



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 1, 2021 – 10:04 AM EDT

PDB ID : 7KX0
Title : Crystal structure of the CD27:CD70 co-stimulatory complex
Authors : Maben, Z.; Liu, W.; Mosyak, L.; Chaparro-Riggers, J.
Deposited on : 2020-12-02
Resolution : 2.69 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : 2.23.1
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) : 2.23.1

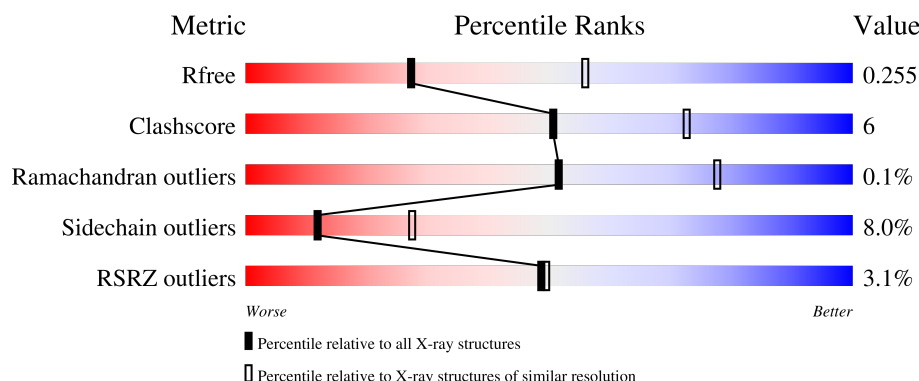
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 ≥ 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	158	<div> <div>4%</div> <div>74%</div> <div>14%</div> <div>•</div> <div>11%</div> </div>
1	B	158	<div> <div>%</div> <div>69%</div> <div>18%</div> <div>•</div> <div>11%</div> </div>
1	C	158	<div> <div>4%</div> <div>71%</div> <div>17%</div> <div>•</div> <div>11%</div> </div>
2	D	114	<div> <div>4%</div> <div>70%</div> <div>16%</div> <div>•</div> <div>12%</div> </div>
2	E	114	<div> <div>%</div> <div>67%</div> <div>18%</div> <div>•</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	114	
3	G	4	
3	I	4	
4	H	4	
5	J	5	
5	L	5	
6	K	5	

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
5	MAN	L	5	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6093 atoms, of which 12 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 CD70 antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	140	Total	C	N	O	S	0	0	0
			1083	678	203	197	5			
1	B	140	Total	C	N	O	S	0	0	0
			1083	678	203	197	5			
1	C	140	Total	C	N	O	S	0	0	0
			1083	678	203	197	5			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	HIS	-	expression tag	UNP P32970
A	37	HIS	-	expression tag	UNP P32970
A	38	HIS	-	expression tag	UNP P32970
A	39	HIS	-	expression tag	UNP P32970
A	40	HIS	-	expression tag	UNP P32970
A	41	HIS	-	expression tag	UNP P32970
A	42	GLY	-	expression tag	UNP P32970
A	43	SER	-	expression tag	UNP P32970
A	44	GLY	-	expression tag	UNP P32970
B	36	HIS	-	expression tag	UNP P32970
B	37	HIS	-	expression tag	UNP P32970
B	38	HIS	-	expression tag	UNP P32970
B	39	HIS	-	expression tag	UNP P32970
B	40	HIS	-	expression tag	UNP P32970
B	41	HIS	-	expression tag	UNP P32970
B	42	GLY	-	expression tag	UNP P32970
B	43	SER	-	expression tag	UNP P32970
B	44	GLY	-	expression tag	UNP P32970
C	36	HIS	-	expression tag	UNP P32970
C	37	HIS	-	expression tag	UNP P32970
C	38	HIS	-	expression tag	UNP P32970
C	39	HIS	-	expression tag	UNP P32970
C	40	HIS	-	expression tag	UNP P32970

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Chain	Residue	Modelled	Actual	Comment	Reference
C	41	HIS	-	expression tag	UNP P32970
C	42	GLY	-	expression tag	UNP P32970
C	43	SER	-	expression tag	UNP P32970
C	44	GLY	-	expression tag	UNP P32970

- Molecule 2 is a protein called CD27 antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	100	Total	C	N	O	S	0	0	0
			775	465	149	144	17			
2	E	99	Total	C	N	O	S	0	0	0
			766	459	147	143	17			
2	F	99	Total	C	N	O	S	0	0	0
			766	459	147	143	17			

There are 27 discrepancies between the modelled and reference sequences:

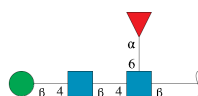
Chain	Residue	Modelled	Actual	Comment	Reference
D	128	GLY	-	expression tag	UNP P26842
D	129	SER	-	expression tag	UNP P26842
D	130	GLY	-	expression tag	UNP P26842
D	131	HIS	-	expression tag	UNP P26842
D	132	HIS	-	expression tag	UNP P26842
D	133	HIS	-	expression tag	UNP P26842
D	134	HIS	-	expression tag	UNP P26842
D	135	HIS	-	expression tag	UNP P26842
D	136	HIS	-	expression tag	UNP P26842
E	128	GLY	-	expression tag	UNP P26842
E	129	SER	-	expression tag	UNP P26842
E	130	GLY	-	expression tag	UNP P26842
E	131	HIS	-	expression tag	UNP P26842
E	132	HIS	-	expression tag	UNP P26842
E	133	HIS	-	expression tag	UNP P26842
E	134	HIS	-	expression tag	UNP P26842
E	135	HIS	-	expression tag	UNP P26842
E	136	HIS	-	expression tag	UNP P26842
F	128	GLY	-	expression tag	UNP P26842
F	129	SER	-	expression tag	UNP P26842
F	130	GLY	-	expression tag	UNP P26842
F	131	HIS	-	expression tag	UNP P26842
F	132	HIS	-	expression tag	UNP P26842
F	133	HIS	-	expression tag	UNP P26842

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Chain	Residue	Modelled	Actual	Comment	Reference
F	134	HIS	-	expression tag	UNP P26842
F	135	HIS	-	expression tag	UNP P26842
F	136	HIS	-	expression tag	UNP P26842

- Molecule 3 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.



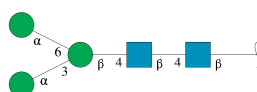
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	4	Total	C	N	O	0	0	0
			49	28	2	19			
3	I	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



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

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



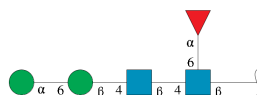
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	J	5	Total	C	N	O	0	0	0
			61	34	2	25			

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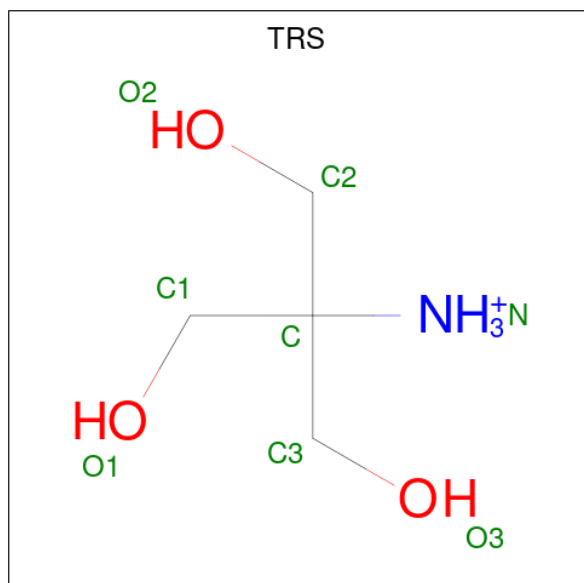
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	L	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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
6	K	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	H	N	O	0	0
			20	4	12	1	3		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

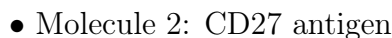
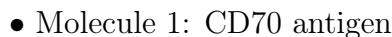
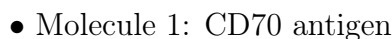


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	F	1	Total	C	N	O	0	0
			14	8	1	5		

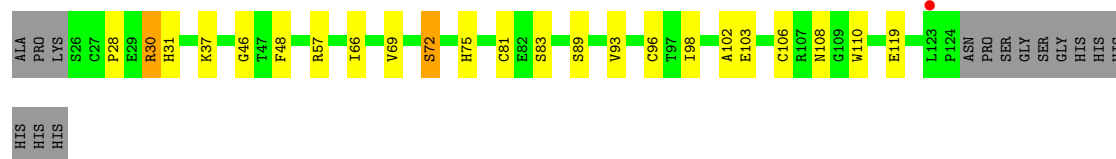
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	27	Total	O	0	0
			27	27		
9	B	33	Total	O	0	0
			33	33		
9	C	28	Total	O	0	0
			28	28		
9	D	17	Total	O	0	0
			17	17		
9	E	13	Total	O	0	0
			13	13		
9	F	27	Total	O	0	0
			27	27		

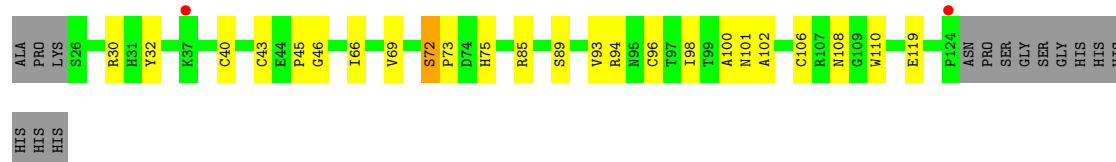
- Molecule 1: CD70 antigen



- Molecule 2: CD27 antigen



- Molecule 2: CD27 antigen



- Molecule 3: 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



- Molecule 3: 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



- Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  40% 60%

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 6: alpha-D-mannopyranose-(1-6)-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 K:  60% 40%

MAG1
MAG2
BMA3
MAN4
FUC5

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	109.53Å 113.63Å 163.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.72 – 2.69 93.31 – 2.69	Depositor EDS
% Data completeness (in resolution range)	64.9 (36.72-2.69) 60.3 (93.31-2.69)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.200 , 0.236 0.213 , 0.255	Depositor DCC
R_{free} test set	915 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 75.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for $-1/2^*h+1/2^*k+1/2^*l, 1/2^*h-1/2^*k+1/2^*l, h+k$ 0.025 for $-1/2^*h+1/2^*k-1/2^*l, 1/2^*h-1/2^*k-1/2^*l, -h-k$ 0.001 for $k, h, -l$ 0.044 for $-1/2^*h-1/2^*k+1/2^*l, -1/2^*h-1/2^*k-1/2^*l, h-k$ 0.019 for $-1/2^*h-1/2^*k-1/2^*l, -1/2^*h-1/2^*k+1/2^*l, -h+k$	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6093	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, NAG, TRS, BMA, 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	0.46	0/1110	0.69	0/1513
1	B	0.46	0/1110	0.70	0/1513
1	C	0.46	0/1110	0.69	0/1513
2	D	0.41	0/795	0.65	0/1076
2	E	0.42	0/786	0.66	0/1065
2	F	0.40	0/786	0.61	0/1065
All	All	0.44	0/5697	0.67	0/7745

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	1083	0	1067	10	0
1	B	1083	0	1067	14	0
1	C	1083	0	1067	13	0
2	D	775	0	705	13	0
2	E	766	0	692	9	0
2	F	766	0	692	12	0
3	G	49	0	43	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	49	0	43	0	0
4	H	50	0	43	0	0
5	J	61	0	52	0	0
5	L	61	0	52	0	0
6	K	60	0	52	0	0
7	C	8	12	12	1	0
8	D	14	0	13	0	0
8	E	14	0	13	0	0
8	F	14	0	13	0	0
9	A	27	0	0	0	0
9	B	33	0	0	1	0
9	C	28	0	0	0	0
9	D	17	0	0	0	0
9	E	13	0	0	0	0
9	F	27	0	0	0	0
All	All	6081	12	5626	66	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 6.

The worst 5 of 66 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:D:30:ARG:HH22	2:D:75:HIS:HD2	1.18	0.91
2:D:30:ARG:HH22	2:D:75:HIS:CD2	1.94	0.85
1:B:57:VAL:HG21	1:C:192:ARG:HG3	1.67	0.76
2:F:45:PRO:HD3	2:F:75:HIS:CE1	2.30	0.66
2:D:89:SER:HB3	2:D:119:GLU:HA	1.86	0.57

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	138/158 (87%)	124 (90%)	14 (10%)	0	100	100
1	B	138/158 (87%)	124 (90%)	13 (9%)	1 (1%)	22	46
1	C	138/158 (87%)	123 (89%)	15 (11%)	0	100	100
2	D	98/114 (86%)	94 (96%)	4 (4%)	0	100	100
2	E	97/114 (85%)	91 (94%)	6 (6%)	0	100	100
2	F	97/114 (85%)	90 (93%)	7 (7%)	0	100	100
All	All	706/816 (86%)	646 (92%)	59 (8%)	1 (0%)	51	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	66	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	119/135 (88%)	110 (92%)	9 (8%)	13	30
1	B	119/135 (88%)	106 (89%)	13 (11%)	6	14
1	C	119/135 (88%)	109 (92%)	10 (8%)	11	25
2	D	89/100 (89%)	83 (93%)	6 (7%)	16	37
2	E	88/100 (88%)	80 (91%)	8 (9%)	9	21
2	F	88/100 (88%)	84 (96%)	4 (4%)	27	55
All	All	622/705 (88%)	572 (92%)	50 (8%)	12	27

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	157	ARG
2	D	93	VAL
2	F	108	ASN
1	C	175	LEU

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Mol	Chain	Res	Type
2	D	30	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	99	HIS
2	F	80	HIS
1	C	107	HIS
2	F	101	ASN
2	E	75	HIS

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 ⓘ

27 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	G	1	1,3	14,14,15	0.33	0	17,19,21	0.68	0
3	NAG	G	2	3	14,14,15	0.38	0	17,19,21	0.97	2 (11%)
3	BMA	G	3	3	11,11,12	0.33	0	15,15,17	0.55	0
3	FUC	G	4	3	10,10,11	0.42	0	14,14,16	0.85	1 (7%)
4	NAG	H	1	1,4	14,14,15	0.33	0	17,19,21	0.76	0
4	NAG	H	2	4	14,14,15	0.31	0	17,19,21	0.78	0
4	BMA	H	3	4	11,11,12	0.33	0	15,15,17	0.87	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	H	4	4	11,11,12	0.38	0	15,15,17	0.80	1 (6%)
3	NAG	I	1	1,3	14,14,15	0.30	0	17,19,21	0.71	0
3	NAG	I	2	3	14,14,15	0.38	0	17,19,21	1.36	2 (11%)
3	BMA	I	3	3	11,11,12	0.33	0	15,15,17	0.79	1 (6%)
3	FUC	I	4	3	10,10,11	0.40	0	14,14,16	0.60	0
5	NAG	J	1	1,5	14,14,15	0.30	0	17,19,21	0.72	0
5	NAG	J	2	5	14,14,15	0.26	0	17,19,21	0.58	0
5	BMA	J	3	5	11,11,12	0.32	0	15,15,17	0.63	0
5	MAN	J	4	5	11,11,12	0.37	0	15,15,17	0.82	1 (6%)
5	MAN	J	5	5	11,11,12	0.34	0	15,15,17	0.95	1 (6%)
6	NAG	K	1	1,6	14,14,15	0.30	0	17,19,21	0.58	0
6	NAG	K	2	6	14,14,15	0.24	0	17,19,21	0.49	0
6	BMA	K	3	6	11,11,12	0.33	0	15,15,17	0.66	0
6	MAN	K	4	6	11,11,12	0.35	0	15,15,17	0.76	1 (6%)
6	FUC	K	5	6	10,10,11	0.42	0	14,14,16	0.81	1 (7%)
5	NAG	L	1	1,5	14,14,15	0.34	0	17,19,21	0.69	0
5	NAG	L	2	5	14,14,15	0.27	0	17,19,21	0.64	0
5	BMA	L	3	5	11,11,12	0.31	0	15,15,17	0.67	1 (6%)
5	MAN	L	4	5	11,11,12	0.38	0	15,15,17	0.84	1 (6%)
5	MAN	L	5	5	11,11,12	0.31	0	15,15,17	0.73	1 (6%)

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	G	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	FUC	G	4	3	-	-	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1
4	MAN	H	4	4	-	0/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
3	FUC	I	4	3	-	-	0/1/1/1
5	NAG	J	1	1,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1
5	BMA	J	3	5	-	0/2/19/22	0/1/1/1
5	MAN	J	4	5	-	0/2/19/22	0/1/1/1
5	MAN	J	5	5	-	0/2/19/22	1/1/1/1
6	NAG	K	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
6	BMA	K	3	6	-	2/2/19/22	0/1/1/1
6	MAN	K	4	6	-	1/2/19/22	1/1/1/1
6	FUC	K	5	6	-	-	0/1/1/1
5	NAG	L	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	L	2	5	-	0/6/23/26	0/1/1/1
5	BMA	L	3	5	-	0/2/19/22	0/1/1/1
5	MAN	L	4	5	-	0/2/19/22	0/1/1/1
5	MAN	L	5	5	-	1/2/19/22	1/1/1/1

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	2	NAG	C1-O5-C5	3.91	117.49	112.19
5	J	5	MAN	C1-O5-C5	3.24	116.58	112.19
3	I	2	NAG	C1-C2-N2	2.79	115.25	110.49
3	G	2	NAG	C1-O5-C5	2.70	115.86	112.19
4	H	3	BMA	C1-O5-C5	2.69	115.83	112.19

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

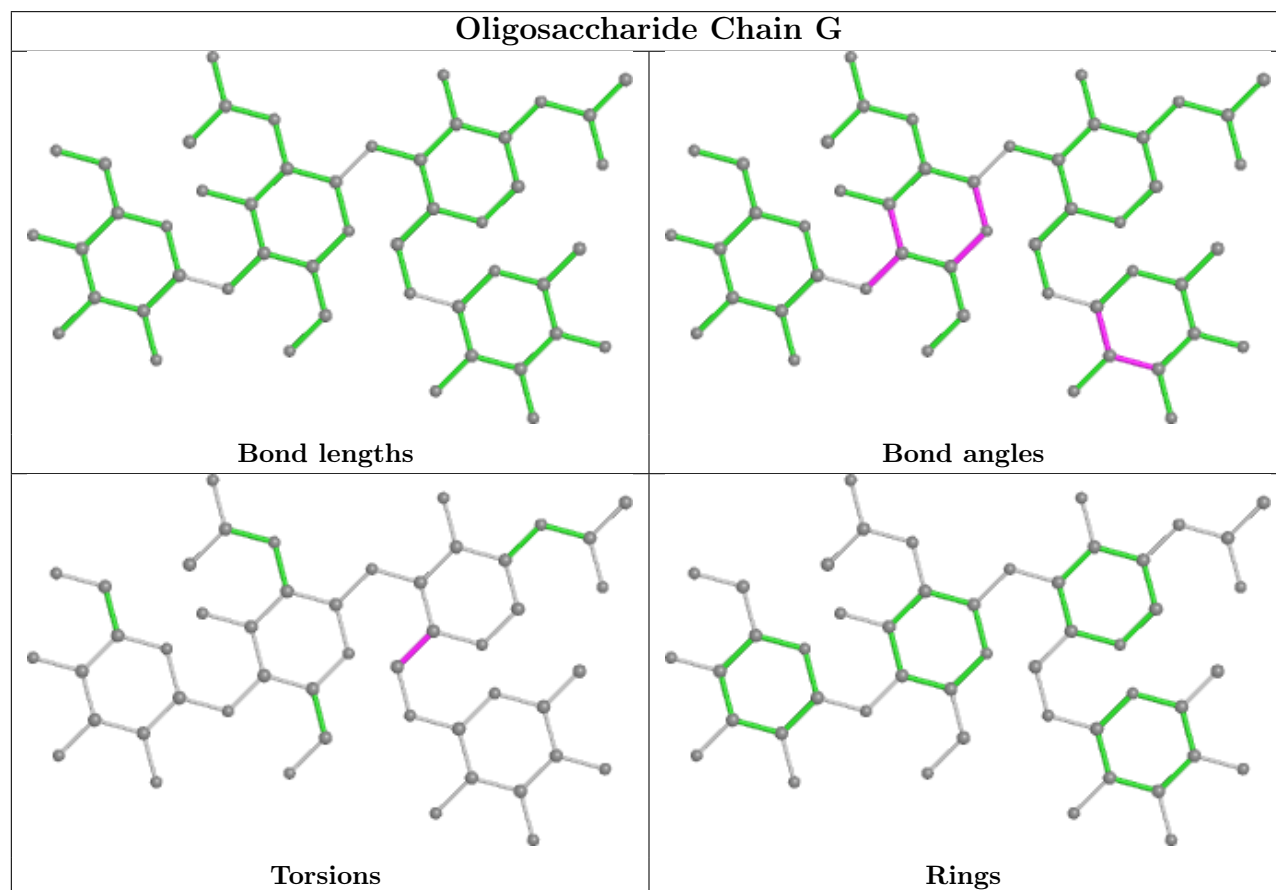
Mol	Chain	Res	Type	Atoms
6	K	4	MAN	O5-C5-C6-O6
5	L	5	MAN	O5-C5-C6-O6
6	K	3	BMA	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6

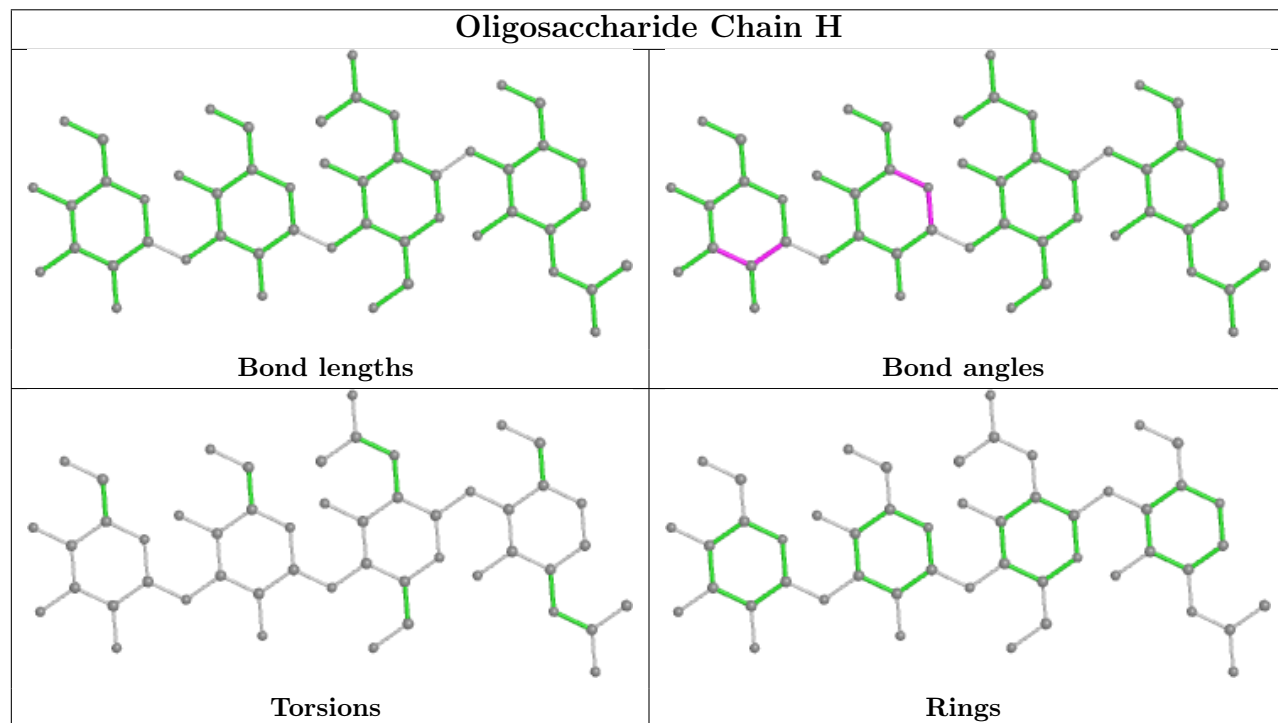
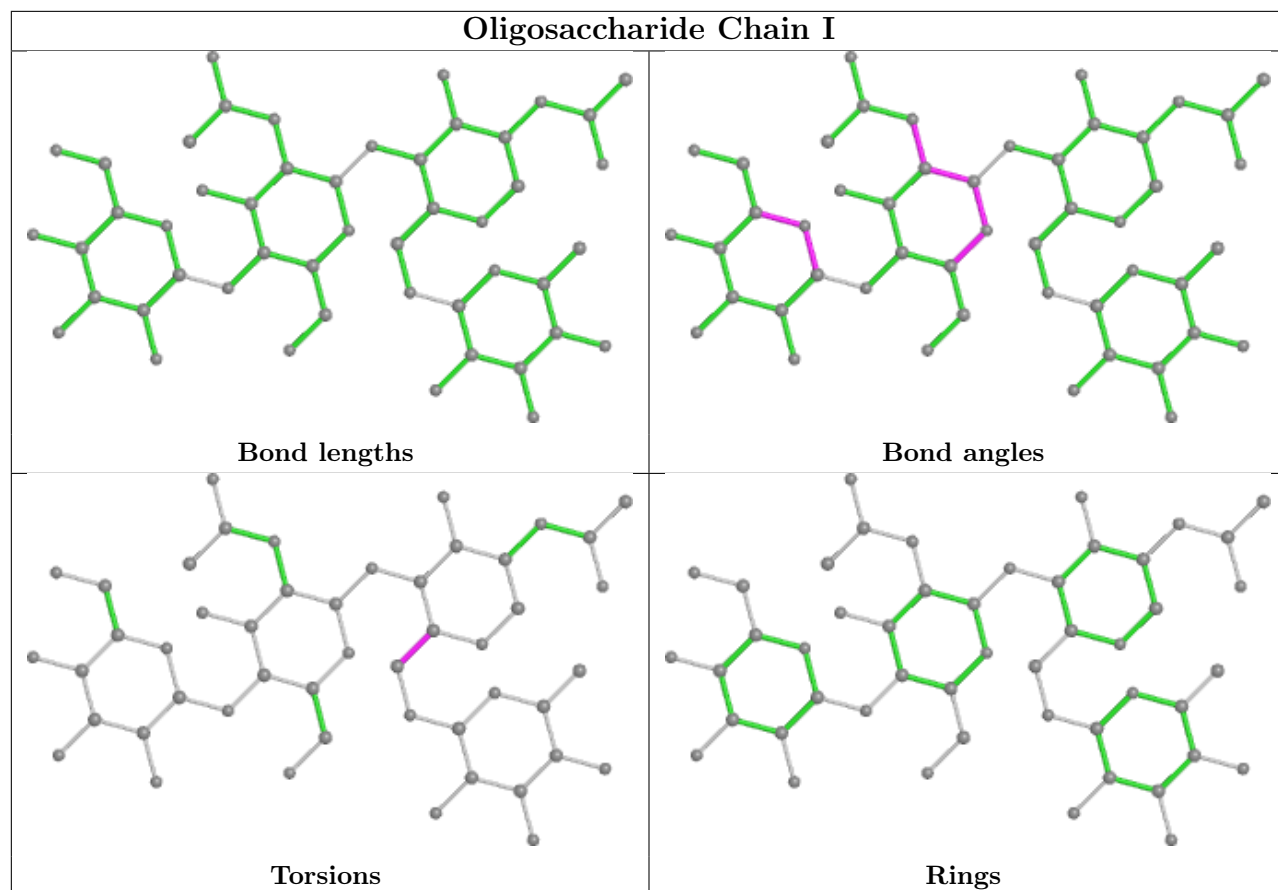
All (3) ring outliers are listed below:

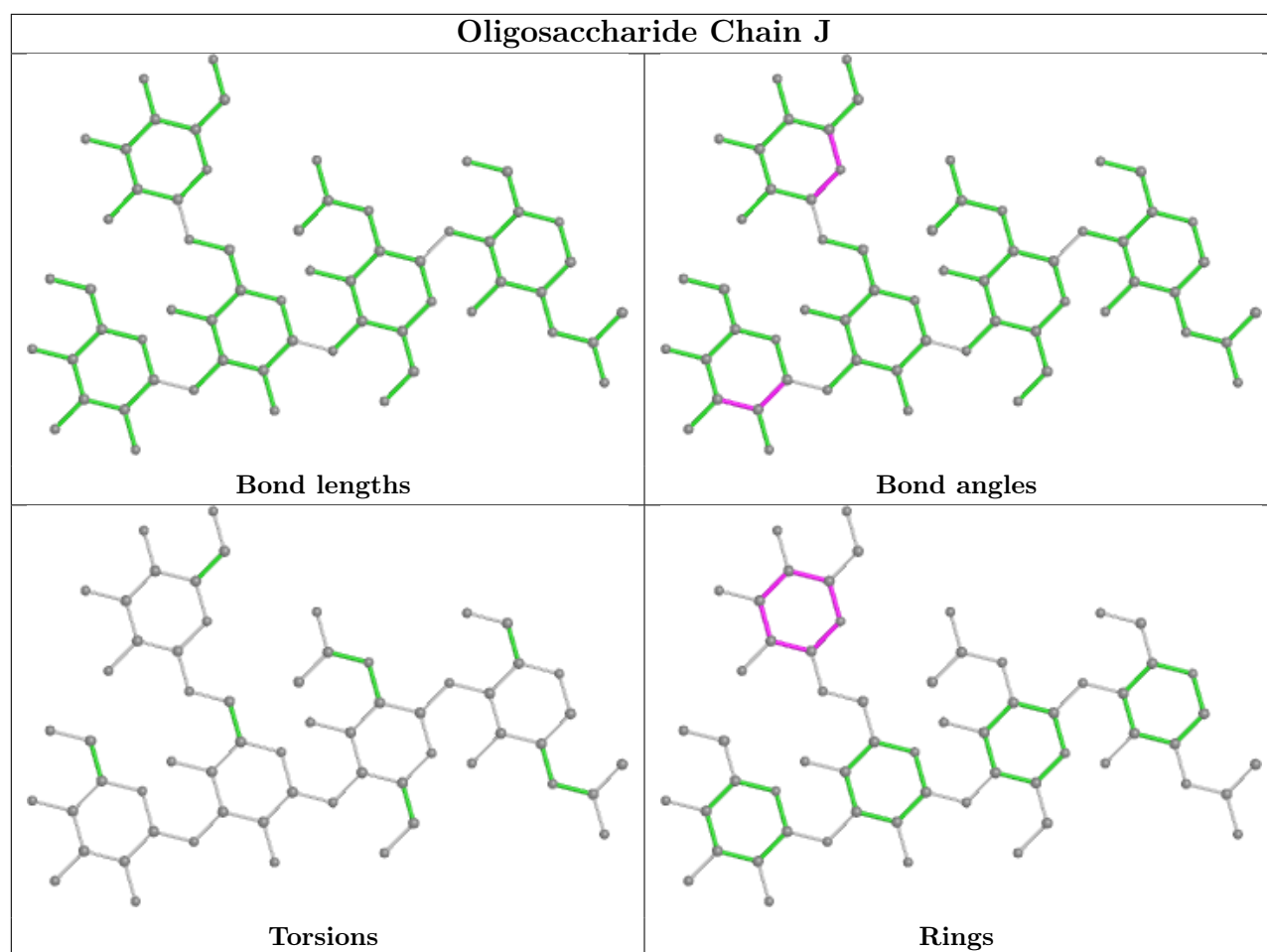
Mol	Chain	Res	Type	Atoms
5	L	5	MAN	C1-C2-C3-C4-C5-O5
5	J	5	MAN	C1-C2-C3-C4-C5-O5
6	K	4	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

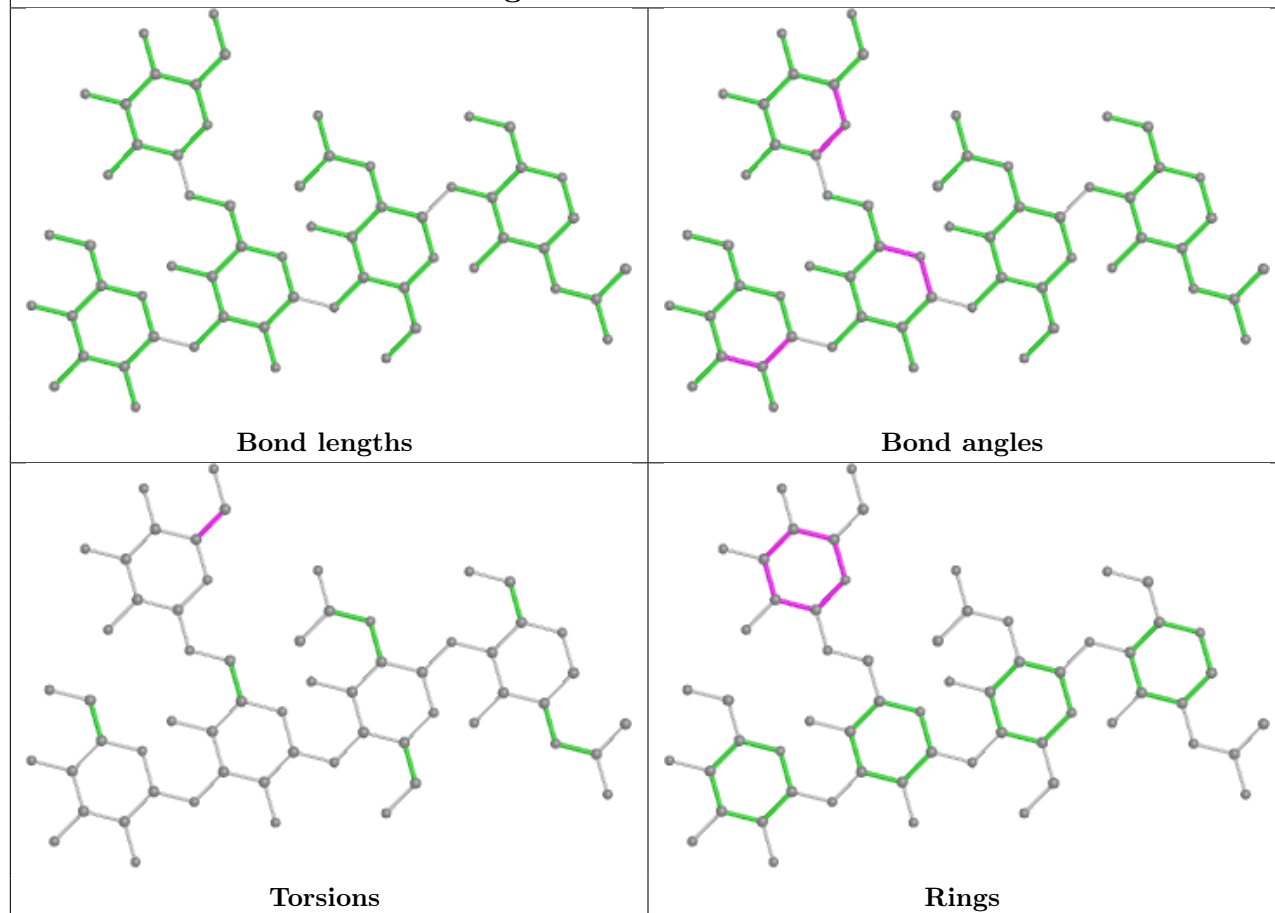
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



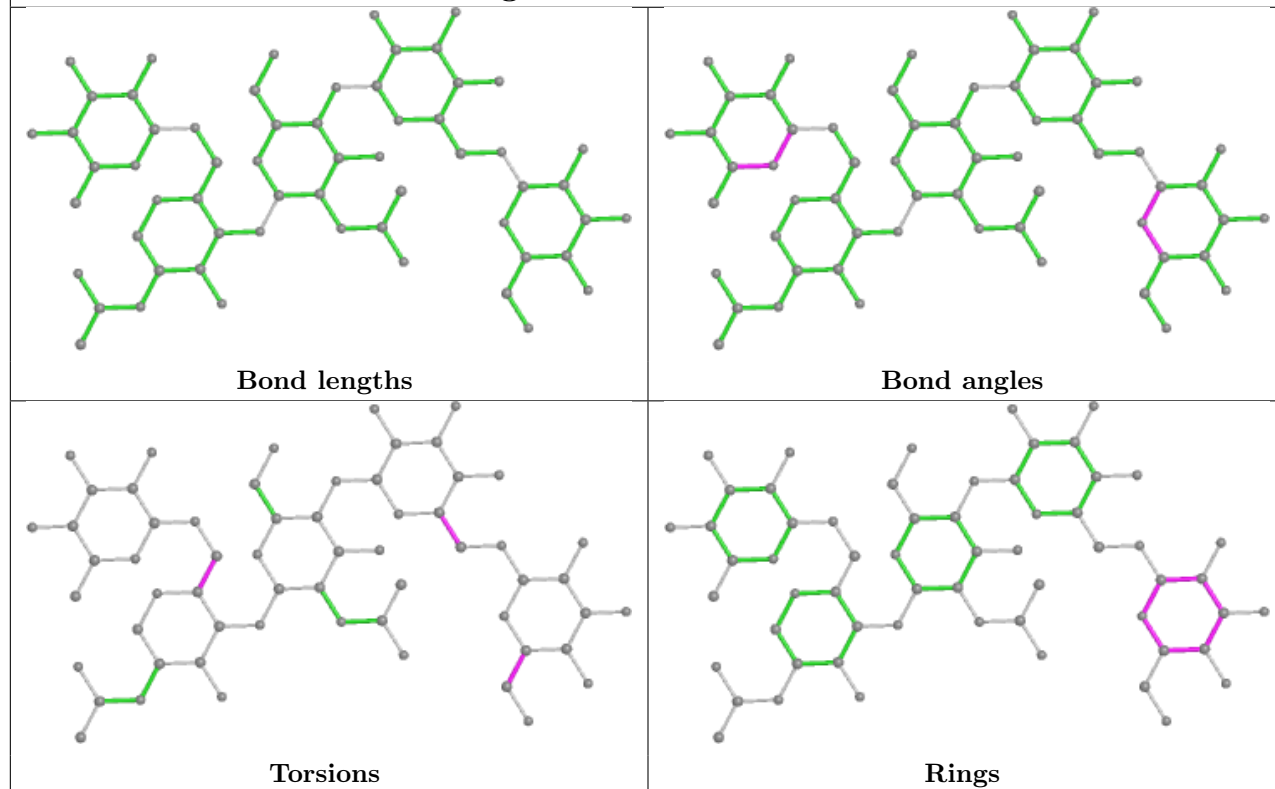




Oligosaccharide Chain L



Oligosaccharide Chain K



5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
8	NAG	E	201	2	14,14,15	0.31	0	17,19,21	0.74	1 (5%)
8	NAG	F	201	2	14,14,15	0.31	0	17,19,21	0.76	1 (5%)
8	NAG	D	201	2	14,14,15	0.30	0	17,19,21	0.73	1 (5%)
7	TRS	C	201	-	7,7,7	0.26	0	9,9,9	0.24	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	E	201	2	-	0/6/23/26	0/1/1/1
8	NAG	F	201	2	-	0/6/23/26	0/1/1/1
8	NAG	D	201	2	-	0/6/23/26	0/1/1/1
7	TRS	C	201	-	-	6/9/9/9	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	201	NAG	C1-O5-C5	2.66	115.80	112.19
8	D	201	NAG	C1-O5-C5	2.42	115.47	112.19
8	E	201	NAG	C1-O5-C5	2.29	115.29	112.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	201	TRS	C1-C-C3-O3

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Mol	Chain	Res	Type	Atoms
7	C	201	TRS	C2-C-C3-O3
7	C	201	TRS	N-C-C3-O3
7	C	201	TRS	C1-C-C2-O2
7	C	201	TRS	C3-C-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	201	TRS	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	140/158 (88%)	0.39	6 (4%) 35 33	58, 80, 119, 155	0
1	B	140/158 (88%)	0.17	1 (0%) 87 89	58, 81, 122, 174	0
1	C	140/158 (88%)	0.33	7 (5%) 28 27	60, 81, 122, 168	0
2	D	100/114 (87%)	0.37	5 (5%) 28 27	71, 97, 202, 267	0
2	E	99/114 (86%)	0.04	1 (1%) 82 83	68, 94, 150, 247	0
2	F	99/114 (86%)	0.01	2 (2%) 65 67	65, 87, 139, 231	0
All	All	718/816 (87%)	0.23	22 (3%) 49 49	58, 87, 142, 267	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	26	SER	4.8
2	D	25	LYS	4.7
2	E	123	LEU	4.0
1	C	55	TRP	3.4
2	F	37	LYS	3.4

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](#)

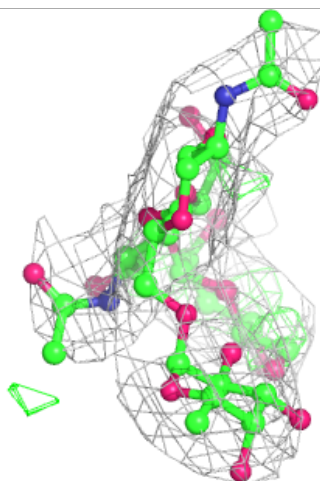
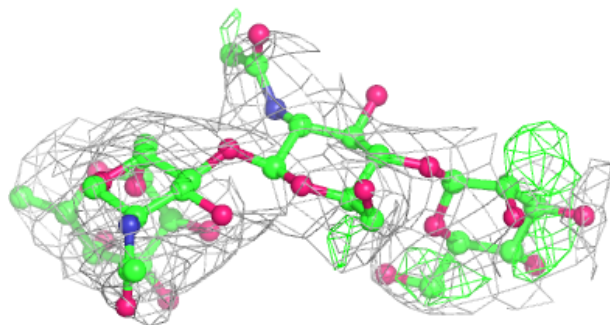
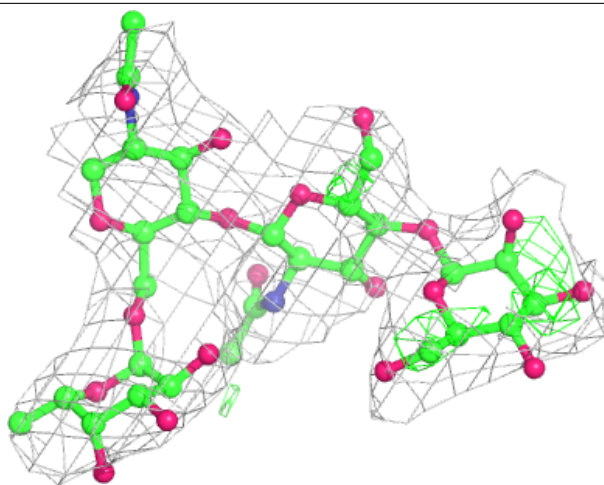
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BMA	I	3	11/12	0.38	0.38	241,248,252,255	0
4	BMA	H	3	11/12	0.39	0.27	233,239,246,252	0
4	MAN	H	4	11/12	0.40	0.40	256,265,275,276	0
5	BMA	L	3	11/12	0.54	0.28	250,256,263,275	0
6	BMA	K	3	11/12	0.63	0.20	230,237,241,245	0
5	BMA	J	3	11/12	0.67	0.25	244,249,260,269	0
6	MAN	K	4	11/12	0.67	0.27	242,248,254,257	0
3	BMA	G	3	11/12	0.68	0.32	238,241,250,250	0
5	MAN	L	5	11/12	0.68	0.43	253,255,258,260	0
5	MAN	J	5	11/12	0.70	0.26	242,244,247,249	0
5	MAN	J	4	11/12	0.72	0.32	273,277,279,281	0
3	NAG	I	2	14/15	0.73	0.26	212,226,232,236	0
5	MAN	L	4	11/12	0.76	0.28	279,283,287,287	0
6	NAG	K	2	14/15	0.80	0.22	191,215,223,224	0
4	NAG	H	2	14/15	0.81	0.26	142,159,207,224	0
3	NAG	G	2	14/15	0.87	0.17	169,206,228,231	0
3	NAG	I	1	14/15	0.87	0.20	117,129,150,191	0
5	NAG	L	1	14/15	0.87	0.23	117,128,139,153	0
4	NAG	H	1	14/15	0.88	0.18	109,118,127,134	0
5	NAG	J	2	14/15	0.89	0.24	150,181,222,236	0
5	NAG	L	2	14/15	0.89	0.29	158,210,233,243	0
3	FUC	G	4	10/11	0.90	0.20	129,132,136,138	0
3	NAG	G	1	14/15	0.90	0.17	107,121,131,145	0
3	FUC	I	4	10/11	0.92	0.19	136,138,142,159	0
6	NAG	K	1	14/15	0.93	0.18	97,117,132,153	0
5	NAG	J	1	14/15	0.95	0.17	114,124,132,141	0
6	FUC	K	5	10/11	0.96	0.15	136,137,139,147	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.

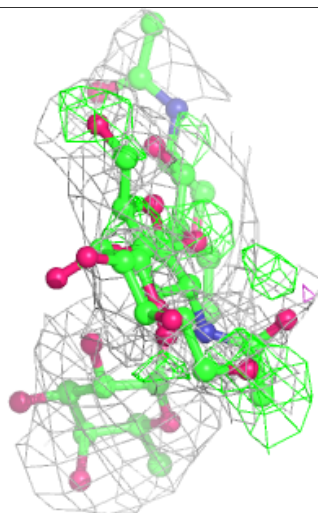
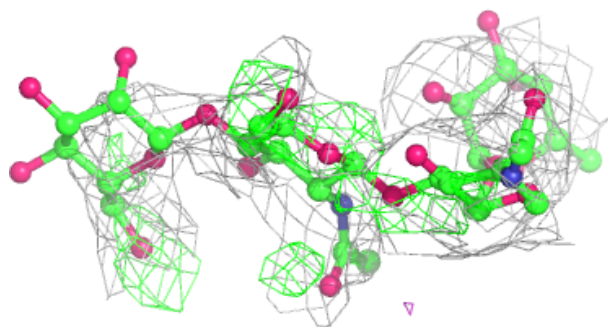
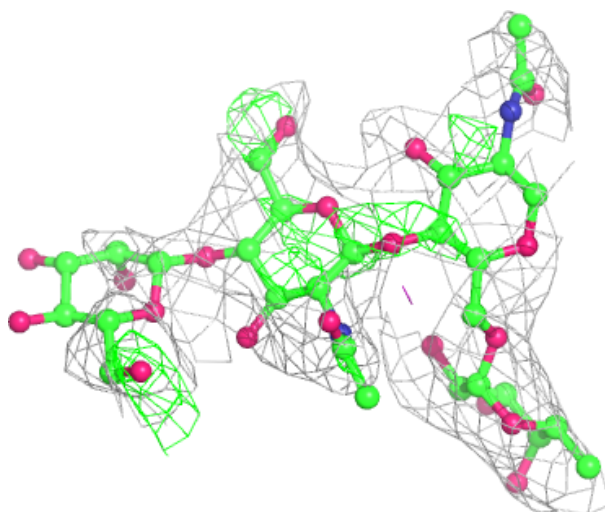
Electron density around Chain G:

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



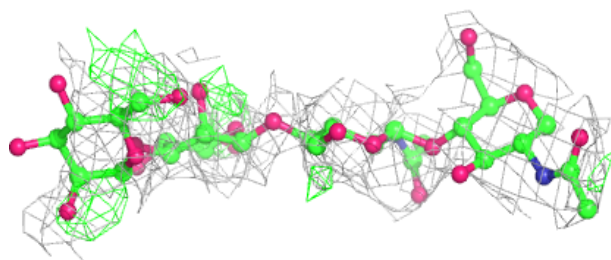
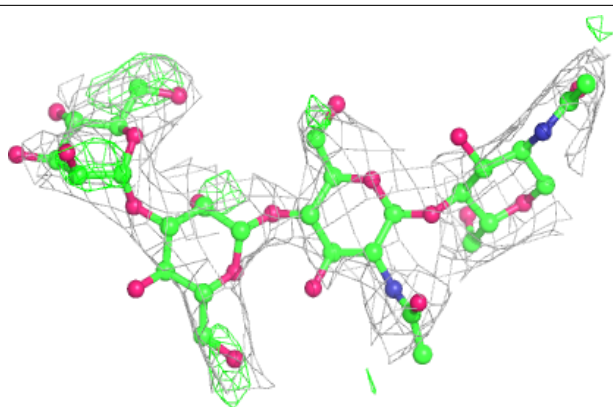
Electron density around Chain I:

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



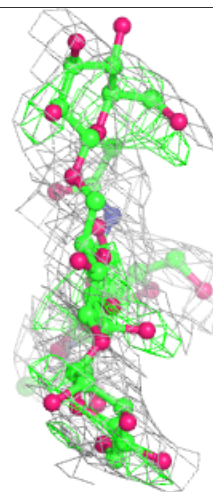
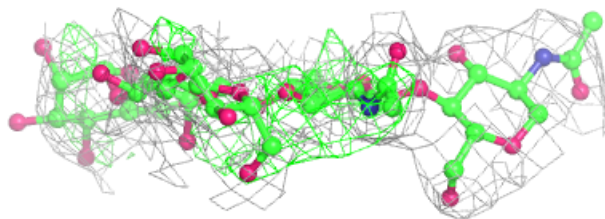
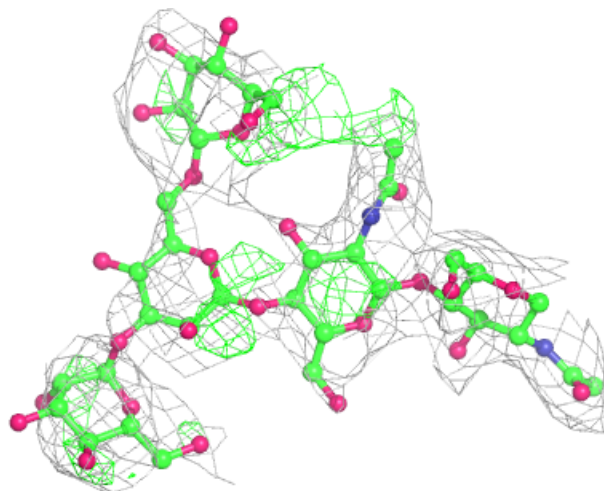
Electron density around Chain H:

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



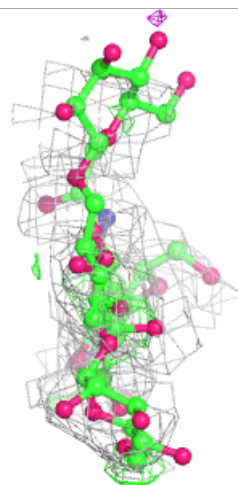
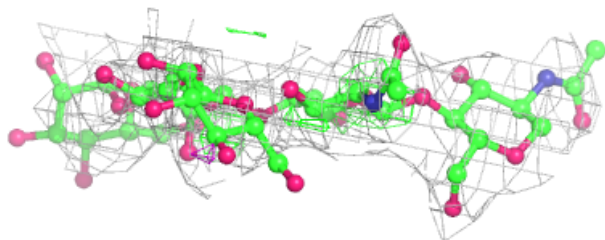
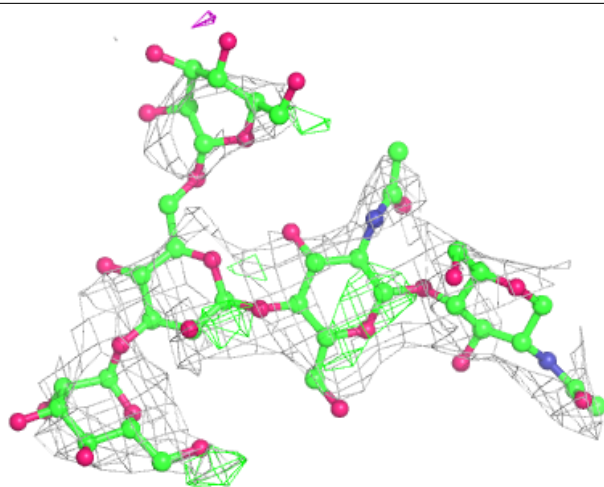
Electron density around Chain J:

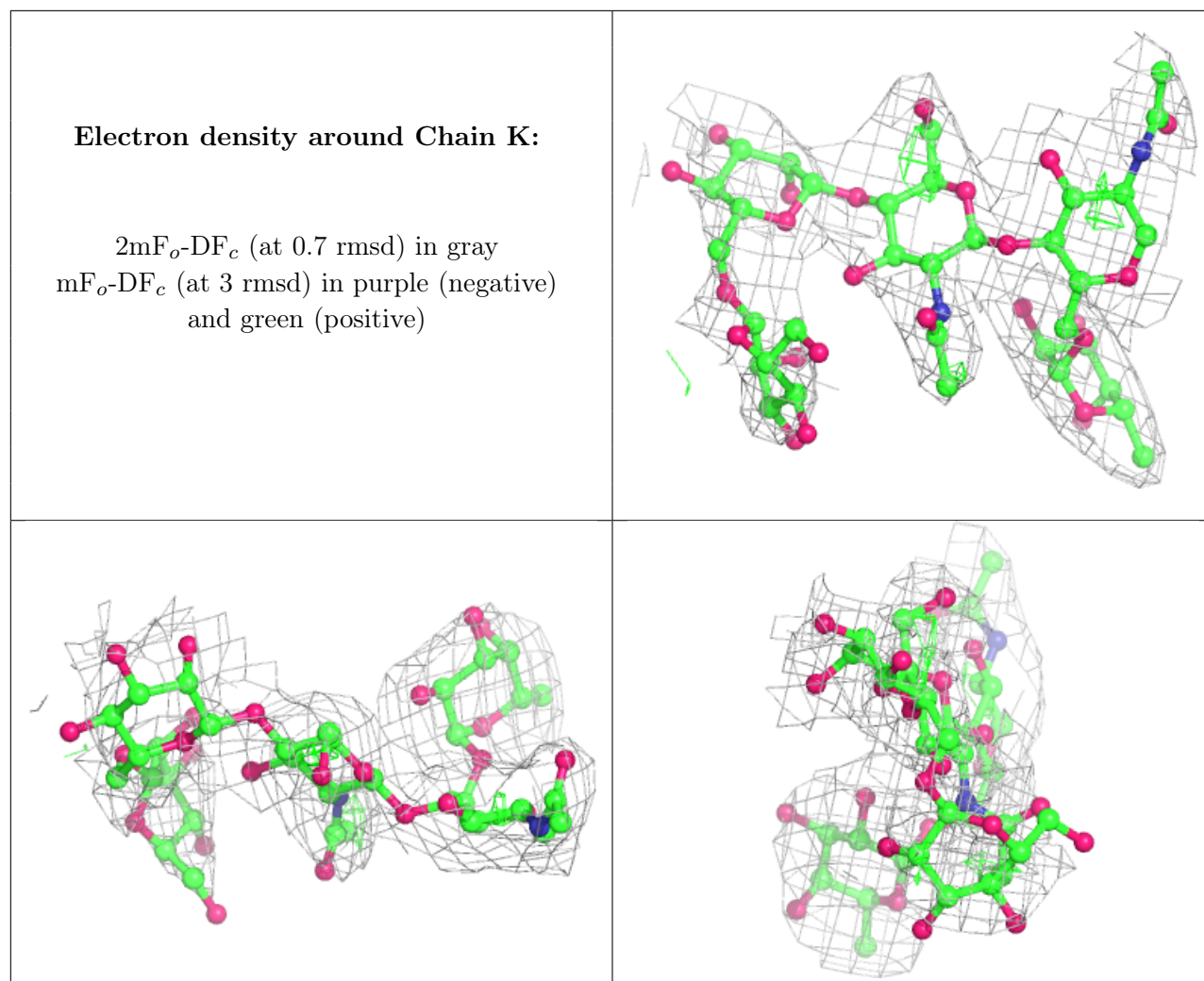
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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, 95th 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(\AA^2)	Q<0.9
8	NAG	D	201	14/15	0.78	0.30	200,229,253,254	0
8	NAG	E	201	14/15	0.83	0.17	158,201,237,239	0
8	NAG	F	201	14/15	0.86	0.26	127,134,147,148	0
7	TRS	C	201	8/8	0.92	0.22	37,39,41,41	20

6.5 Other polymers [i](#)

There are no such residues in this entry.