



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 05:35 AM EDT

PDB ID : 6NMY  
Title : A Cytokine-receptor complex  
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Deposited on : 2019-01-13  
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

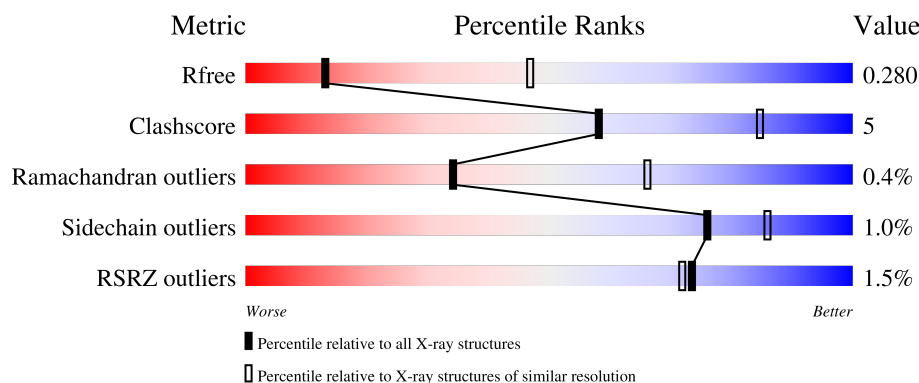
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	F	288	<div> <div>2%</div> <div>81% 12% 6%</div> </div>
1	M	288	<div> <div>4%</div> <div>76% 14% 9%</div> </div>
2	A	216	<div> <div>2%</div> <div>85% 13%</div> </div>
2	C	216	<div> <div>0%</div> <div>86% 14%</div> </div>
3	I	118	<div> <div>0%</div> <div>81% 9% 8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	J	118	 84% 6% 8%
4	B	198	 88% 11%
4	D	198	 89% 10%
5	E	4	 50% 25% 25%
5	G	4	 50% 25% 25%
6	H	3	 33% 33% 33%
6	K	3	 67% 33%
6	N	3	 100%
7	L	2	 100%
7	O	2	 100%

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12975 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 Interleukin-3 receptor subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	270	Total	C	N	O	S	0	0	0
			2189	1381	392	400	16			
1	M	262	Total	C	N	O	S	0	0	0
			2128	1341	383	388	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	212	GLN	ASN	engineered mutation	UNP P26951
M	212	GLN	ASN	engineered mutation	UNP P26951

- Molecule 2 is a protein called Cytokine receptor common subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	215	Total	C	N	O	S	0	0	0
			1722	1079	304	329	10			
2	C	215	Total	C	N	O	S	0	0	0
			1722	1079	304	329	10			

- Molecule 3 is a protein called Interleukin-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	108	Total	C	N	O	S	0	0	0
			874	554	155	161	4			
3	J	108	Total	C	N	O	S	0	0	0
			874	554	155	161	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	8	GLY	-	expression tag	UNP P08700
I	9	ALA	-	expression tag	UNP P08700

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Chain	Residue	Modelled	Actual	Comment	Reference
I	10	MET	-	expression tag	UNP P08700
I	11	GLY	-	expression tag	UNP P08700
I	13	TYR	TRP	engineered mutation	UNP P08700
J	8	GLY	-	expression tag	UNP P08700
J	9	ALA	-	expression tag	UNP P08700
J	10	MET	-	expression tag	UNP P08700
J	11	GLY	-	expression tag	UNP P08700
J	13	TYR	TRP	engineered mutation	UNP P08700

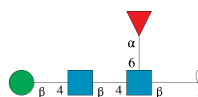
- Molecule 4 is a protein called Cytokine receptor common subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	196	Total	C	N	O	S	0	0	0
			1580	987	283	302	8			
4	D	197	Total	C	N	O	S	0	0	0
			1589	992	284	305	8			

There are 2 discrepancies between the modelled and reference sequences:

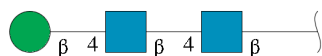
Chain	Residue	Modelled	Actual	Comment	Reference
B	346	GLN	ASN	engineered mutation	UNP P32927
D	346	GLN	ASN	engineered mutation	UNP P32927

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	4	Total	C	N	O		0	0	0
			49	28	2	19				
5	G	4	Total	C	N	O		0	0	0
			49	28	2	19				

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



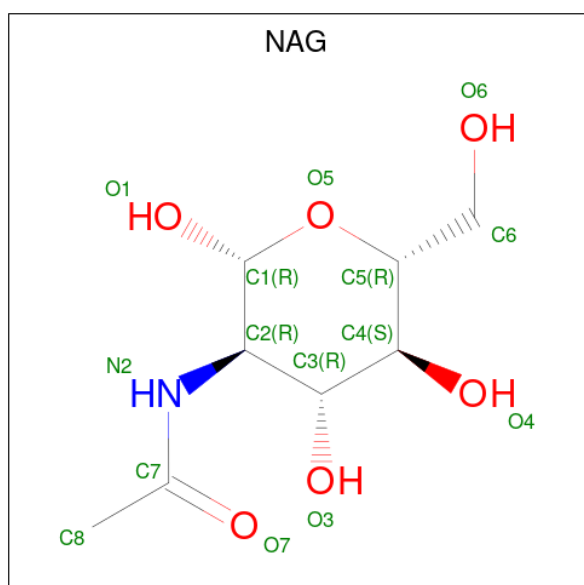
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 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
7	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	O	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

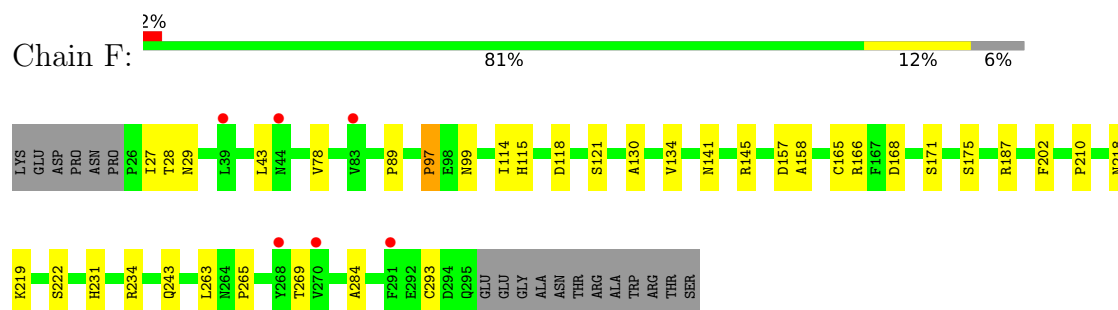
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	F	2	Total	O	0	0
			2	2		
9	M	2	Total	O	0	0
			2	2		
9	A	1	Total	O	0	0
			1	1		
9	C	1	Total	O	0	0
			1	1		
9	I	1	Total	O	0	0
			1	1		
9	J	2	Total	O	0	0
			2	2		
9	B	2	Total	O	0	0
			2	2		
9	D	1	Total	O	0	0
			1	1		

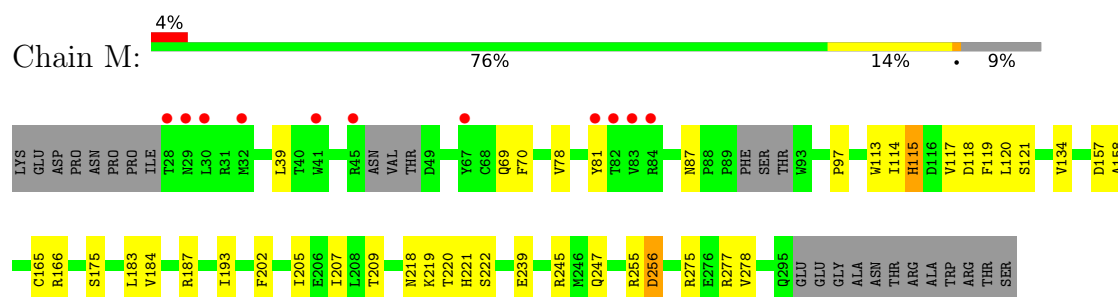
### 3 Residue-property plots [i](#)

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.

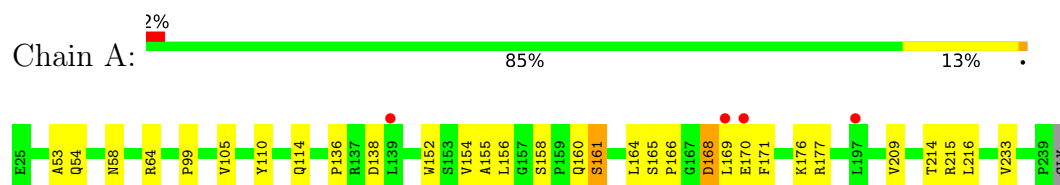
- Molecule 1: Interleukin-3 receptor subunit alpha



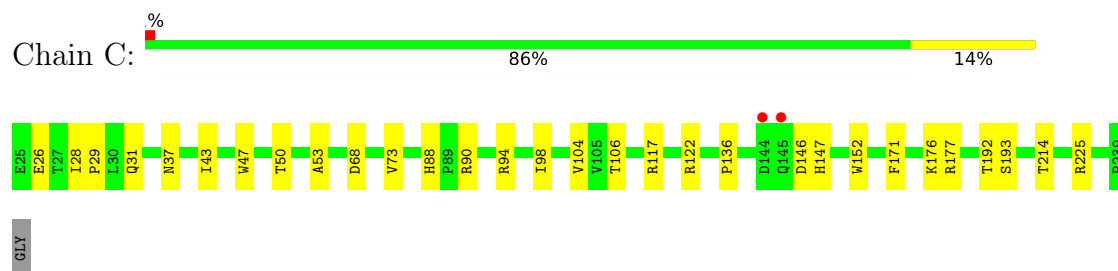
- Molecule 1: Interleukin-3 receptor subunit alpha



- Molecule 2: Cytokine receptor common subunit beta




- Molecule 2: Cytokine receptor common subunit beta






- Molecule 3: Interleukin-3

Chain I:  81% 9% 8%



- Molecule 3: Interleukin-3

Chain J:  84% 6% 8%




- Molecule 4: Cytokine receptor common subunit beta

Chain B:  88% 11% .



- Molecule 4: Cytokine receptor common subunit beta

Chain D:  89% 10% ..



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

Chain E:  50% 25% 25%



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

Chain G:  50% 25% 25%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  33% 33% 33%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  67% 33%

NAG1  
NAG2  
BMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

NAG1  
NAG2  
BMA3

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%

NAG1  
NAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%

NAG1  
NAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.65Å 157.25Å 168.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.45 – 3.30 47.76 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.45-3.30) 99.8 (47.76-3.30)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 3.33Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.236 , 0.278 0.238 , 0.280	Depositor DCC
$R_{free}$ test set	2233 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	95.0	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 29.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	12975	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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: BMA, 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	F	0.27	0/2246	0.48	0/3048
1	M	0.25	0/2181	0.48	0/2955
2	A	0.24	0/1771	0.47	0/2429
2	C	0.25	0/1771	0.47	0/2429
3	I	0.24	0/892	0.41	0/1212
3	J	0.25	0/892	0.42	0/1212
4	B	0.25	0/1625	0.45	0/2208
4	D	0.26	0/1634	0.45	0/2220
All	All	0.25	0/13012	0.46	0/17713

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	F	2189	0	2113	24	0
1	M	2128	0	2050	25	0
2	A	1722	0	1654	17	0
2	C	1722	0	1653	21	0
3	I	874	0	879	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	874	0	879	7	0
4	B	1580	0	1499	14	0
4	D	1589	0	1505	15	0
5	E	49	0	43	1	0
5	G	49	0	43	1	0
6	H	39	0	34	1	0
6	K	39	0	34	0	0
6	N	39	0	34	0	0
7	L	28	0	25	0	0
7	O	28	0	25	0	0
8	C	14	0	13	0	0
9	A	1	0	0	0	0
9	B	2	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	F	2	0	0	1	0
9	I	1	0	0	0	0
9	J	2	0	0	0	0
9	M	2	0	0	0	0
All	All	12975	0	12483	121	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 5.

The worst 5 of 121 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:F:218:ASN:N	1:F:293:CYS:SG	2.67	0.68
1:M:278:VAL:HG11	3:I:116:LYS:HB2	1.76	0.68
2:A:136:PRO:HG3	2:A:214:THR:HG23	1.78	0.65
2:C:26:GLU:HG3	2:C:31:GLN:HG3	1.78	0.64
2:C:146:ASP:O	2:C:147:HIS:ND1	2.31	0.64

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	F	268/288 (93%)	245 (91%)	21 (8%)	2 (1%)	22	54
1	M	256/288 (89%)	235 (92%)	20 (8%)	1 (0%)	34	66
2	A	213/216 (99%)	196 (92%)	15 (7%)	2 (1%)	17	48
2	C	213/216 (99%)	195 (92%)	18 (8%)	0	100	100
3	I	106/118 (90%)	101 (95%)	5 (5%)	0	100	100
3	J	106/118 (90%)	99 (93%)	6 (6%)	1 (1%)	17	48
4	B	194/198 (98%)	178 (92%)	16 (8%)	0	100	100
4	D	195/198 (98%)	174 (89%)	21 (11%)	0	100	100
All	All	1551/1640 (95%)	1423 (92%)	122 (8%)	6 (0%)	34	66

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	175	SER
3	J	30	PRO
1	M	175	SER
2	A	161	SER
1	F	89	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	F	241/256 (94%)	239 (99%)	2 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	233/256 (91%)	229 (98%)	4 (2%)	60	78
2	A	200/200 (100%)	196 (98%)	4 (2%)	55	76
2	C	200/200 (100%)	199 (100%)	1 (0%)	88	93
3	I	99/104 (95%)	98 (99%)	1 (1%)	76	86
3	J	99/104 (95%)	98 (99%)	1 (1%)	76	86
4	B	173/175 (99%)	173 (100%)	0	100	100
4	D	174/175 (99%)	173 (99%)	1 (1%)	86	91
All	All	1419/1470 (96%)	1405 (99%)	14 (1%)	76	86

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	160	GLN
2	A	165	SER
4	D	261	SER
3	I	108	ARG
3	J	13	TYR

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 ⓘ

21 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	E	1	1,5	14,14,15	0.29	0	17,19,21	0.55	0
5	NAG	E	2	5	14,14,15	0.48	0	17,19,21	0.59	0
5	BMA	E	3	5	11,11,12	1.09	1 (9%)	15,15,17	0.99	1 (6%)
5	FUC	E	4	5	10,10,11	0.79	0	14,14,16	0.85	0
5	NAG	G	1	1,5	14,14,15	1.02	1 (7%)	17,19,21	1.39	3 (17%)
5	NAG	G	2	5	14,14,15	0.31	0	17,19,21	0.38	0
5	BMA	G	3	5	11,11,12	0.70	0	15,15,17	0.72	0
5	FUC	G	4	5	10,10,11	1.78	2 (20%)	14,14,16	1.74	3 (21%)
6	NAG	H	1	1,6	14,14,15	0.73	0	17,19,21	1.12	2 (11%)
6	NAG	H	2	6	14,14,15	0.44	0	17,19,21	1.28	1 (5%)
6	BMA	H	3	6	11,11,12	0.79	0	15,15,17	0.87	0
6	NAG	K	1	1,6	14,14,15	0.36	0	17,19,21	0.83	1 (5%)
6	NAG	K	2	6	14,14,15	0.31	0	17,19,21	0.67	0
6	BMA	K	3	6	11,11,12	0.80	0	15,15,17	0.83	0
7	NAG	L	1	1,7	14,14,15	0.39	0	17,19,21	0.57	0
7	NAG	L	2	7	14,14,15	0.63	0	17,19,21	0.43	0
6	NAG	N	1	2,6	14,14,15	0.63	1 (7%)	17,19,21	0.91	1 (5%)
6	NAG	N	2	6	14,14,15	1.64	2 (14%)	17,19,21	1.12	3 (17%)
6	BMA	N	3	6	11,11,12	0.90	0	15,15,17	1.26	1 (6%)
7	NAG	O	1	2,7	14,14,15	0.35	0	17,19,21	0.70	0
7	NAG	O	2	7	14,14,15	0.24	0	17,19,21	0.49	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	E	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1
5	BMA	E	3	5	-	1/2/19/22	0/1/1/1
5	FUC	E	4	5	-	-	0/1/1/1
5	NAG	G	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	2/2/19/22	0/1/1/1
5	FUC	G	4	5	-	-	0/1/1/1
6	NAG	H	1	1,6	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	H	2	6	-	2/6/23/26	0/1/1/1
6	BMA	H	3	6	-	0/2/19/22	0/1/1/1
6	NAG	K	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	K	2	6	-	3/6/23/26	0/1/1/1
6	BMA	K	3	6	-	0/2/19/22	0/1/1/1
7	NAG	L	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	L	2	7	-	0/6/23/26	0/1/1/1
6	NAG	N	1	2,6	-	1/6/23/26	0/1/1/1
6	NAG	N	2	6	-	2/6/23/26	0/1/1/1
6	BMA	N	3	6	-	2/2/19/22	0/1/1/1
7	NAG	O	1	2,7	-	1/6/23/26	0/1/1/1
7	NAG	O	2	7	-	0/6/23/26	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	2	NAG	O5-C1	-5.34	1.35	1.43
5	G	4	FUC	C1-C2	3.90	1.61	1.52
5	G	4	FUC	O5-C1	3.59	1.49	1.43
5	G	1	NAG	O5-C1	-3.53	1.38	1.43
5	E	3	BMA	C1-C2	3.12	1.59	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	2	NAG	C1-O5-C5	4.44	118.21	112.19
5	G	4	FUC	C1-O5-C5	4.17	122.23	112.78
5	G	1	NAG	C1-O5-C5	3.77	117.31	112.19
5	G	4	FUC	C1-C2-C3	3.34	113.77	109.67
6	N	3	BMA	C1-C2-C3	-3.06	105.91	109.67

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

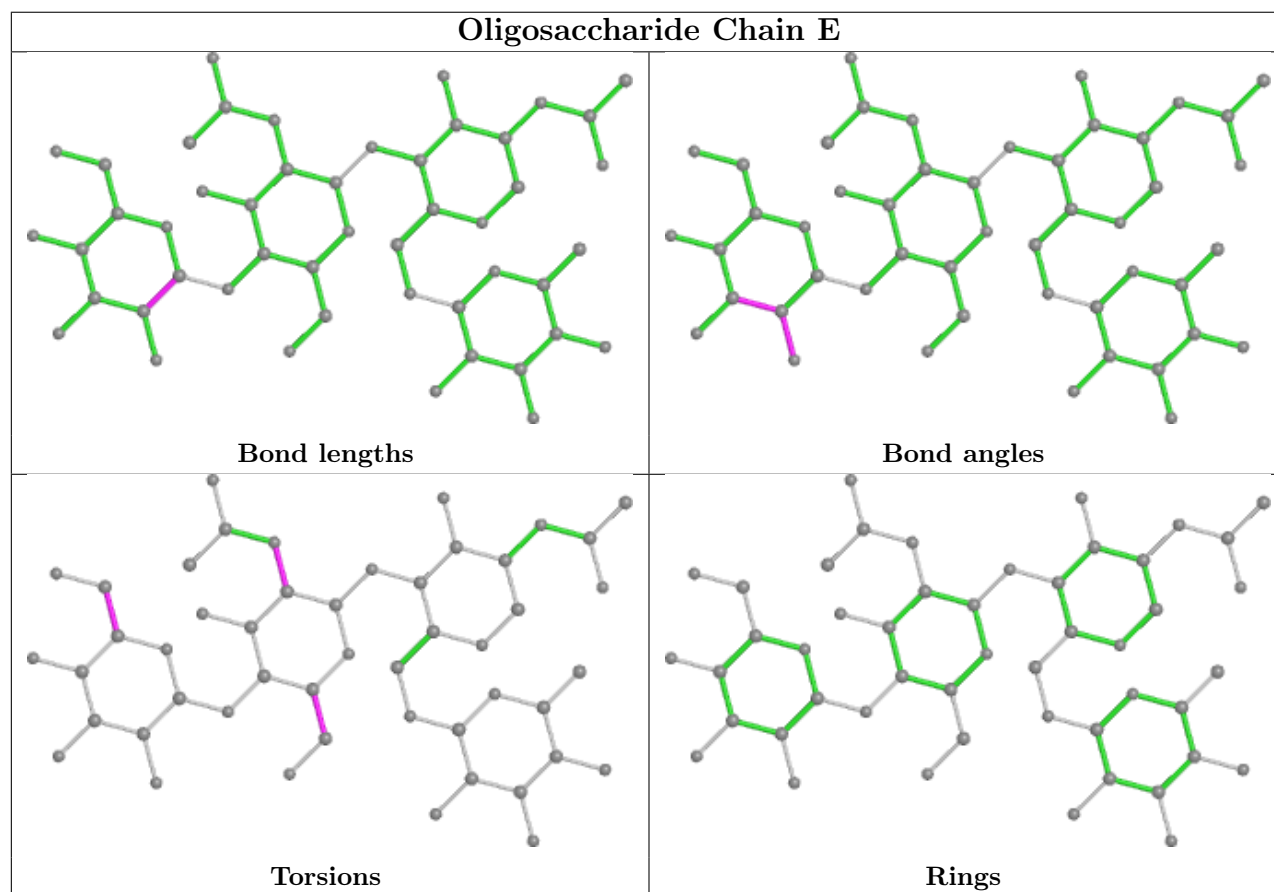
Mol	Chain	Res	Type	Atoms
5	E	2	NAG	O5-C5-C6-O6
7	L	1	NAG	O5-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
6	N	2	NAG	C4-C5-C6-O6
6	H	1	NAG	O5-C5-C6-O6

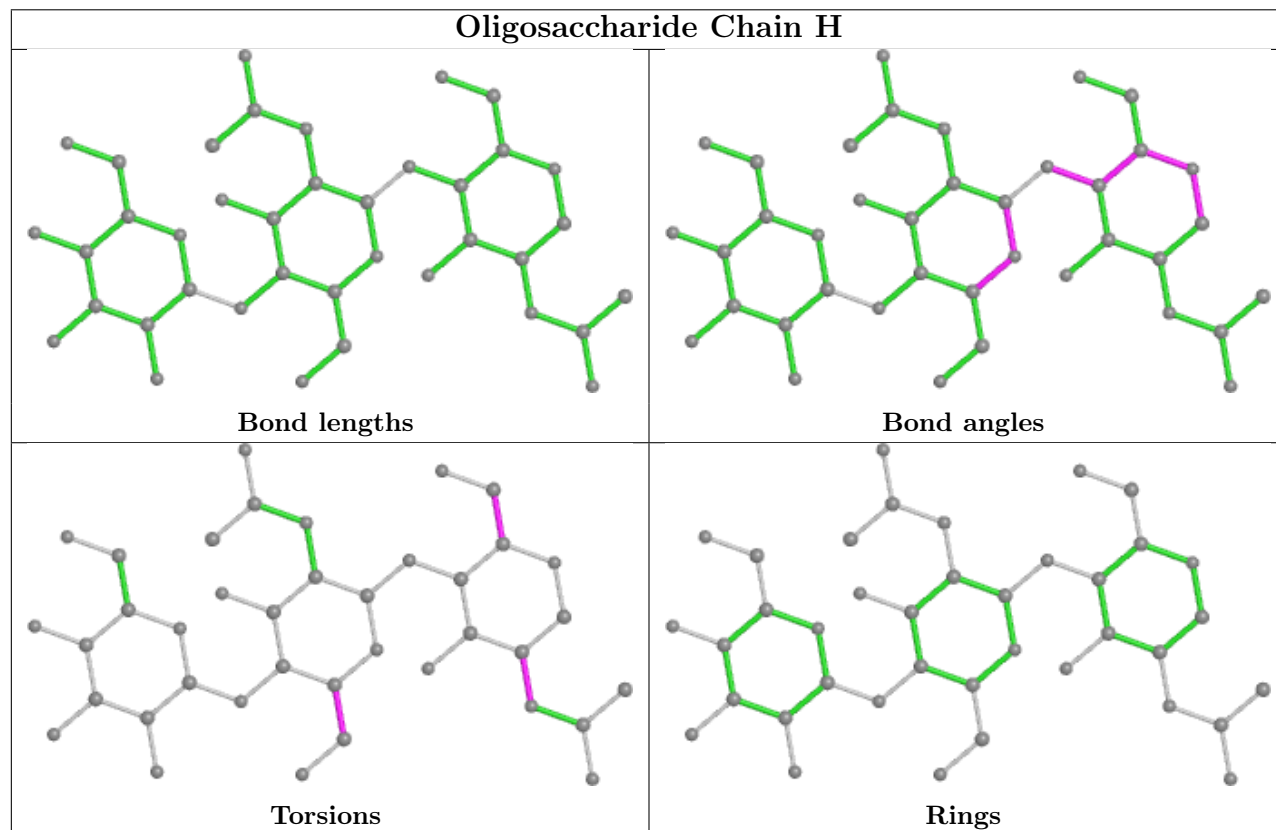
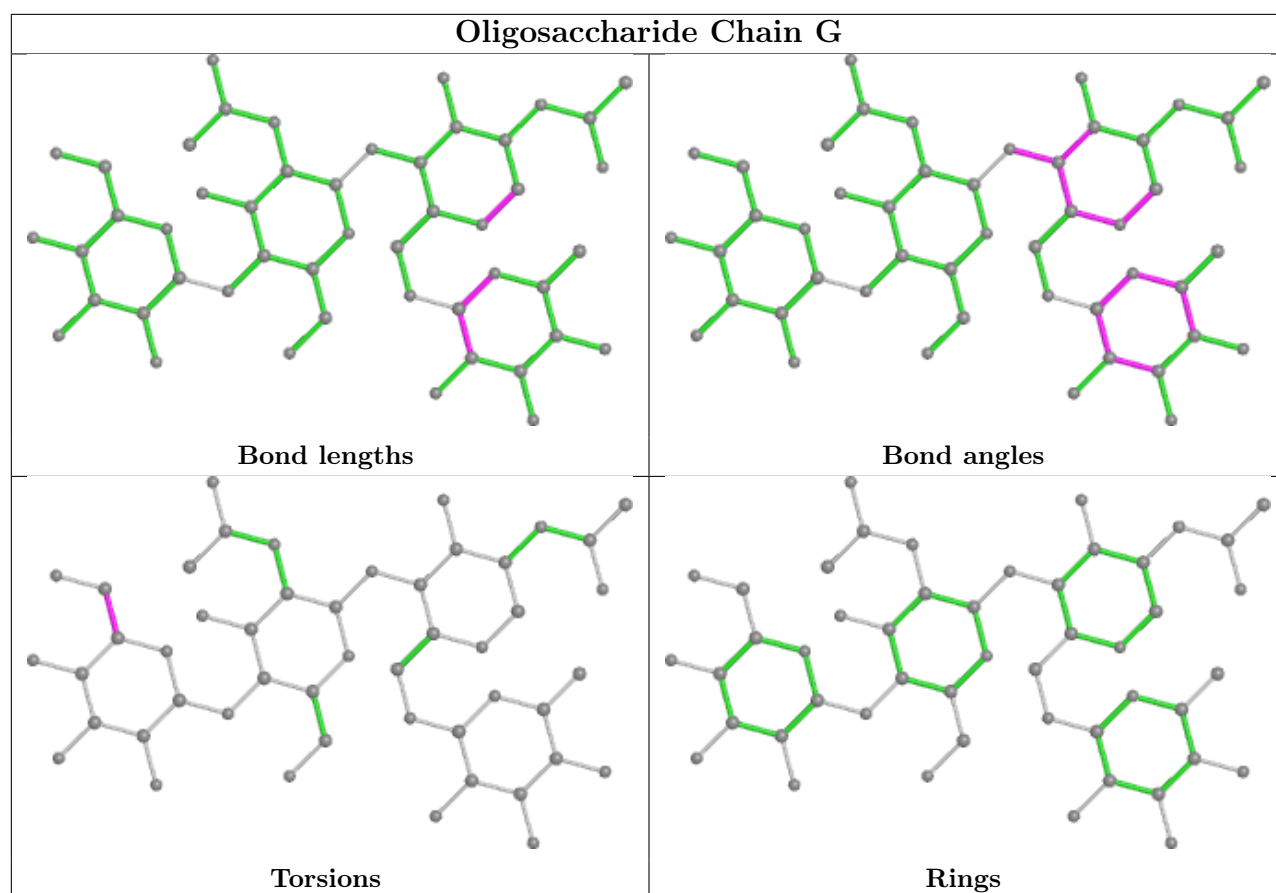
There are no ring outliers.

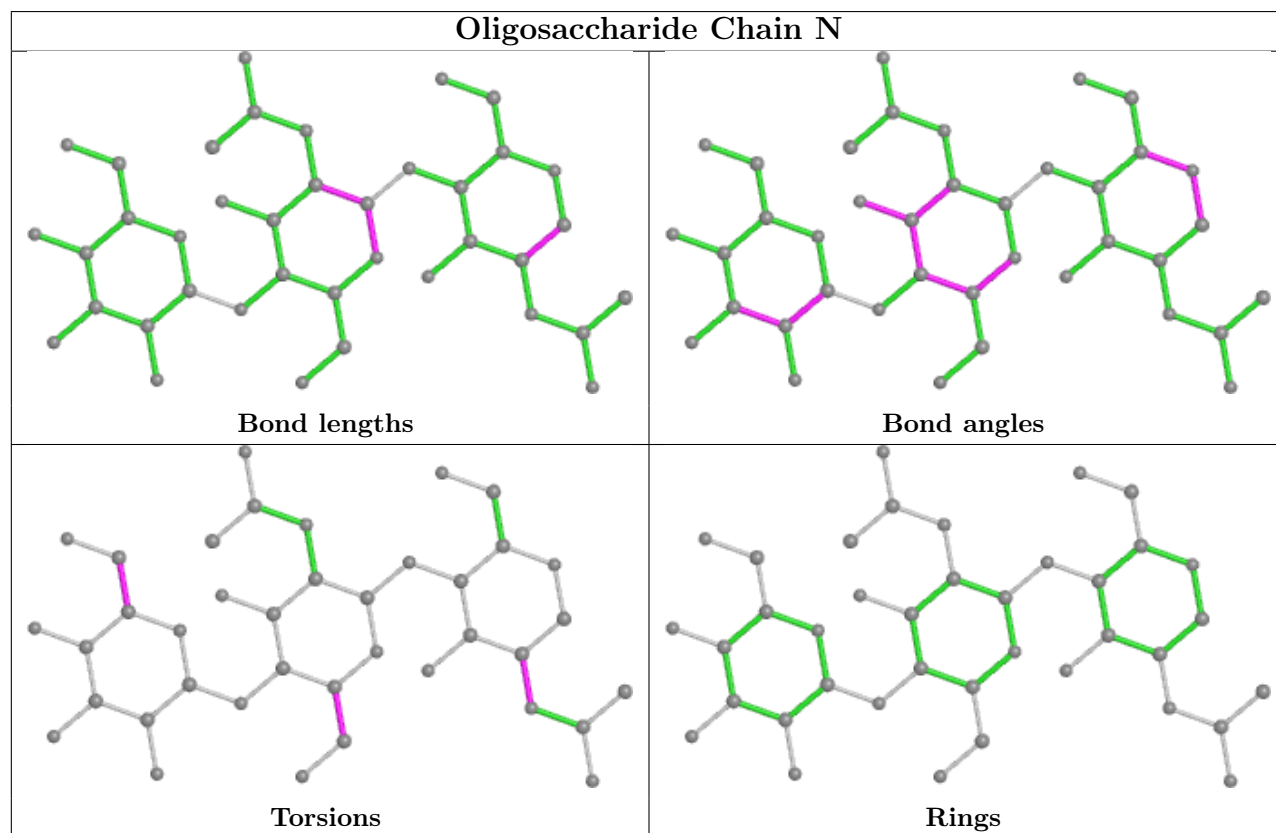
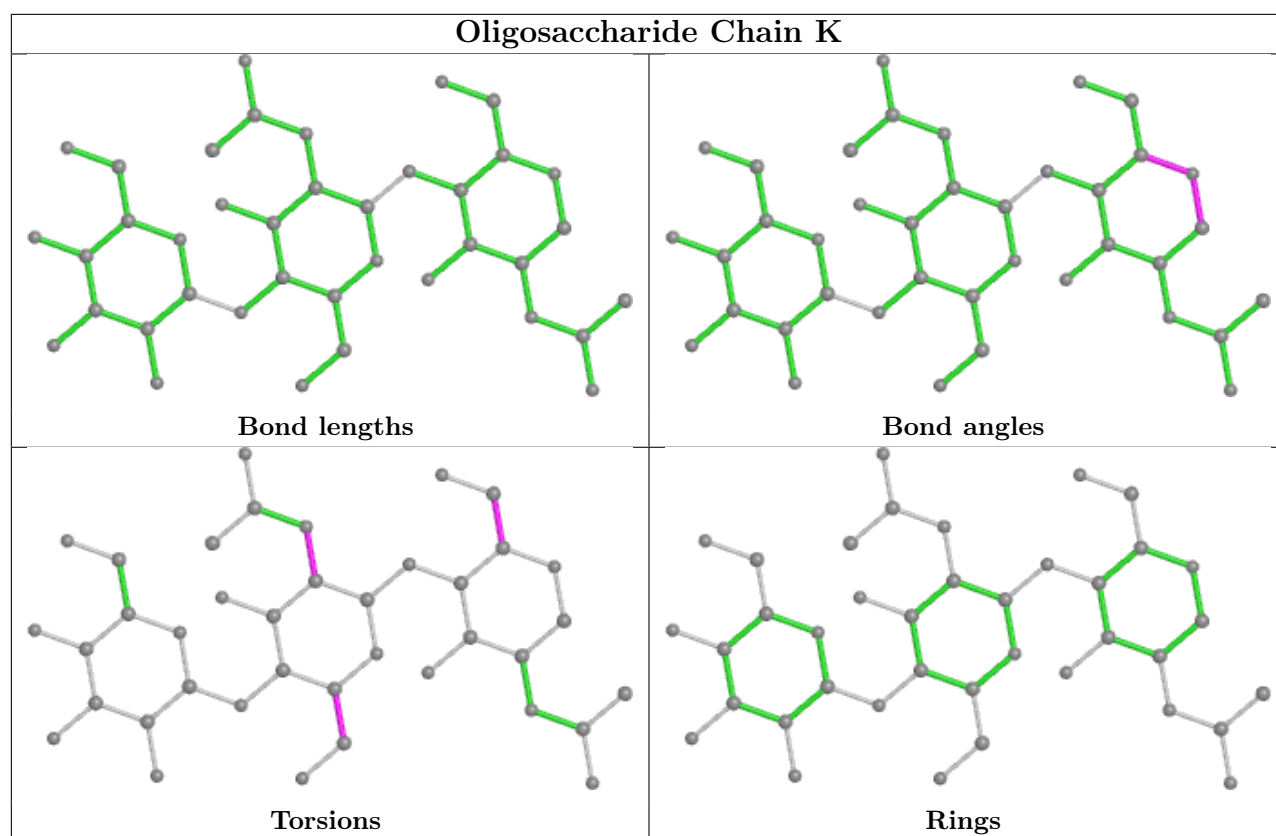
4 monomers are involved in 3 short contacts:

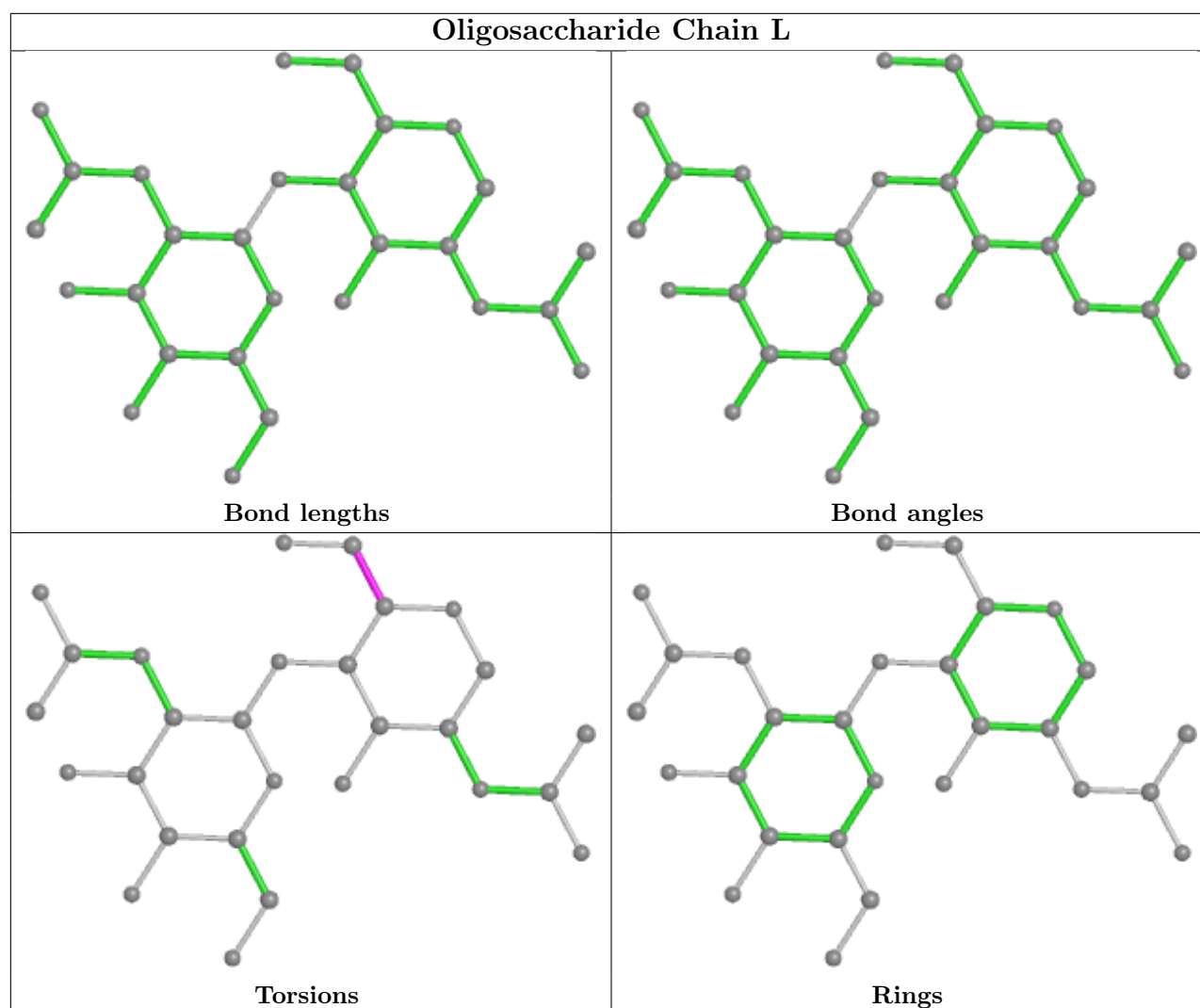
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	1	NAG	1	0
6	H	1	NAG	1	0
5	E	3	BMA	1	0
5	E	2	NAG	1	0

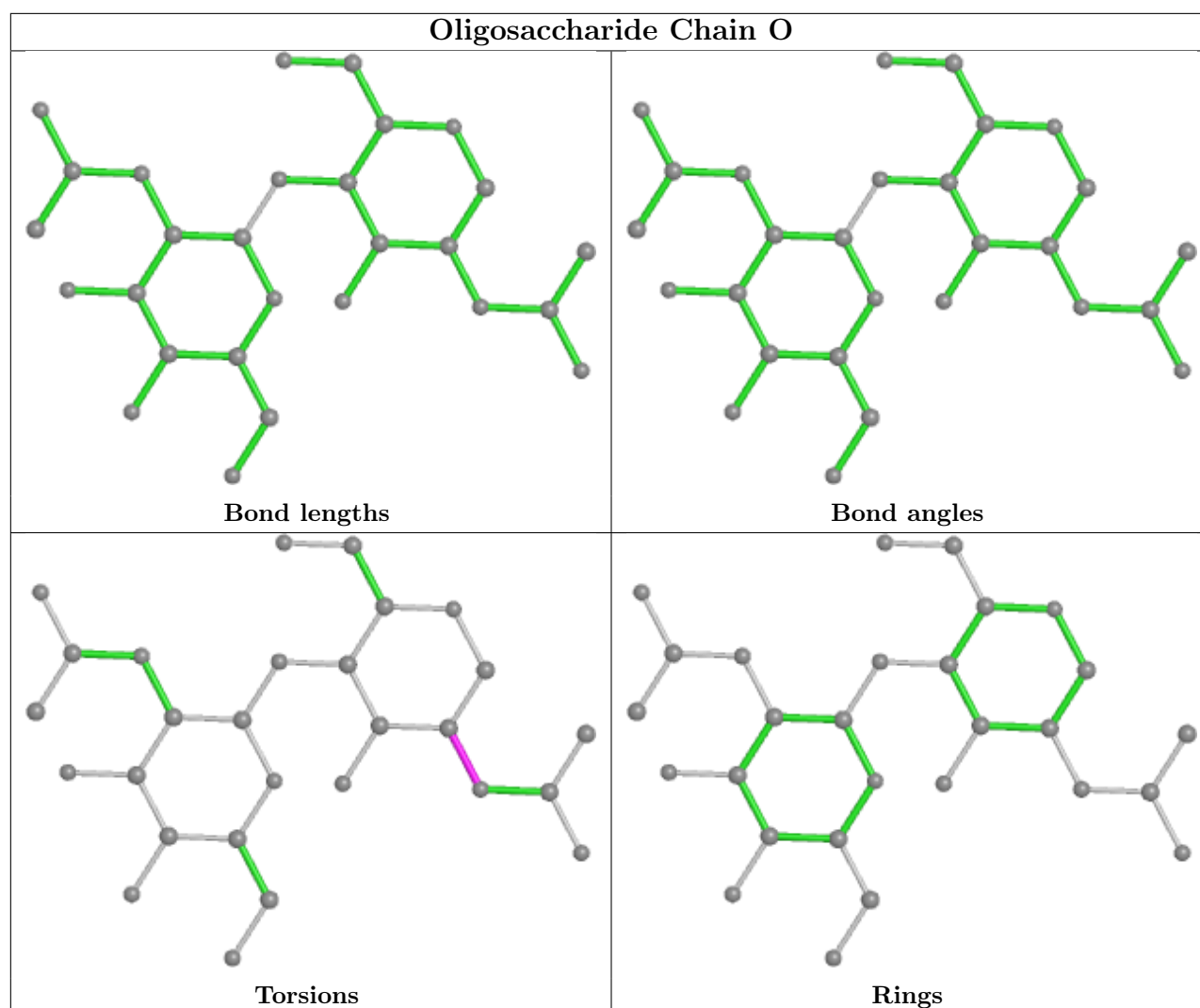
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
8	NAG	C	301	2	14,14,15	0.46	0	17,19,21	0.65	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
8	NAG	C	301	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	301	NAG	C1-O5-C5	2.30	115.30	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [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	F	270/288 (93%)	0.14	6 (2%) 62 60	62, 83, 126, 154	0
1	M	262/288 (90%)	0.30	11 (4%) 36 34	56, 119, 156, 171	0
2	A	215/216 (99%)	0.13	4 (1%) 66 65	74, 103, 142, 165	0
2	C	215/216 (99%)	0.03	2 (0%) 84 84	63, 83, 121, 143	0
3	I	108/118 (91%)	0.08	0 100 100	69, 92, 121, 128	0
3	J	108/118 (91%)	0.04	0 100 100	61, 75, 95, 122	0
4	B	196/198 (98%)	-0.12	0 100 100	68, 94, 125, 132	0
4	D	197/198 (99%)	-0.05	0 100 100	63, 75, 102, 120	0
All	All	1571/1640 (95%)	0.08	23 (1%) 73 72	56, 90, 140, 171	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	28	THR	6.2
1	M	41	TRP	3.5
1	F	44	ASN	3.1
2	A	169	LEU	3.1
1	M	30	LEU	2.8

### 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,



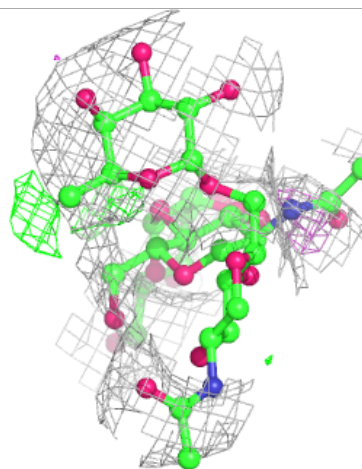
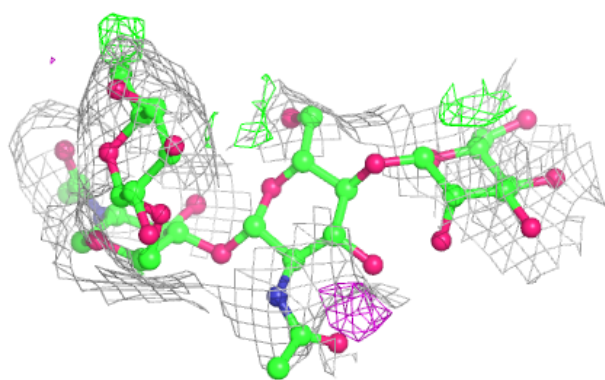
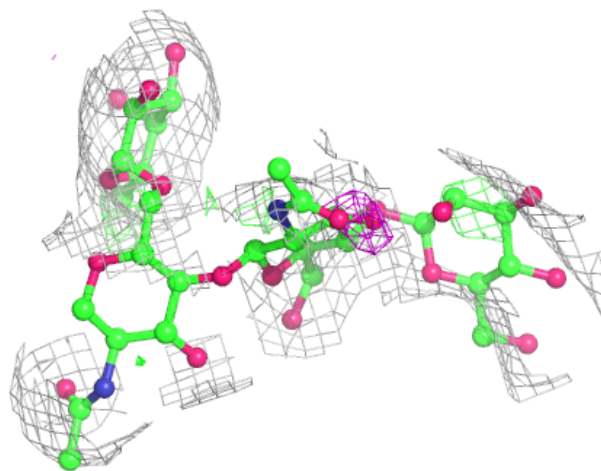
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	BMA	E	3	11/12	0.65	0.24	134,143,152,155	0
6	BMA	H	3	11/12	0.70	0.22	95,110,119,120	0
7	NAG	L	2	14/15	0.74	0.34	132,148,154,154	0
5	NAG	E	2	14/15	0.80	0.24	125,134,146,151	0
6	NAG	K	2	14/15	0.80	0.16	148,159,166,172	0
6	NAG	H	1	14/15	0.80	0.20	108,113,118,127	0
6	NAG	N	1	14/15	0.81	0.18	106,124,126,129	0
6	BMA	N	3	11/12	0.81	0.17	125,145,145,152	0
5	NAG	G	2	14/15	0.81	0.26	152,162,170,176	0
5	BMA	G	3	11/12	0.82	0.15	160,166,173,176	0
7	NAG	O	2	14/15	0.83	0.28	122,123,124,124	0
7	NAG	O	1	14/15	0.84	0.22	104,104,105,105	0
6	BMA	K	3	11/12	0.84	0.13	156,168,172,180	0
6	NAG	N	2	14/15	0.86	0.24	121,129,143,155	0
5	NAG	E	1	14/15	0.88	0.13	93,102,109,111	0
6	NAG	K	1	14/15	0.88	0.13	125,137,143,144	0
5	FUC	G	4	10/11	0.89	0.18	130,135,141,141	0
5	NAG	G	1	14/15	0.89	0.14	130,134,140,142	0
7	NAG	L	1	14/15	0.90	0.34	134,145,149,154	0
6	NAG	H	2	14/15	0.90	0.17	112,119,121,129	0
5	FUC	E	4	10/11	0.91	0.15	97,104,111,115	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.

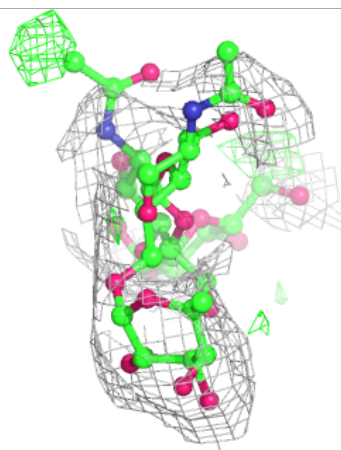
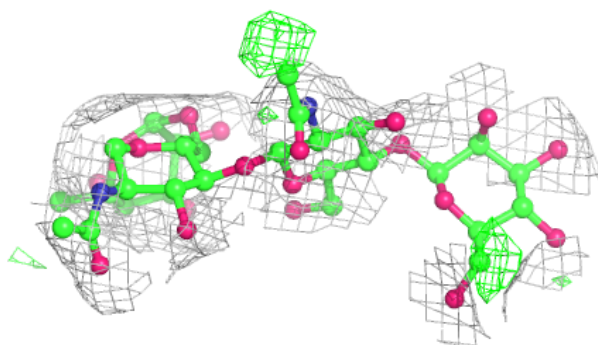
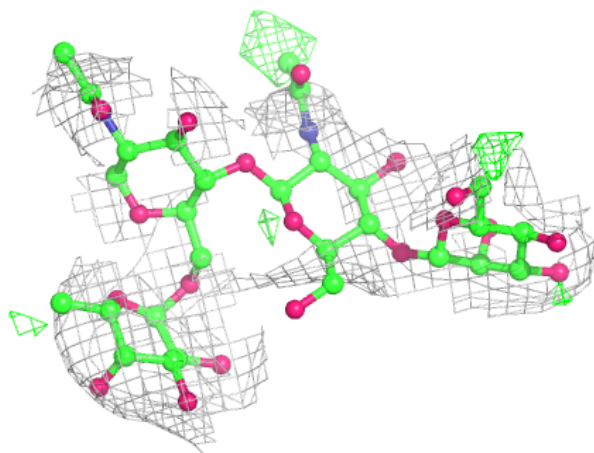
**Electron density around Chain E:**

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



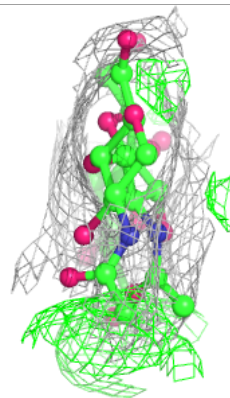
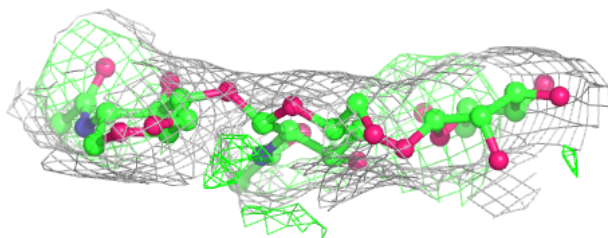
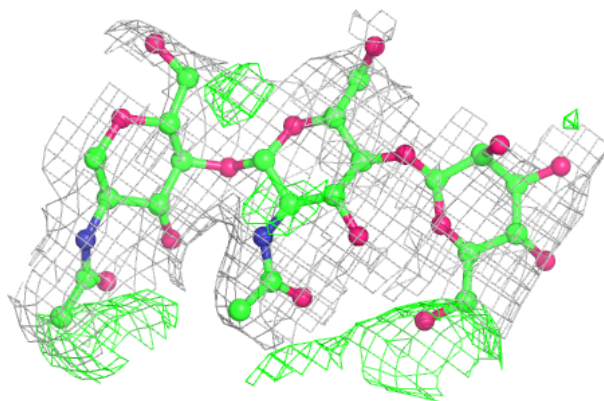
**Electron density around Chain G:**

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



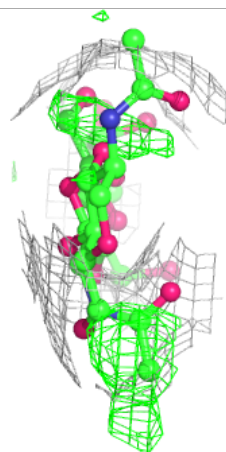
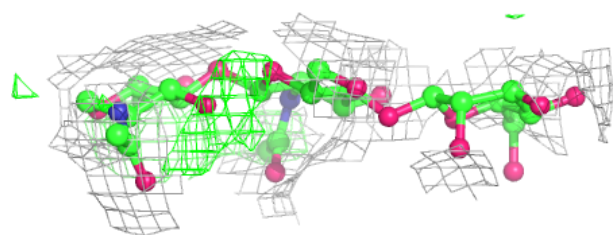
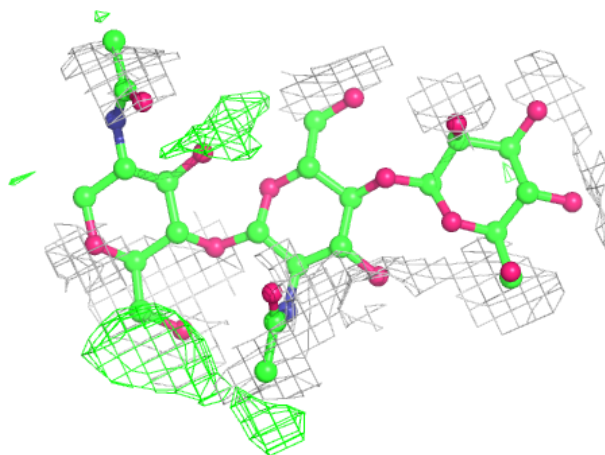
**Electron density around Chain H:**

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



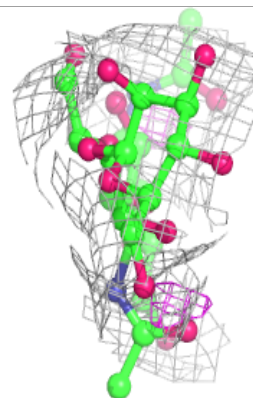
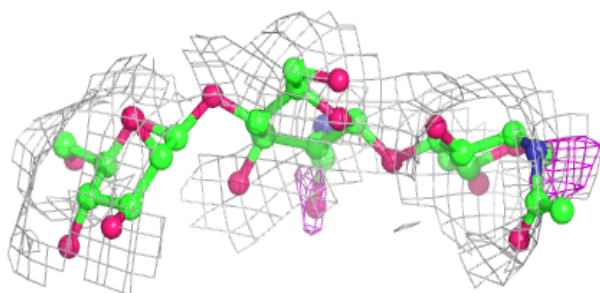
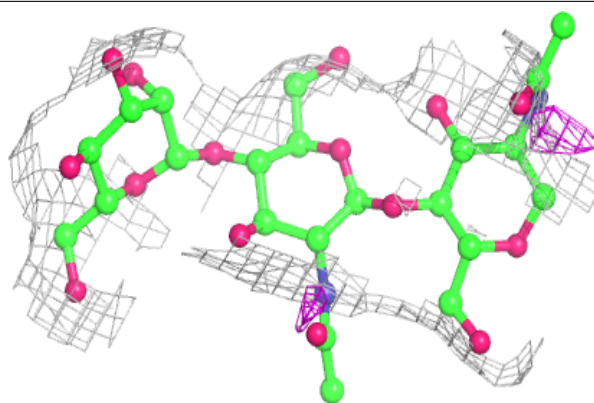
**Electron density around Chain K:**

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

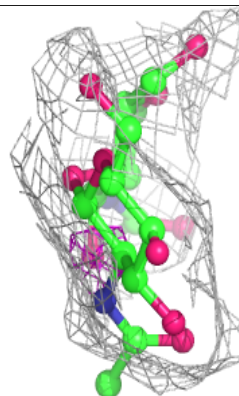
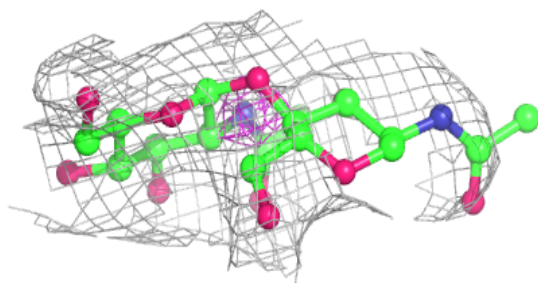
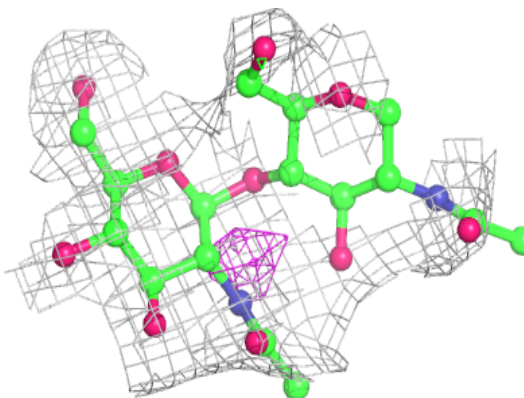


**Electron density around Chain N:**

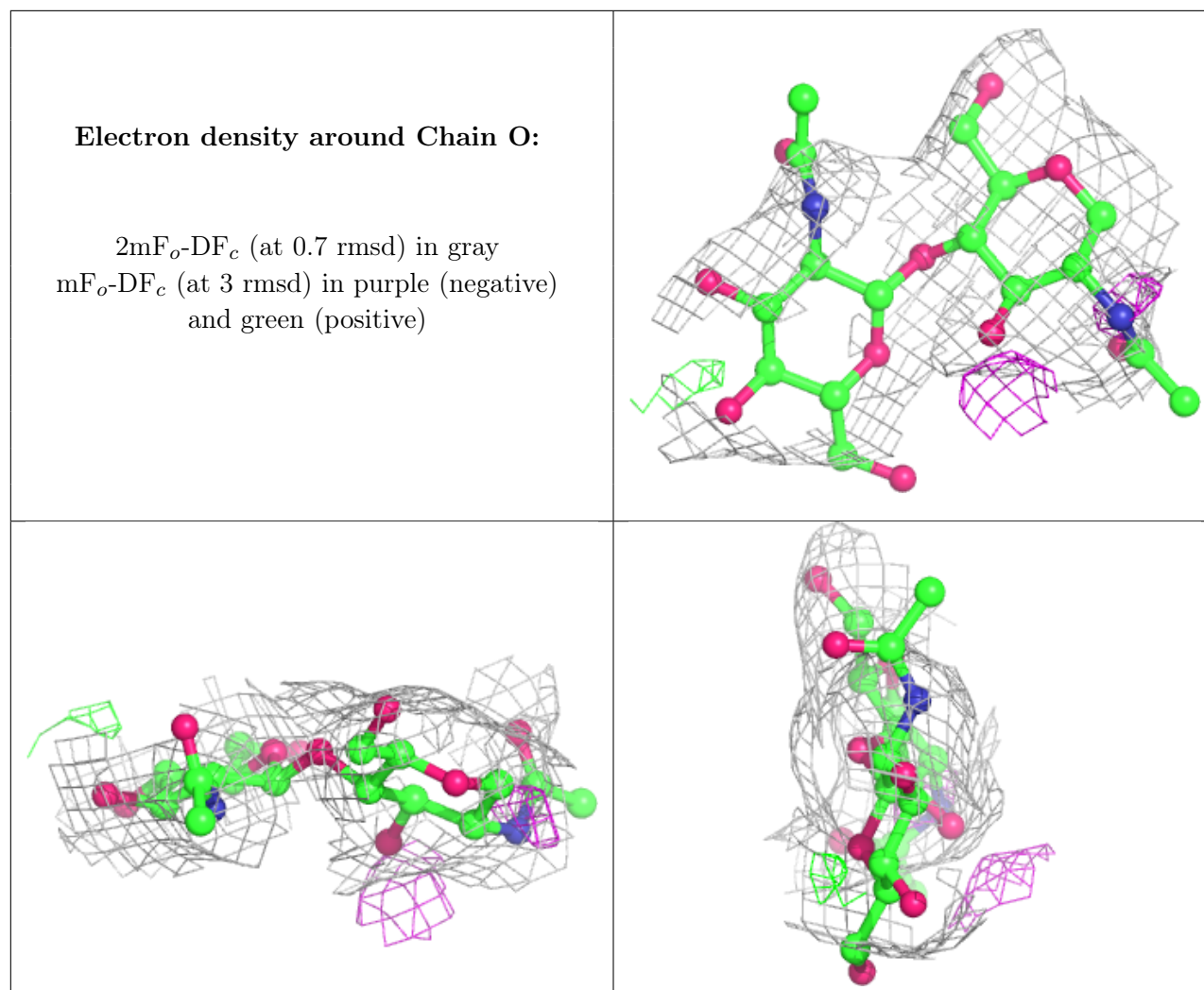
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**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 ⓘ

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	C	301	14/15	0.71	0.22	116,127,134,134	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.