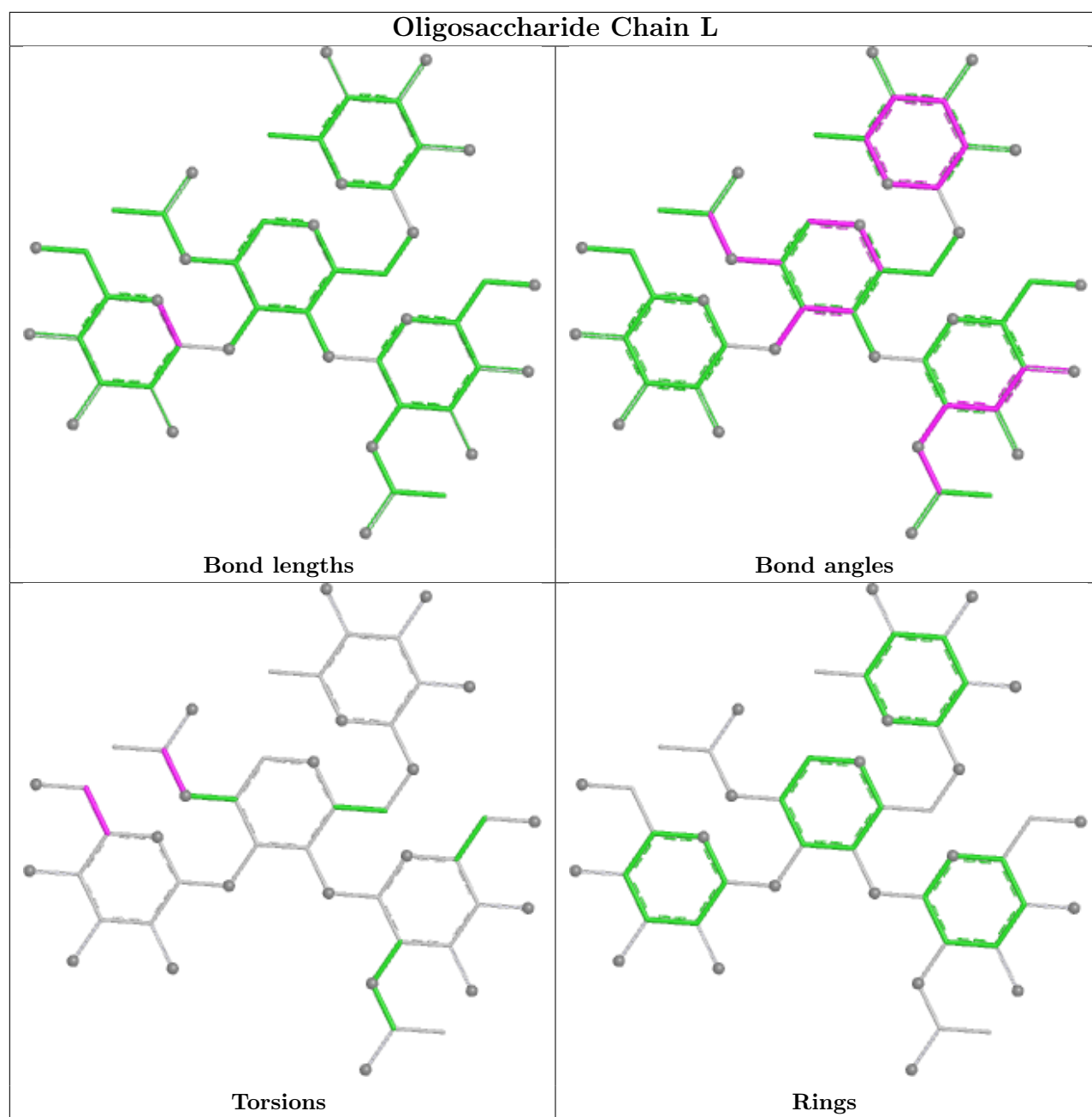


## Oligosaccharide Chain K

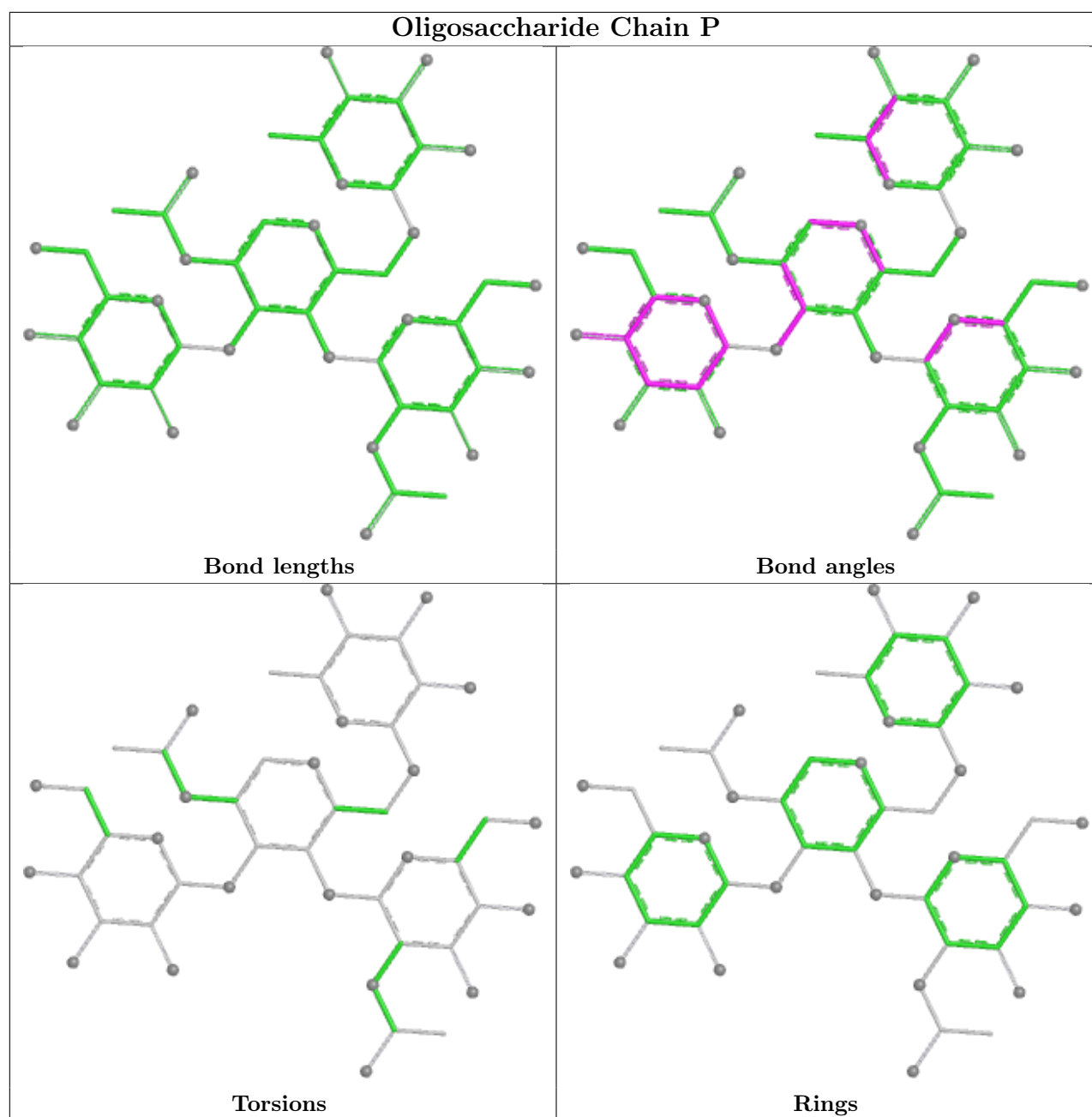


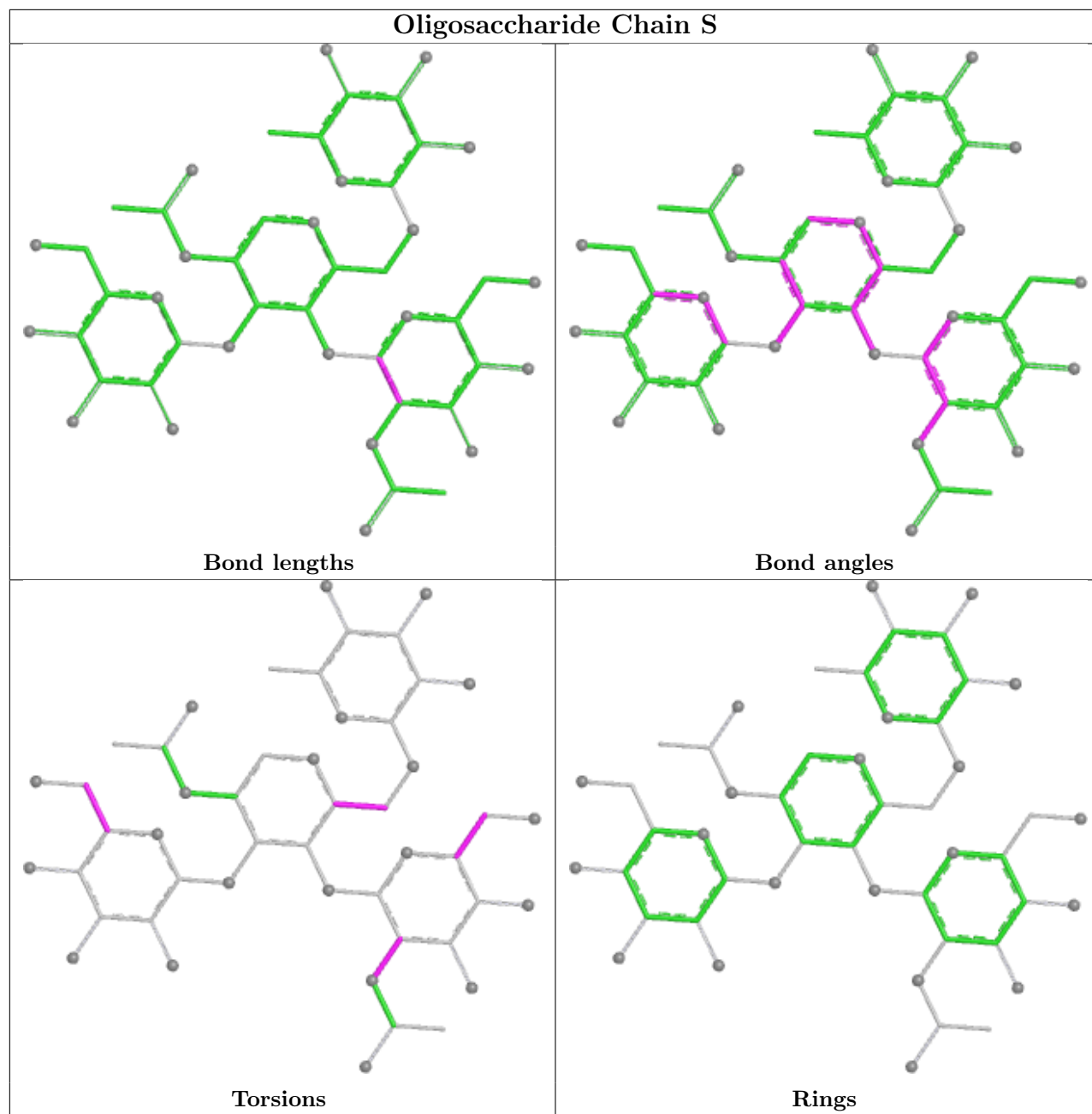
## Oligosaccharide Chain O

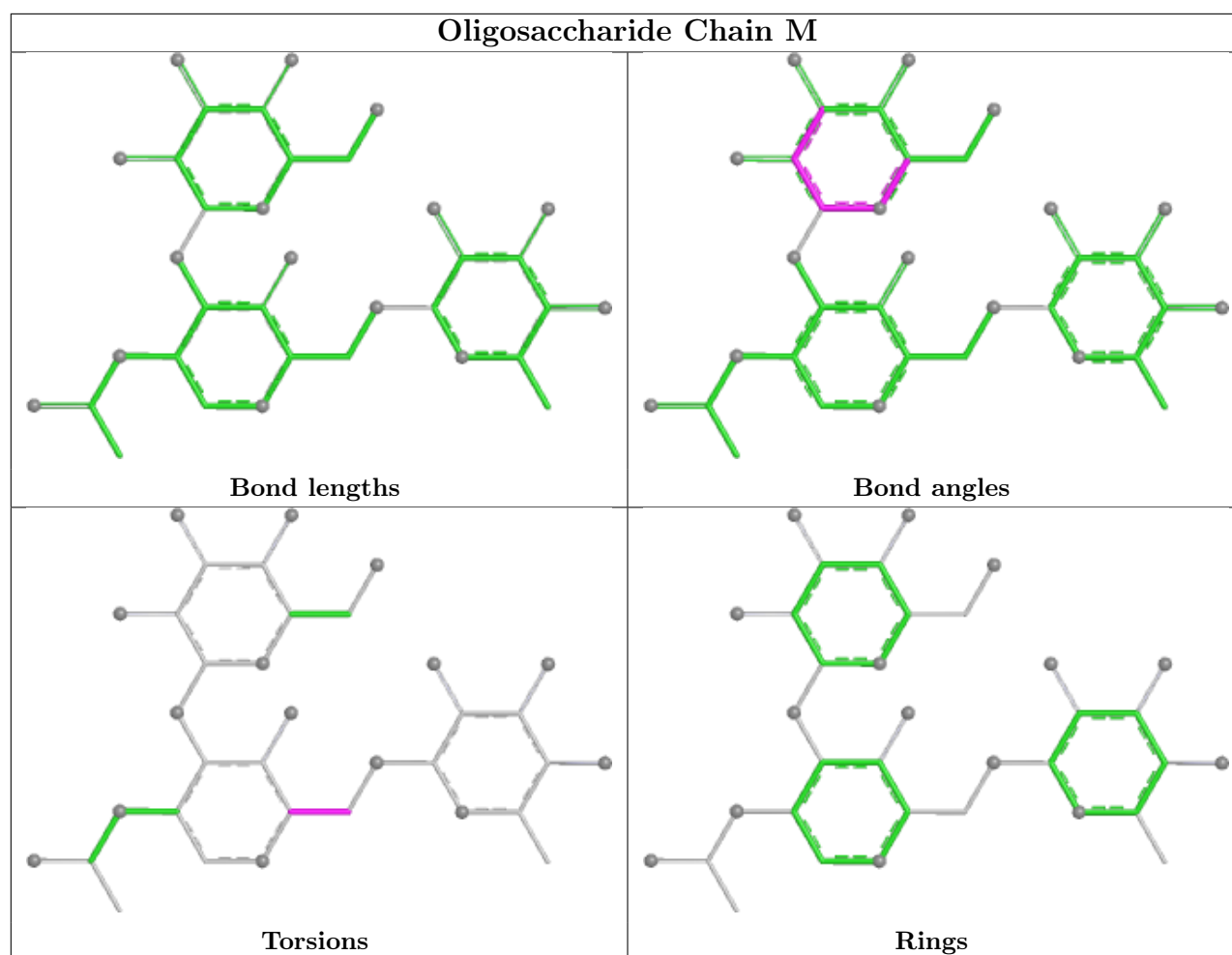












## 5.6 Ligand geometry [i](#)

13 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	$\# Z  > 2$
9	SCN	G	201	-	1,2,2	0.51	0	0,1,1	-	-
8	NAG	A	401	1	14,14,15	0.66	0	17,19,21	1.19	2 (11%)
9	SCN	D	402	-	1,2,2	0.55	0	0,1,1	-	-
8	NAG	A	402	1	14,14,15	0.80	1 (7%)	17,19,21	2.10	5 (29%)
11	SO4	F	201	-	4,4,4	0.72	0	6,6,6	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	GOL	E	201	-	5,5,5	0.28	0	5,5,5	0.39	0
9	SCN	A	403	-	1,2,2	0.58	0	0,1,1	-	-
8	NAG	B	401	1	14,14,15	0.68	0	17,19,21	1.58	2 (11%)
9	SCN	D	403	-	1,2,2	0.57	0	0,1,1	-	-
9	SCN	D	404	-	1,2,2	0.53	0	0,1,1	-	-
8	NAG	C	401	1	14,14,15	0.72	0	17,19,21	1.34	1 (5%)
8	NAG	D	401	1	14,14,15	0.83	1 (7%)	17,19,21	2.00	4 (23%)
11	SO4	E	202	-	4,4,4	0.74	0	6,6,6	0.26	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
8	NAG	A	401	1	-	4/6/23/26	0/1/1/1
8	NAG	A	402	1	-	3/6/23/26	0/1/1/1
10	GOL	E	201	-	-	1/4/4/4	-
8	NAG	B	401	1	-	5/6/23/26	0/1/1/1
8	NAG	C	401	1	-	0/6/23/26	0/1/1/1
8	NAG	D	401	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	401	NAG	C1-C2	2.30	1.55	1.52
8	A	402	NAG	C1-C2	2.21	1.55	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	402	NAG	C1-O5-C5	5.35	119.36	112.19
8	D	401	NAG	C1-O5-C5	5.07	118.97	112.19
8	A	402	NAG	C2-N2-C7	4.83	129.37	122.90
8	B	401	NAG	C2-N2-C7	4.72	129.22	122.90
8	C	401	NAG	C1-O5-C5	4.26	117.89	112.19

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	402	NAG	C3-C2-N2-C7
8	B	401	NAG	C1-C2-N2-C7
8	D	401	NAG	C3-C2-N2-C7
8	A	402	NAG	C4-C5-C6-O6
8	A	401	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	403	SCN	1	0
8	B	401	NAG	7	0
8	C	401	NAG	1	0
8	D	401	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 ⓘ

### 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	284/304 (93%)	-0.15	8 (2%) 55 51	47, 69, 125, 157	0
1	B	298/304 (98%)	0.08	17 (5%) 30 26	52, 79, 133, 156	0
1	C	295/304 (97%)	0.11	20 (6%) 25 20	50, 83, 130, 152	0
1	D	291/304 (95%)	-0.24	5 (1%) 69 65	46, 65, 105, 137	0
2	E	120/120 (100%)	-0.54	0 100 100	36, 62, 81, 106	1 (0%)
2	F	120/120 (100%)	-0.35	1 (0%) 82 81	41, 68, 90, 105	1 (0%)
2	G	120/120 (100%)	-0.19	0 100 100	43, 75, 101, 116	1 (0%)
2	H	120/120 (100%)	-0.06	0 100 100	42, 74, 104, 120	1 (0%)
All	All	1648/1696 (97%)	-0.12	51 (3%) 51 47	36, 71, 123, 157	4 (0%)

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	25	ILE	4.7
1	B	239	ILE	4.6
1	B	321	HIS	4.4
1	C	263	GLN	4.2
1	D	317	GLU	4.2

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

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

### 6.3 Carbohydrates ⓘ

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.

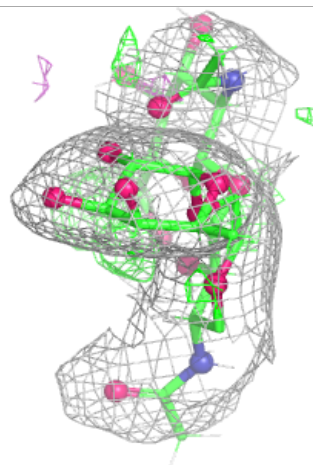
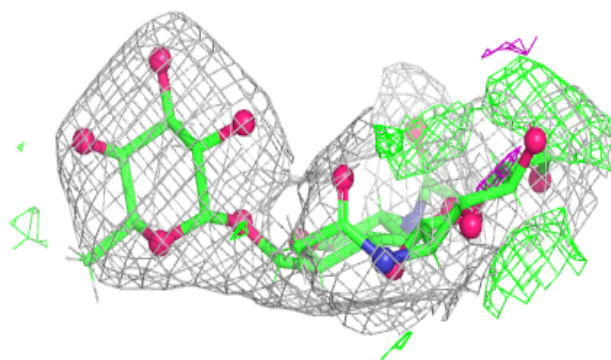
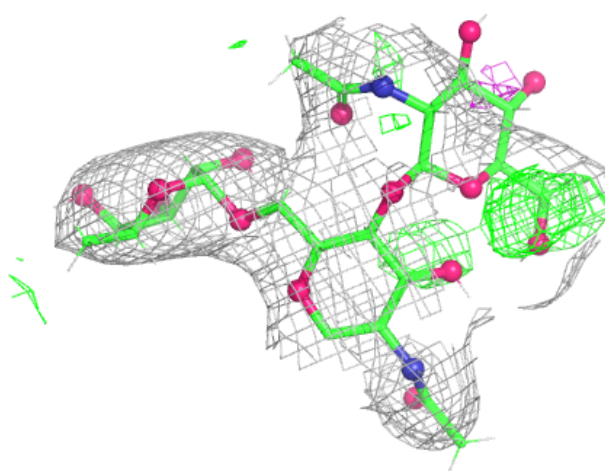
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	S	3	14/15	0.49	0.20	95,118,150,176	0
7	MAN	M	2	11/12	0.55	0.18	72,118,152,160	0
3	NAG	I	2	14/15	0.57	0.21	84,115,163,175	0
6	MAN	P	2	11/12	0.58	0.16	90,111,134,136	0
5	NAG	O	3	14/15	0.63	0.17	88,110,135,146	0
6	MAN	S	2	11/12	0.63	0.15	92,113,136,140	0
4	NAG	R	2	14/15	0.64	0.12	111,133,159,170	0
6	NAG	L	1	14/15	0.64	0.14	91,123,151,154	0
6	NAG	L	3	14/15	0.66	0.18	94,118,142,167	0
6	FUC	L	4	10/11	0.67	0.13	103,128,151,154	0
5	FUC	O	4	10/11	0.69	0.14	98,123,148,150	0
4	NAG	N	2	14/15	0.69	0.15	104,125,149,162	0
5	MAN	K	2	11/12	0.70	0.16	100,120,143,148	0
4	NAG	N	1	14/15	0.70	0.14	93,119,135,143	0
4	NAG	Q	2	14/15	0.71	0.15	76,114,139,158	0
6	MAN	L	2	11/12	0.72	0.17	95,121,145,151	0
4	NAG	U	2	14/15	0.73	0.14	89,117,155,161	0
5	MAN	O	2	11/12	0.79	0.14	87,115,140,147	0
3	NAG	T	2	14/15	0.80	0.12	73,114,137,141	0
6	NAG	P	3	14/15	0.80	0.11	80,101,124,133	0
6	FUC	P	4	10/11	0.80	0.17	79,105,132,136	0
3	NAG	T	1	14/15	0.81	0.11	75,91,112,115	0
4	NAG	Q	1	14/15	0.83	0.12	69,91,107,112	0
4	NAG	J	2	14/15	0.83	0.13	75,105,129,132	0
4	NAG	R	1	14/15	0.84	0.12	93,119,144,145	0
5	NAG	K	3	14/15	0.85	0.12	86,117,140,142	0
5	FUC	K	4	10/11	0.86	0.11	71,94,113,115	0
3	FUC	T	3	10/11	0.86	0.17	85,113,138,155	0
7	FUC	M	3	10/11	0.86	0.20	96,120,151,153	0
4	NAG	U	1	14/15	0.88	0.11	73,89,110,119	0
5	NAG	O	1	14/15	0.88	0.10	95,114,135,144	0
4	NAG	J	1	14/15	0.91	0.10	71,86,104,104	0
6	FUC	S	4	10/11	0.91	0.09	59,71,89,97	0
3	NAG	I	1	14/15	0.92	0.09	57,86,110,118	0
6	NAG	P	1	14/15	0.92	0.09	67,92,100,113	0
5	NAG	K	1	14/15	0.93	0.09	73,90,108,115	0
6	NAG	S	1	14/15	0.94	0.08	63,82,108,112	0
7	NAG	M	1	14/15	0.94	0.09	78,94,113,118	0
3	FUC	I	3	10/11	0.95	0.09	61,77,90,92	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain I:**

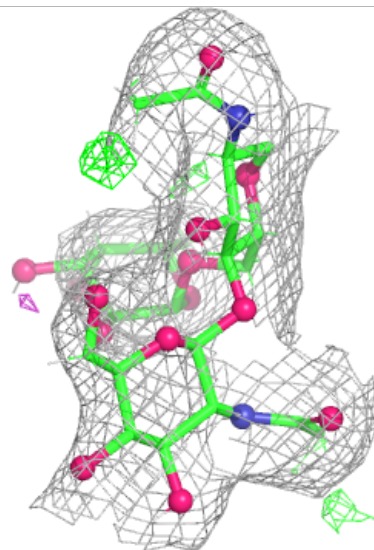
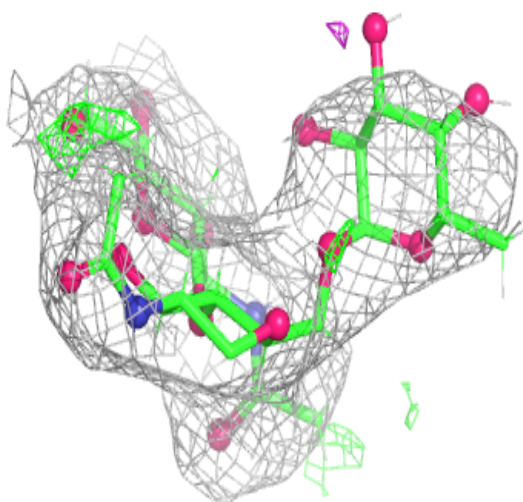
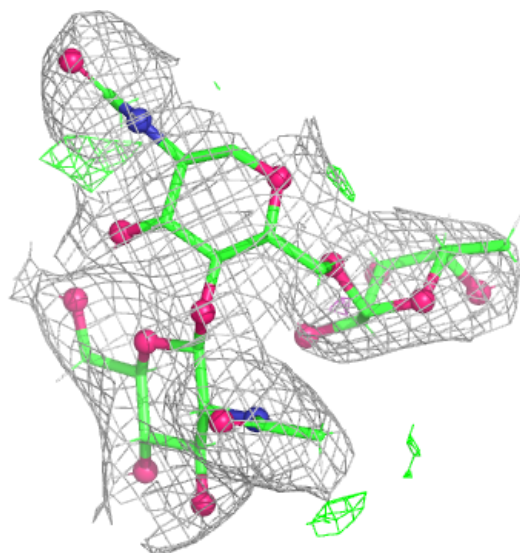
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





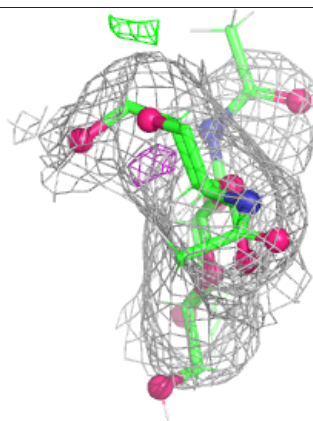
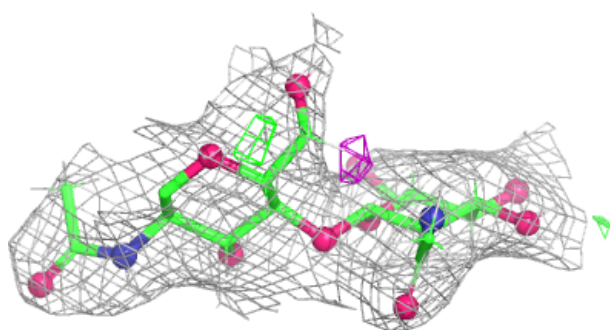
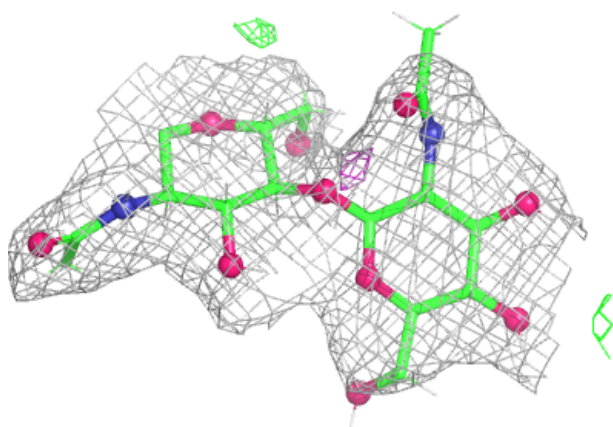
**Electron density around Chain T:**

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and green (positive)



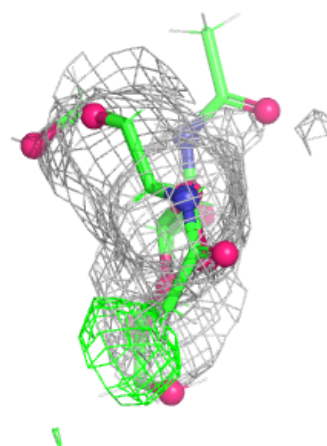
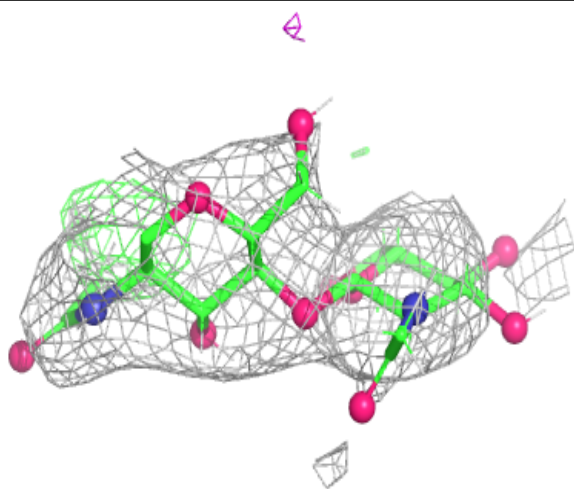
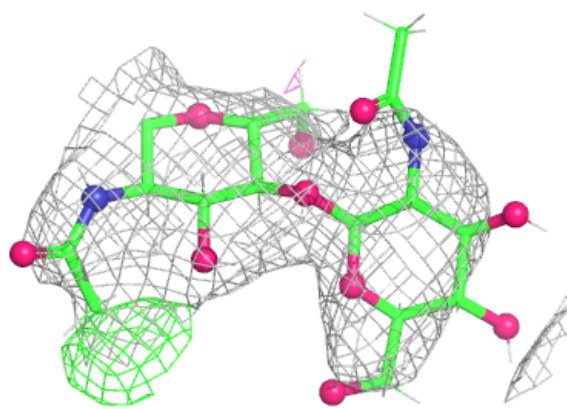
**Electron density around Chain J:**

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



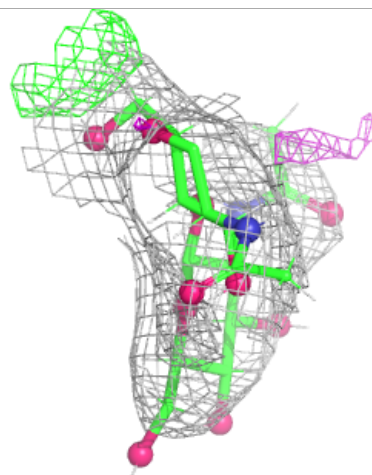
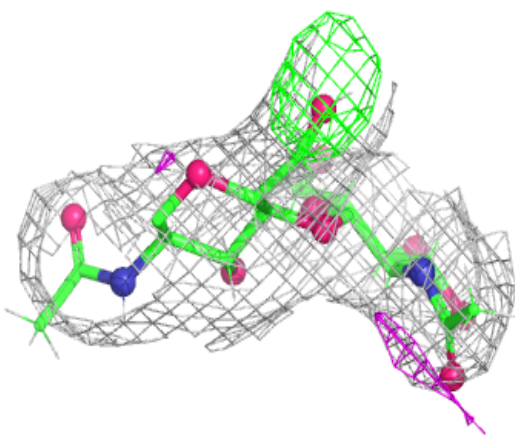
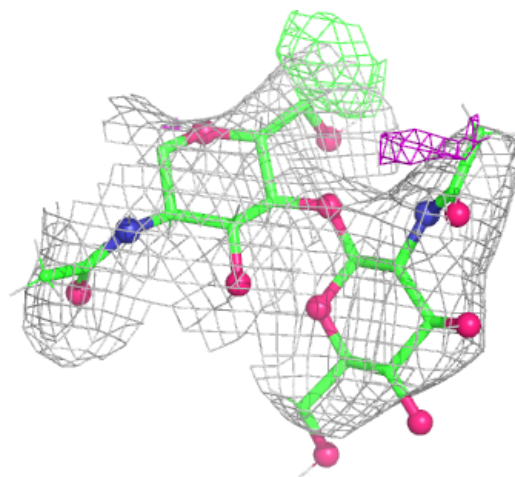
**Electron density around Chain N:**

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



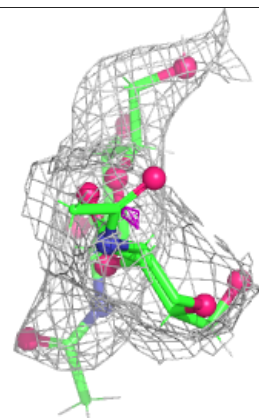
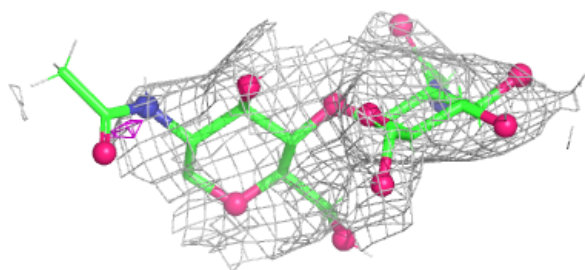
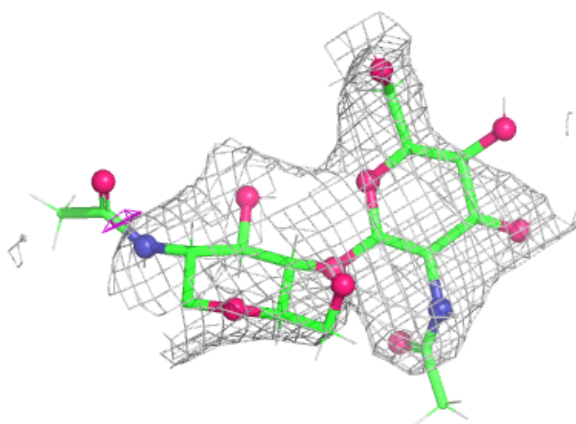
**Electron density around Chain Q:**

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and green (positive)

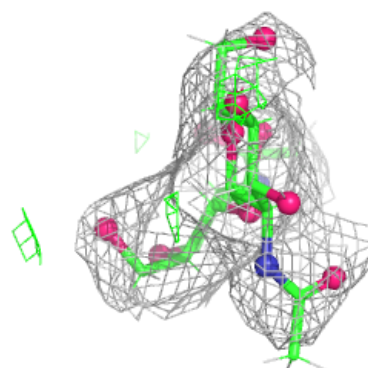
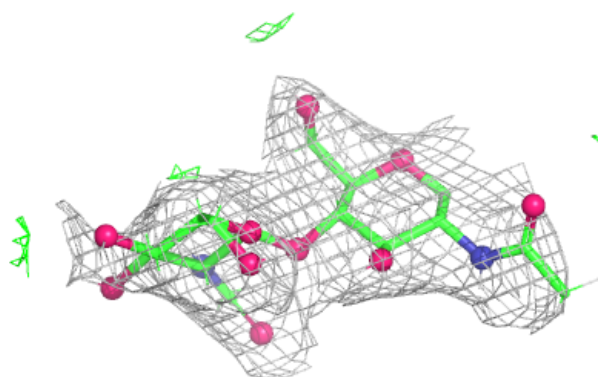
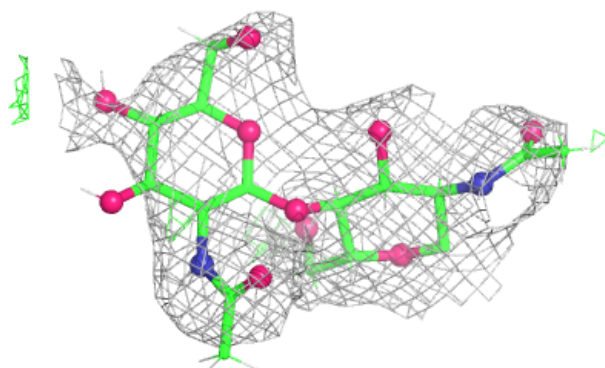


**Electron density around Chain R:**

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

**Electron density around Chain U:**

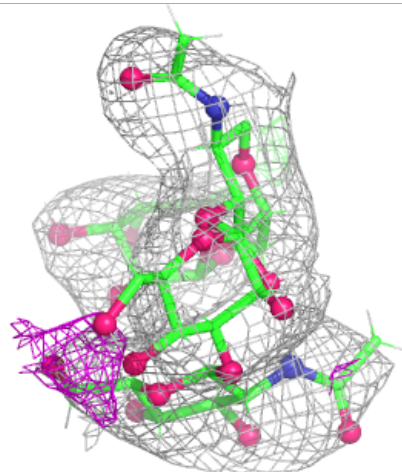
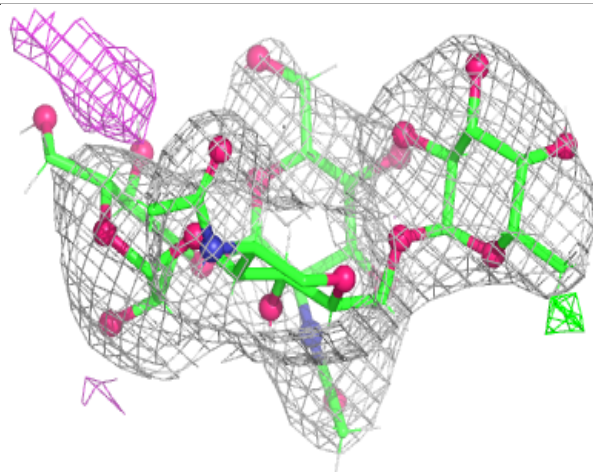
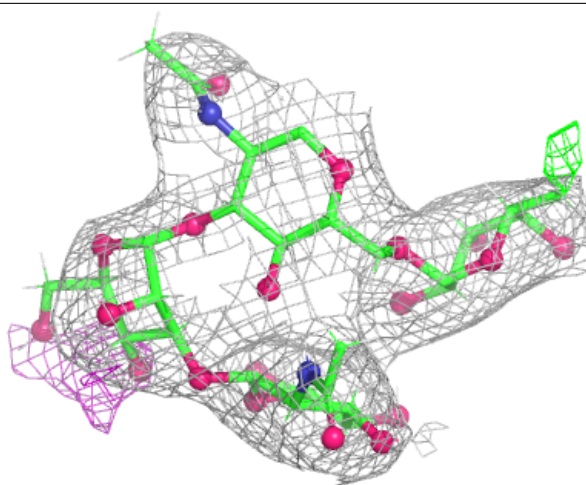
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





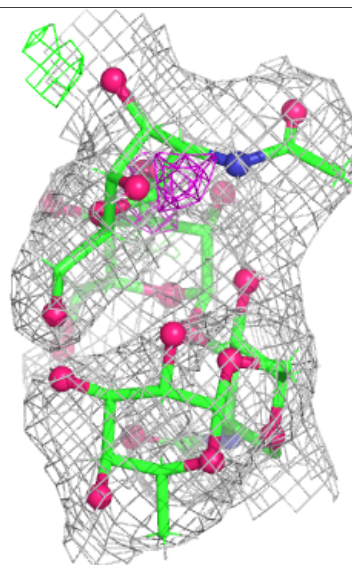
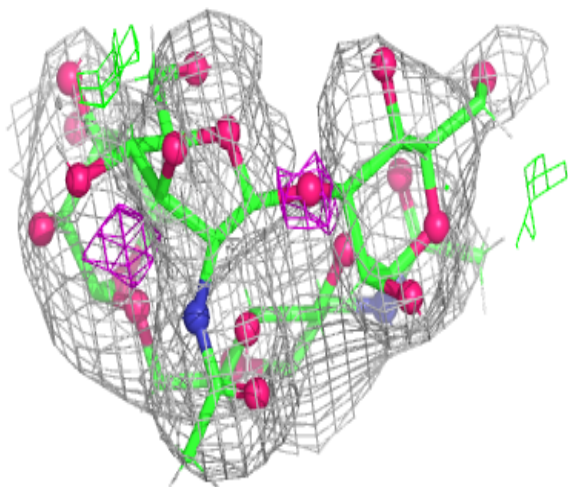
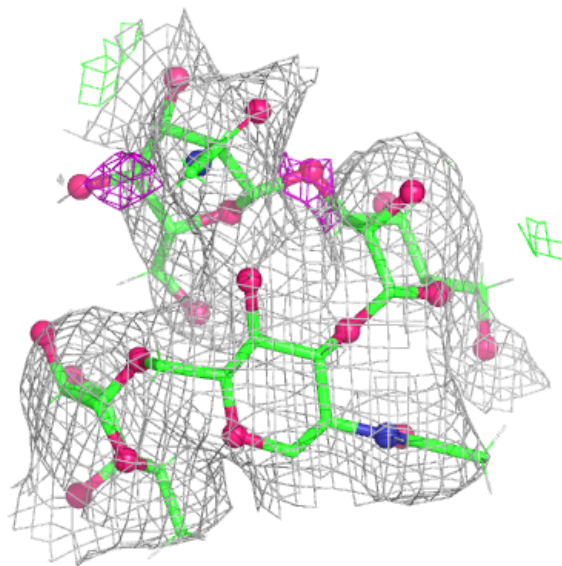
**Electron density around Chain K:**

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



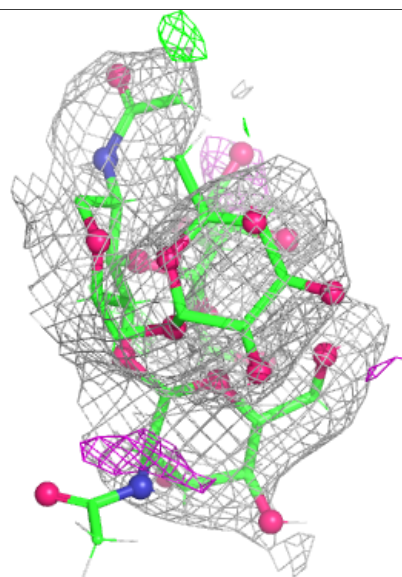
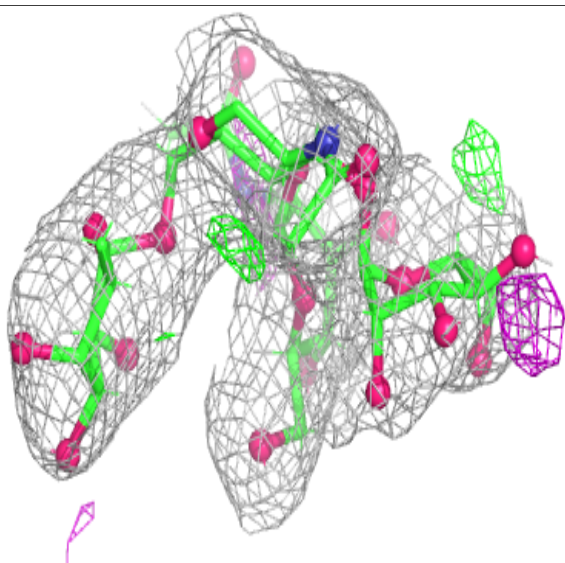
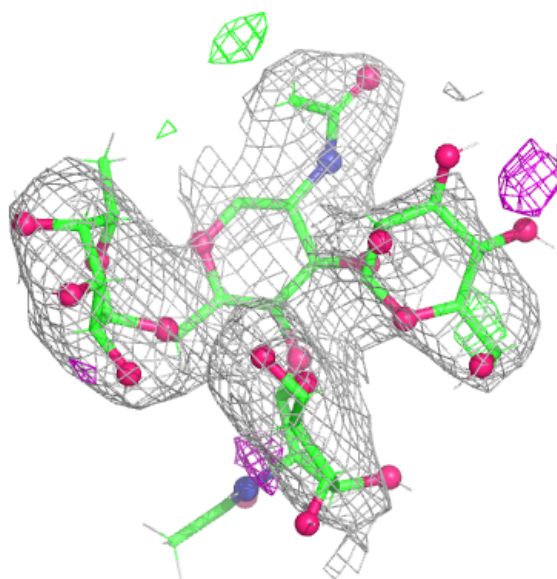
**Electron density around Chain O:**

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



**Electron density around Chain L:**

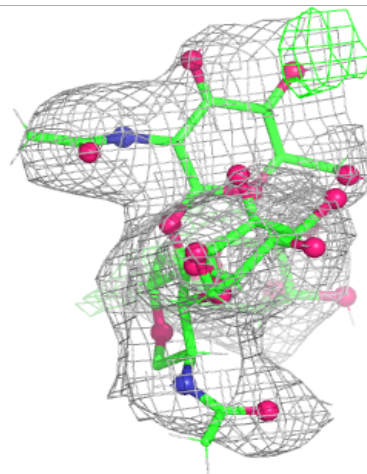
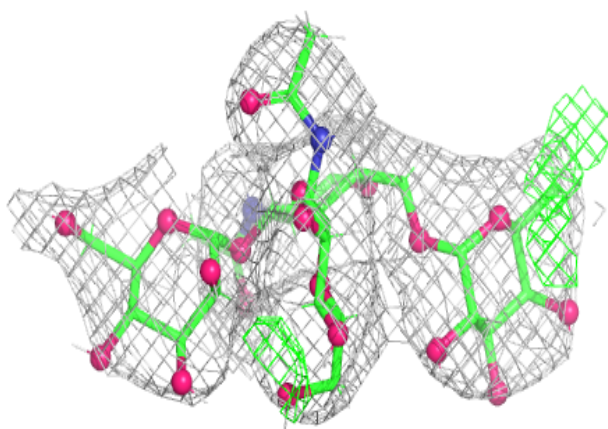
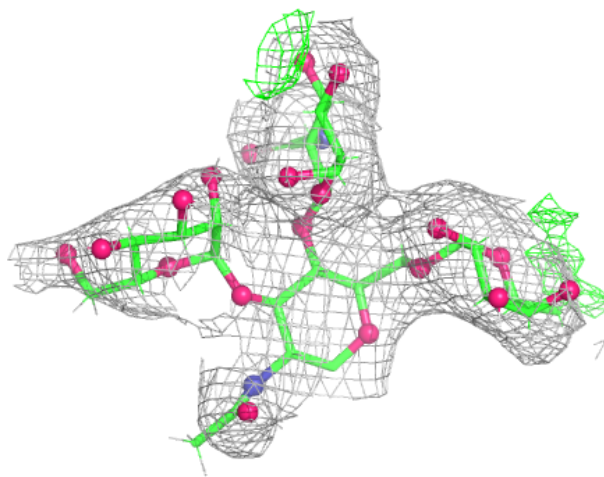
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





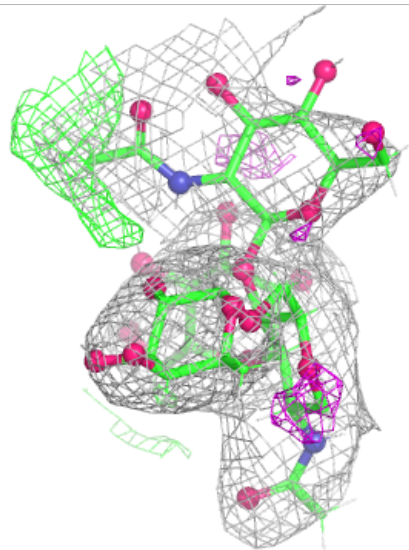
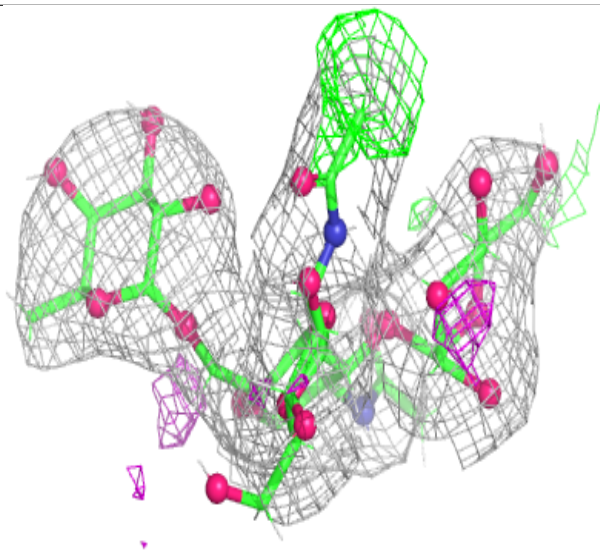
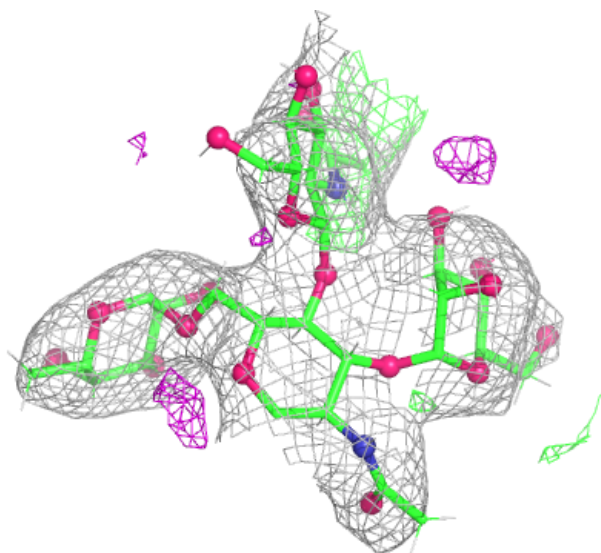
**Electron density around Chain P:**

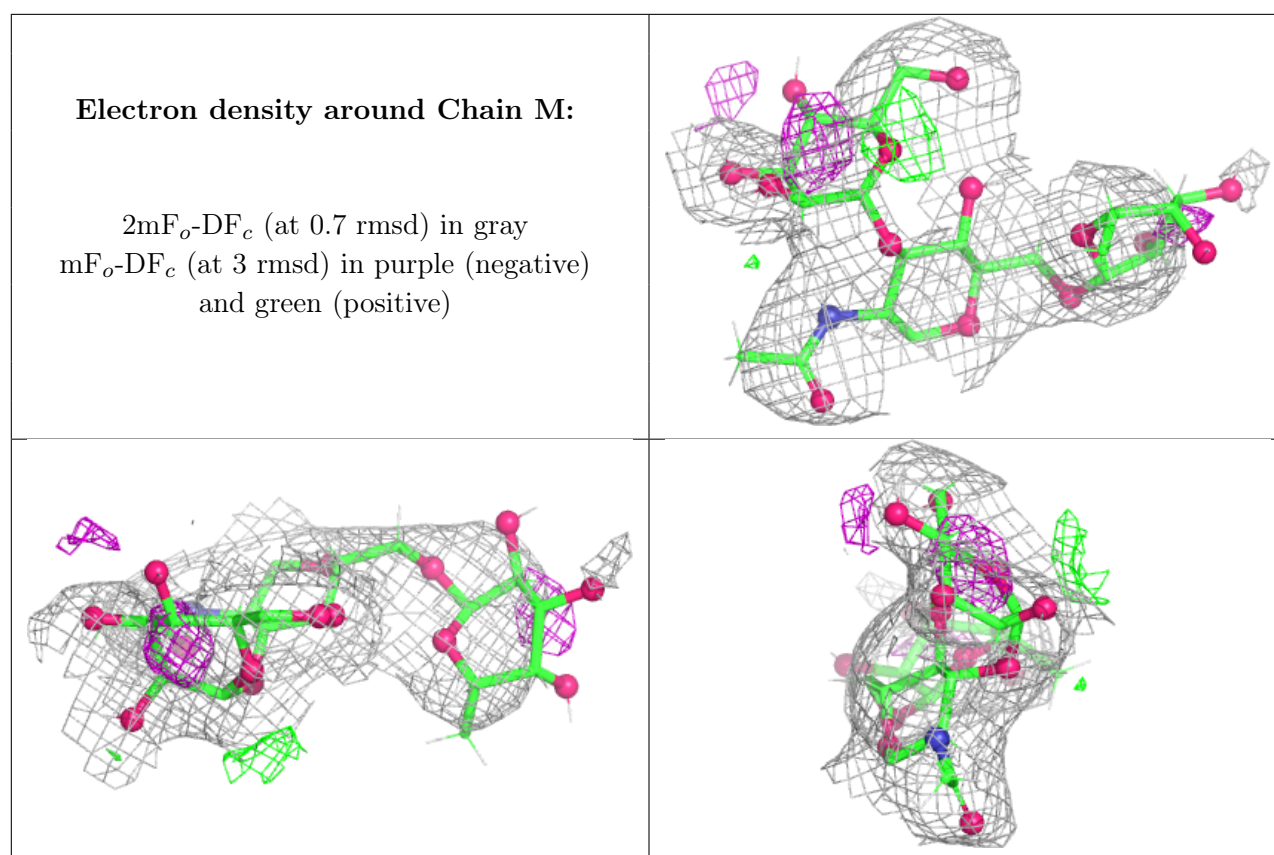
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain S:**

$2mF_o-DF_c$  (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
8	NAG	B	401	14/15	0.64	0.18	99,126,154,158	0
8	NAG	D	401	14/15	0.69	0.14	64,88,105,124	0
8	NAG	C	401	14/15	0.78	0.14	90,120,145,146	0
8	NAG	A	402	14/15	0.81	0.13	64,92,115,120	0
8	NAG	A	401	14/15	0.83	0.15	83,102,127,130	0
10	GOL	E	201	6/6	0.84	0.20	76,107,129,129	0
11	SO4	F	201	5/5	0.92	0.09	94,98,116,131	0
9	SCN	D	403	3/3	0.94	0.07	62,62,73,83	0
11	SO4	E	202	5/5	0.94	0.26	64,76,88,99	0
9	SCN	D	404	3/3	0.94	0.11	46,46,52,71	0
9	SCN	G	201	3/3	0.95	0.12	49,49,53,77	0
9	SCN	A	403	3/3	0.96	0.12	57,57,58,64	0
9	SCN	D	402	3/3	0.98	0.07	55,55,59,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.