



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 12:21 AM EDT

PDB ID : 7KDM  
Title : Ricin bound to VHH antibody V5G6  
Authors : Rudolph, M.J.  
Deposited on : 2020-10-08  
Resolution : 2.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

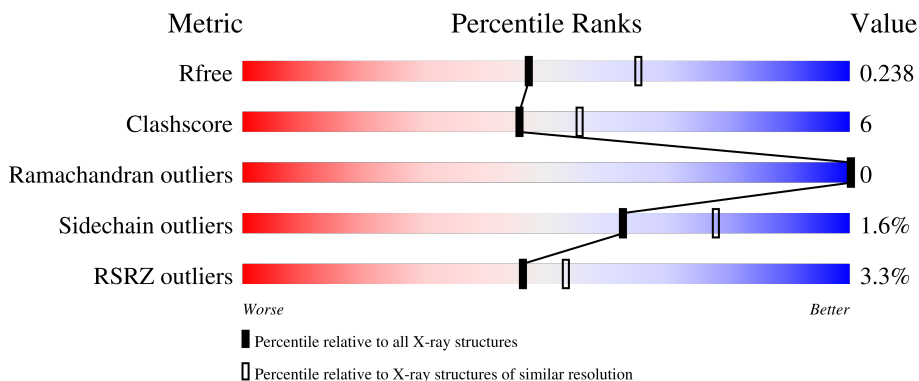
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	267	 88% 9%
1	D	267	 82% 13%
2	B	262	 85% 14%
2	E	262	 87% 11%
3	C	130	 15% 73% 9% 16%

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Mol	Chain	Length	Quality of chain
3	F	130	
4	G	2	
4	J	2	
5	H	2	
5	K	2	
6	I	3	
6	L	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	CL	B	302	-	-	X	-
8	CL	D	305	-	-	X	-
8	CL	E	302	-	-	X	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 10550 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 Ricin chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	257	Total	C	N	O	S	0	1	0
			2039	1290	361	383	5			
1	D	258	Total	C	N	O	S	0	0	0
			2039	1291	361	382	5			

- Molecule 2 is a protein called Ricin chain B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	259	Total	C	N	O	S	0	0	0
			2013	1261	354	386	12			
2	E	260	Total	C	N	O	S	0	1	0
			2027	1268	356	390	13			

- Molecule 3 is a protein called Anti-RON nanobody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	109	Total	C	N	O	S	0	0	0
			816	510	136	166	4			
3	F	109	Total	C	N	O	S	0	0	0
			816	510	136	166	4			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	G	2	Total	C	N	O	0	0	0
			24	14	1	9			

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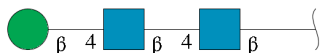
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 5 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
5	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	L	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	Zn	0	0
			3	3		
7	B	1	Total	Zn	0	0
			1	1		
7	D	4	Total	Zn	0	0
			4	4		
7	E	1	Total	Zn	0	0
			1	1		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Cl 1 1	0	0
8	D	1	Total Cl 1 1	0	0
8	E	1	Total Cl 1 1	0	0


- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	151	Total O 151 151	0	0
9	B	145	Total O 145 145	0	0
9	C	13	Total O 13 13	0	0
9	D	137	Total O 137 137	0	0
9	E	149	Total O 149 149	0	0
9	F	11	Total O 11 11	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.

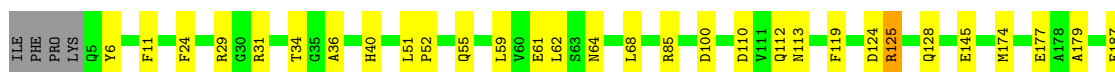
- Molecule 1: Ricin chain A

Chain A: 




- Molecule 1: Ricin chain A

Chain D: 




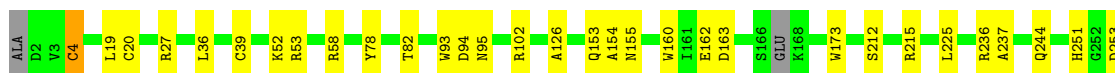
- Molecule 2: Ricin chain B

Chain B: 

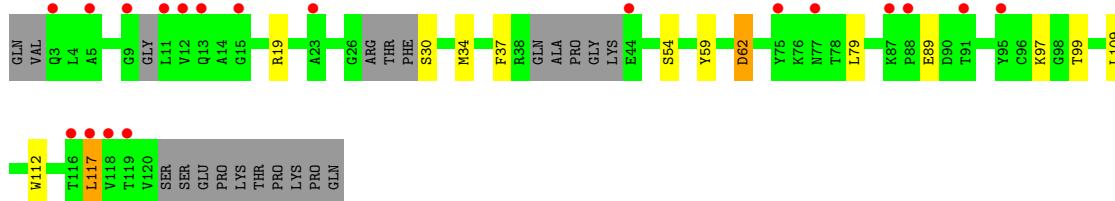
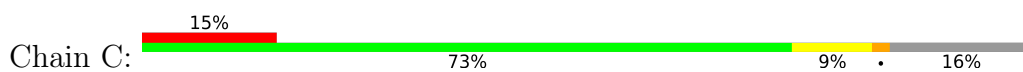


- Molecule 2: Ricin chain B

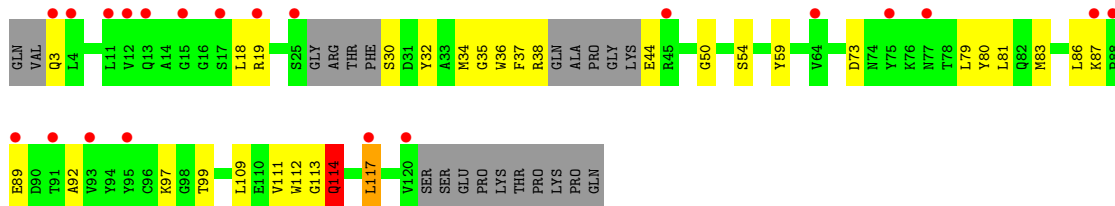
Chain E: 



- Molecule 3: Anti-RON nanobody



- Molecule 3: Anti-RON nanobody



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



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



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose




- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





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

Chain I:  33% 67%

MAG1  
MAG2  
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 L:  67% 33%

MAG1  
MAG2  
BMA3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.34Å 77.44Å 101.58Å 89.97° 90.18° 89.98°	Depositor
Resolution (Å)	19.65 – 2.30 19.65 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.0 (19.65-2.30) 95.9 (19.65-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.68 (at 2.30Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.187 , 0.238 0.187 , 0.238	Depositor DCC
$R_{free}$ test set	2742 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtrriage
Anisotropy	0.515	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 25.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.025 for h,-k,-l 0.470 for -h,k,-l 0.022 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10550	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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, ZN, NAG, FUC, CL

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	0.32	0/2082	0.50	0/2833
1	D	0.35	0/2083	0.72	2/2835 (0.1%)
2	B	0.30	0/2057	0.53	0/2809
2	E	0.30	0/2071	0.54	1/2828 (0.0%)
3	C	0.28	0/828	0.51	0/1114
3	F	0.38	0/829	0.77	3/1117 (0.3%)
All	All	0.32	0/9950	0.59	6/13536 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	F	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	125	ARG	NE-CZ-NH1	-21.32	109.64	120.30
1	D	125	ARG	NE-CZ-NH2	14.10	127.35	120.30
3	F	113	GLY	C-N-CA	-10.70	94.96	121.70
3	F	111	VAL	CG1-CB-CG2	8.21	124.04	110.90
3	F	114	GLN	CB-CG-CD	-6.46	94.79	111.60
2	E	225	LEU	CA-CB-CG	5.06	126.93	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	114	GLN	Sidechain

## 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	2039	0	2004	19	0
1	D	2039	0	2005	29	0
2	B	2013	0	1957	29	0
2	E	2027	0	1965	21	0
3	C	816	0	774	9	0
3	F	816	0	775	20	0
4	G	24	0	22	0	0
4	J	24	0	22	0	0
5	H	28	0	25	1	0
5	K	28	0	25	1	0
6	I	39	0	34	1	0
6	L	39	0	34	0	0
7	A	3	0	0	0	0
7	B	1	0	0	0	0
7	D	4	0	0	0	0
7	E	1	0	0	0	0
8	B	1	0	0	2	0
8	D	1	0	0	2	0
8	E	1	0	0	5	0
9	A	151	0	0	7	0
9	B	145	0	0	3	0
9	C	13	0	0	2	0
9	D	137	0	0	4	0
9	E	149	0	0	5	0
9	F	11	0	0	1	0
All	All	10550	0	9642	125	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.

All (125) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:HIS:ND1	8:E:302:CL:CL	2.32	0.97
1:D:34:THR:HG23	1:D:36:ALA:H	1.34	0.91
8:E:302:CL:CL	9:E:501:HOH:O	2.26	0.91
8:E:302:CL:CL	9:E:438:HOH:O	2.31	0.85
2:B:106:VAL:HG13	8:B:302:CL:CL	2.20	0.79
1:D:40:HIS:NE2	8:D:305:CL:CL	2.54	0.78
1:A:34:THR:HG23	1:A:36:ALA:H	1.50	0.77
3:C:62:ASP:OD2	9:C:201:HOH:O	2.02	0.77
1:A:102:GLU:OE2	9:A:401:HOH:O	2.03	0.76
1:D:125:ARG:HA	1:D:128:GLN:HE21	1.52	0.74
2:B:56:THR:HG21	2:B:58:ARG:HE	1.55	0.71
1:D:85:ARG:NH2	1:D:110:ASP:OD2	2.25	0.70
3:F:114:GLN:O	3:F:114:GLN:HG3	1.91	0.69
1:D:61:GLU:OE2	9:D:401:HOH:O	2.12	0.68
2:B:52:LYS:HG3	2:B:58:ARG:HG3	1.77	0.66
3:F:89:GLU:N	3:F:89:GLU:OE1	2.28	0.66
1:A:100:ASP:OD2	9:A:402:HOH:O	2.13	0.65
2:E:102:ARG:NH1	9:E:401:HOH:O	2.16	0.65
1:A:138:GLU:OE2	9:A:403:HOH:O	2.14	0.64
3:F:73:ASP:OD1	9:F:201:HOH:O	2.15	0.64
3:C:97:LYS:NZ	9:C:204:HOH:O	2.33	0.62
3:C:89:GLU:N	3:C:89:GLU:OE1	2.32	0.61
3:F:114:GLN:O	3:F:114:GLN:CG	2.47	0.61
3:F:83:MET:HE2	3:F:86:LEU:HD21	1.83	0.61
2:E:27:ARG:NH2	9:E:402:HOH:O	2.27	0.60
1:A:65:HIS:ND1	1:A:145:GLU:OE2	2.36	0.59
1:A:125:ARG:NH1	1:A:128:GLN:OE1	2.37	0.58
2:E:20[B]:CYS:HB3	2:E:39:CYS:SG	2.44	0.57
2:E:78:TYR:HE2	2:E:82:THR:HG22	1.69	0.57
3:F:38:ARG:HG3	3:F:92:ALA:HB3	1.87	0.56
1:A:111:VAL:O	9:A:404:HOH:O	2.18	0.56
2:E:155:ASN:ND2	2:E:160:TRP:CZ2	2.74	0.56
2:B:27:ARG:NH2	9:B:404:HOH:O	2.34	0.56
1:D:6:TYR:HB2	1:D:59:LEU:CD2	2.35	0.56
1:A:67:GLU:OE1	9:A:405:HOH:O	2.18	0.55
2:E:94:ASP:OD2	8:E:302:CL:CL	2.62	0.55
1:D:40:HIS:CE1	8:E:302:CL:CL	2.96	0.54
2:B:19:LEU:HD12	2:B:36:LEU:HD13	1.89	0.53
1:A:85:ARG:NH1	9:A:412:HOH:O	2.42	0.53
1:D:174:MET:HG2	1:D:188:MET:HE2	1.91	0.52
3:F:19:ARG:HH11	3:F:80:TYR:HB3	1.75	0.52
2:E:154:ALA:HB2	2:E:173:TRP:CH2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:ASP:HB3	2:B:82:THR:OG1	2.10	0.51
1:D:125:ARG:HA	1:D:128:GLN:NE2	2.22	0.51
2:E:126:ALA:HA	2:E:212:SER:HA	1.92	0.51
2:B:10:ILE:HG21	6:I:2:NAG:H83	1.91	0.51
2:E:52:LYS:HG3	2:E:58:ARG:HG3	1.93	0.51
2:B:165:SER:OG	2:B:168:LYS:HG3	2.11	0.51
1:D:100:ASP:OD2	9:D:402:HOH:O	2.19	0.51
1:D:187:GLU:OE2	9:D:403:HOH:O	2.19	0.50
3:C:37:PHE:CE1	3:C:97:LYS:HD3	2.46	0.50
2:E:237:ALA:HA	3:F:59:TYR:CD2	2.47	0.50
2:B:98:ILE:N	8:B:302:CL:CL	2.65	0.50
3:F:37:PHE:CE1	3:F:97:LYS:HD3	2.47	0.49
3:C:97:LYS:HD2	3:C:112:TRP:CH2	2.48	0.49
1:D:195:ASN:HD22	1:D:195:ASN:C	2.16	0.49
2:B:54:ASP:OD1	2:B:56:THR:HB	2.13	0.48
2:E:236:ARG:HH11	2:E:244:GLN:HE22	1.61	0.48
2:B:24:ARG:HD3	2:B:35:GLN:OE1	2.13	0.48
2:E:95:ASN:O	2:E:215:ARG:NH2	2.42	0.48
2:E:162:GLU:HG2	2:E:163:ASP:N	2.29	0.48
2:E:19:LEU:HD12	2:E:36:LEU:HD13	1.95	0.48
1:A:112:GLN:HG3	1:A:113:ASN:OD1	2.14	0.48
3:C:34:MET:HB2	3:C:79:LEU:HD13	1.95	0.48
1:D:222:ASN:HD22	1:D:222:ASN:C	2.17	0.48
1:D:6:TYR:HB2	1:D:59:LEU:HD21	1.95	0.47
1:D:29:ARG:HD3	1:D:179:ALA:O	2.14	0.47
1:A:113:ASN:HB3	1:A:115:TYR:CZ	2.49	0.47
3:F:97:LYS:HD2	3:F:112:TRP:CH2	2.49	0.47
3:F:32:TYR:HB3	3:F:34:MET:HE2	1.97	0.47
2:B:197:ILE:H	2:B:197:ILE:HD12	1.80	0.47
3:C:117:LEU:HD23	3:C:117:LEU:H	1.79	0.47
1:A:113:ASN:HB3	1:A:115:TYR:CE1	2.50	0.47
1:D:40:HIS:CE1	8:D:305:CL:CL	3.04	0.46
1:D:177:GLU:CD	1:D:208:GLU:HG2	2.35	0.46
1:D:220:GLU:HG2	2:E:4:CYS:HB3	1.98	0.46
1:D:124:ASP:O	1:D:128:GLN:HG2	2.16	0.46
3:F:36:TRP:NE1	3:F:81:LEU:HB2	2.31	0.46
1:D:64:ASN:HB2	1:D:145:GLU:HG3	1.97	0.46
2:B:56:THR:CG2	2:B:58:ARG:HE	2.26	0.45
1:D:31:ARG:HA	1:D:31:ARG:HD2	1.75	0.45
1:D:119:PHE:HB2	1:D:125:ARG:HG2	1.99	0.45
2:B:79:ASP:OD2	9:B:401:HOH:O	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:CD	1:A:208:GLU:HG2	2.37	0.45
1:D:222:ASN:HD22	1:D:223:GLN:HG3	1.82	0.45
1:D:31:ARG:NH1	9:D:404:HOH:O	2.33	0.44
1:D:112:GLN:HG3	1:D:113:ASN:OD1	2.17	0.44
2:E:20[B]:CYS:SG	2:E:39:CYS:HA	2.57	0.44
1:A:166:ARG:HD2	9:A:532:HOH:O	2.17	0.44
2:B:93:TRP:CE3	5:H:1:NAG:H5	2.53	0.44
2:B:183:PRO:HD2	2:B:189:ASN:O	2.18	0.44
2:B:237:ALA:HA	3:C:59:TYR:CD2	2.52	0.44
3:F:87:LYS:HB3	3:F:89:GLU:OE1	2.18	0.44
1:D:206:THR:HG21	1:D:232:LEU:HA	1.99	0.43
2:E:93:TRP:CE3	5:K:1:NAG:H5	2.54	0.43
2:B:196:ASN:HD21	2:B:228:TYR:HE2	1.60	0.43
2:B:78:TYR:HE2	2:B:82:THR:HG1	1.66	0.42
2:B:176:TYR:CD1	2:B:182:ARG:HG3	2.54	0.42
3:F:117:LEU:H	3:F:117:LEU:HD23	1.83	0.42
2:B:192:THR:HG23	2:B:214:GLN:HG3	2.01	0.42
2:E:53:ARG:NH2	9:E:414:HOH:O	2.53	0.42
1:D:11:PHE:HB2	1:D:24:PHE:CD1	2.55	0.42
1:A:39:ARG:NE	1:A:261:PRO:HG3	2.35	0.42
2:E:162:GLU:HG2	2:E:163:ASP:H	1.85	0.42
3:F:18:LEU:HD23	3:F:18:LEU:HA	1.92	0.42
3:F:97:LYS:HD2	3:F:112:TRP:CZ2	2.55	0.42
2:B:23:VAL:HB	2:B:46:ASN:HB2	2.02	0.41
2:B:53:ARG:NH2	9:B:416:HOH:O	2.52	0.41
1:A:234:ARG:HA	2:B:262:PHE:HD1	1.86	0.41
2:B:56:THR:HG22	2:B:58:ARG:HG2	2.03	0.41
2:E:251:HIS:CE1	2:E:253:ASP:HB2	2.55	0.41
2:B:195:SER:HB2	2:B:197:ILE:HD12	2.02	0.41
1:D:52:PRO:HD2	1:D:55:GLN:HE21	1.86	0.41
2:B:225:LEU:HD23	2:B:227:LEU:HD23	2.03	0.41
3:C:99:THR:HA	3:C:109:LEU:O	2.21	0.41
3:F:35:GLY:HA2	3:F:50:GLY:HA2	2.02	0.41
2:B:34:ILE:HG13	2:B:64:LEU:HD12	2.03	0.40
1:A:124:ASP:O	1:A:128:GLN:HG2	2.22	0.40
2:B:27:ARG:HD2	2:B:27:ARG:HA	1.69	0.40
3:F:34:MET:CB	3:F:79:LEU:HD13	2.51	0.40
1:A:110:ASP:N	1:A:110:ASP:OD1	2.54	0.40
3:F:44:GLU:N	3:F:44:GLU:OE1	2.54	0.40
1:A:39:ARG:CZ	1:A:261:PRO:HG3	2.51	0.40
2:E:153:GLN:HE21	2:E:155:ASN:HD21	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:99:THR:HA	3:F:109:LEU:O	2.22	0.40

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	256/267 (96%)	251 (98%)	5 (2%)	0	100	100
1	D	256/267 (96%)	253 (99%)	3 (1%)	0	100	100
2	B	255/262 (97%)	251 (98%)	4 (2%)	0	100	100
2	E	257/262 (98%)	253 (98%)	4 (2%)	0	100	100
3	C	101/130 (78%)	97 (96%)	4 (4%)	0	100	100
3	F	103/130 (79%)	100 (97%)	3 (3%)	0	100	100
All	All	1228/1318 (93%)	1205 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	217/226 (96%)	217 (100%)	0	100	100
1	D	217/226 (96%)	211 (97%)	6 (3%)	43	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	225/227 (99%)	224 (100%)	1 (0%)	91	96
2	E	227/227 (100%)	226 (100%)	1 (0%)	91	96
3	C	84/102 (82%)	79 (94%)	5 (6%)	19	26
3	F	84/102 (82%)	80 (95%)	4 (5%)	25	36
All	All	1054/1110 (95%)	1037 (98%)	17 (2%)	62	78

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	165	SER
3	C	19	ARG
3	C	30	SER
3	C	54	SER
3	C	62	ASP
3	C	117	LEU
1	D	51	LEU
1	D	62	LEU
1	D	68	LEU
1	D	195	ASN
1	D	222	ASN
1	D	238	SER
2	E	4	CYS
3	F	3	GLN
3	F	30	SER
3	F	54	SER
3	F	117	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	106	HIS
1	A	141	ASN
2	B	186	ASN
1	D	55	GLN
1	D	106	HIS
1	D	128	GLN
1	D	195	ASN
1	D	222	ASN
2	E	244	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

14 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
4	NAG	G	1	4,1	14,14,15	0.77	1 (7%)	17,19,21	0.82	0
4	FUC	G	2	4	10,10,11	0.71	0	14,14,16	0.85	0
5	NAG	H	1	2,5	14,14,15	0.67	0	17,19,21	1.22	2 (11%)
5	NAG	H	2	5	14,14,15	0.20	0	17,19,21	0.53	0
6	NAG	I	1	2,6	14,14,15	0.69	0	17,19,21	1.10	1 (5%)
6	NAG	I	2	6	14,14,15	0.57	0	17,19,21	0.45	0
6	BMA	I	3	6	11,11,12	0.73	0	15,15,17	0.68	0
4	NAG	J	1	4,1	14,14,15	0.79	1 (7%)	17,19,21	0.81	0
4	FUC	J	2	4	10,10,11	0.99	1 (10%)	14,14,16	1.20	2 (14%)
5	NAG	K	1	2,5	14,14,15	0.62	0	17,19,21	1.14	2 (11%)
5	NAG	K	2	5	14,14,15	0.24	0	17,19,21	0.58	0
6	NAG	L	1	2,6	14,14,15	0.68	0	17,19,21	0.98	1 (5%)
6	NAG	L	2	6	14,14,15	0.60	0	17,19,21	0.45	0
6	BMA	L	3	6	11,11,12	0.76	0	15,15,17	0.72	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
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	FUC	G	2	4	-	-	0/1/1/1
5	NAG	H	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	1/6/23/26	0/1/1/1
6	NAG	I	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	4/6/23/26	0/1/1/1
6	BMA	I	3	6	-	0/2/19/22	0/1/1/1
4	NAG	J	1	4,1	-	2/6/23/26	0/1/1/1
4	FUC	J	2	4	-	-	0/1/1/1
5	NAG	K	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
6	NAG	L	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	4/6/23/26	0/1/1/1
6	BMA	L	3	6	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	2	FUC	C1-C2	2.54	1.58	1.52
4	J	1	NAG	C1-C2	2.31	1.55	1.52
4	G	1	NAG	C1-C2	2.12	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	1	NAG	O4-C4-C3	-2.98	103.46	110.35
5	K	1	NAG	O4-C4-C3	-2.97	103.48	110.35
5	H	1	NAG	C1-C2-N2	2.97	115.56	110.49
4	J	2	FUC	C1-C2-C3	2.92	113.25	109.67
6	I	1	NAG	C1-C2-N2	2.73	115.16	110.49
5	K	1	NAG	C1-C2-N2	2.30	114.41	110.49
4	J	2	FUC	C1-O5-C5	2.22	117.80	112.78
6	L	1	NAG	C1-C2-N2	2.12	114.12	110.49

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	1	NAG	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
6	I	2	NAG	C8-C7-N2-C2

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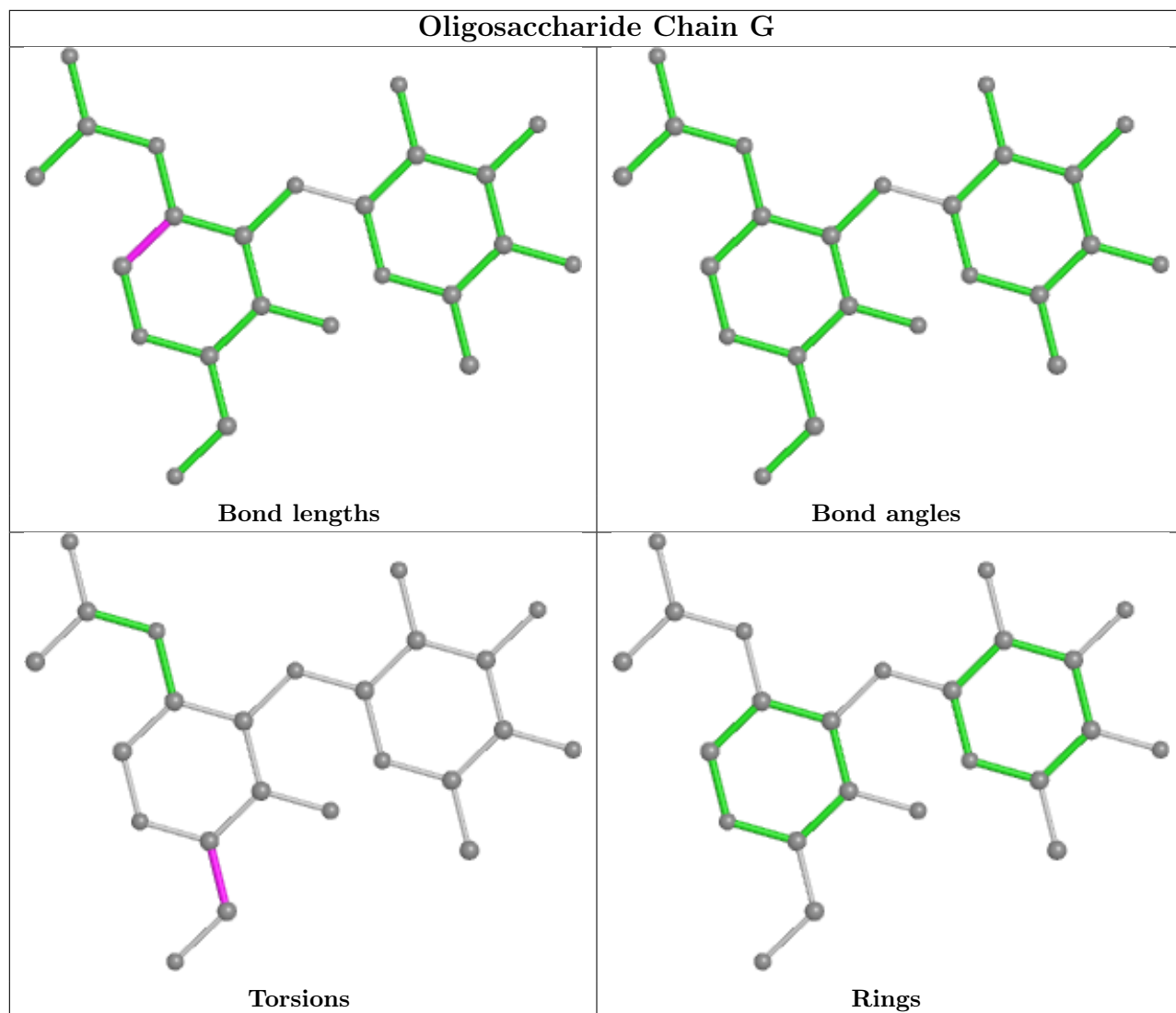
Mol	Chain	Res	Type	Atoms
6	I	2	NAG	O7-C7-N2-C2
6	L	2	NAG	C8-C7-N2-C2
6	L	2	NAG	O7-C7-N2-C2
6	I	2	NAG	O5-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6
6	L	2	NAG	C4-C5-C6-O6
6	L	2	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
5	H	2	NAG	C3-C2-N2-C7
5	K	2	NAG	C3-C2-N2-C7
5	K	2	NAG	C1-C2-N2-C7

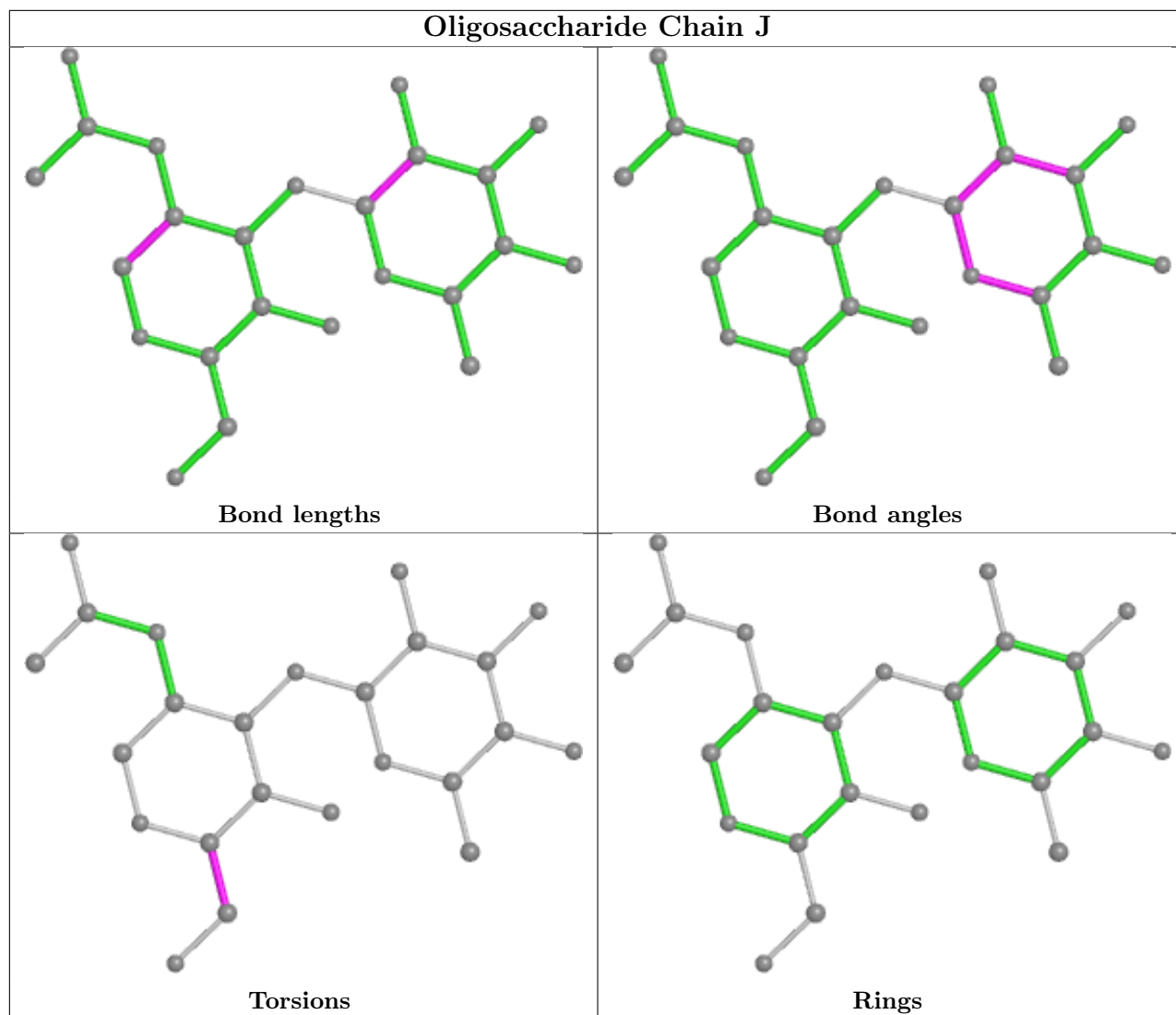
There are no ring outliers.

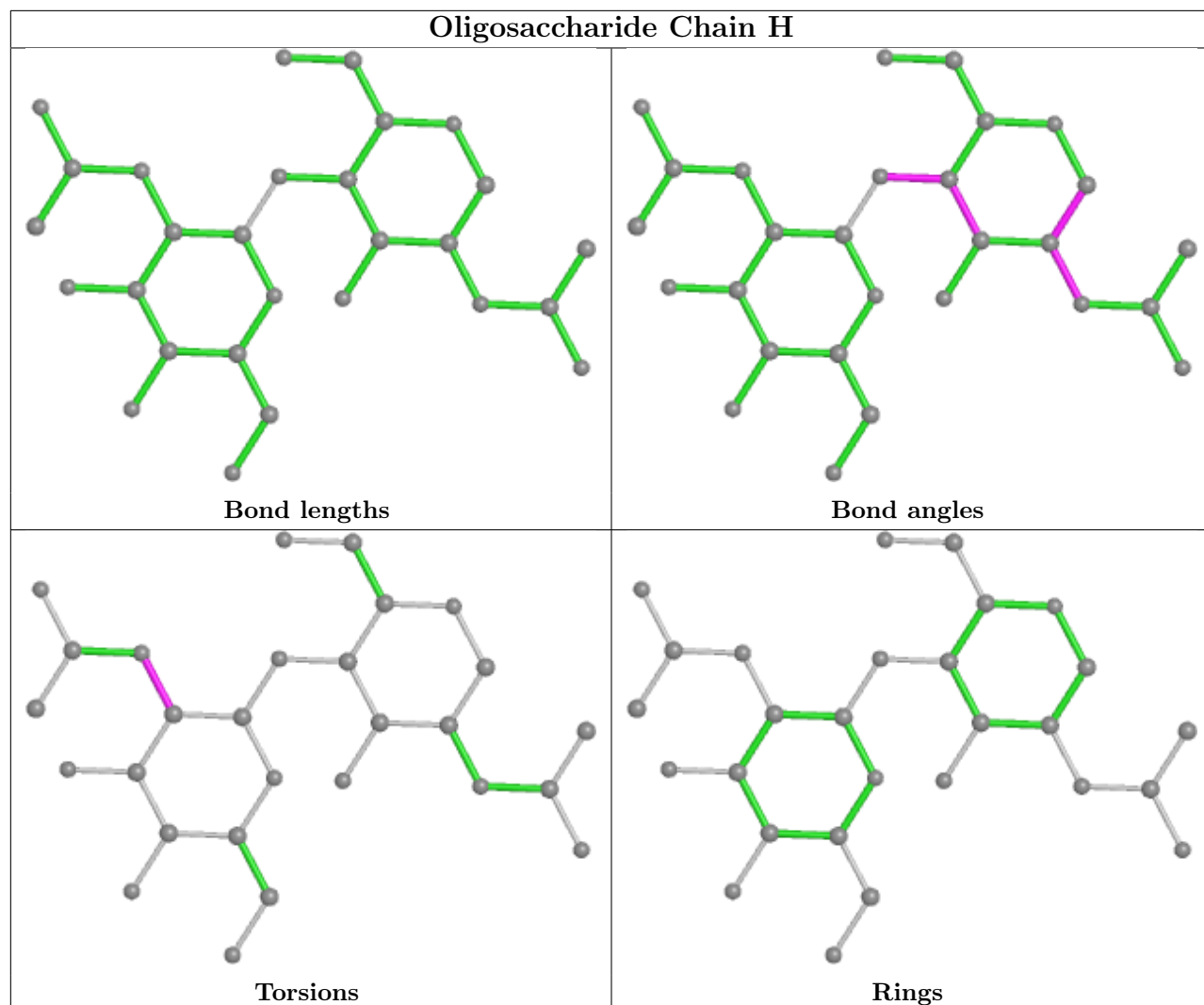
3 monomers are involved in 3 short contacts:

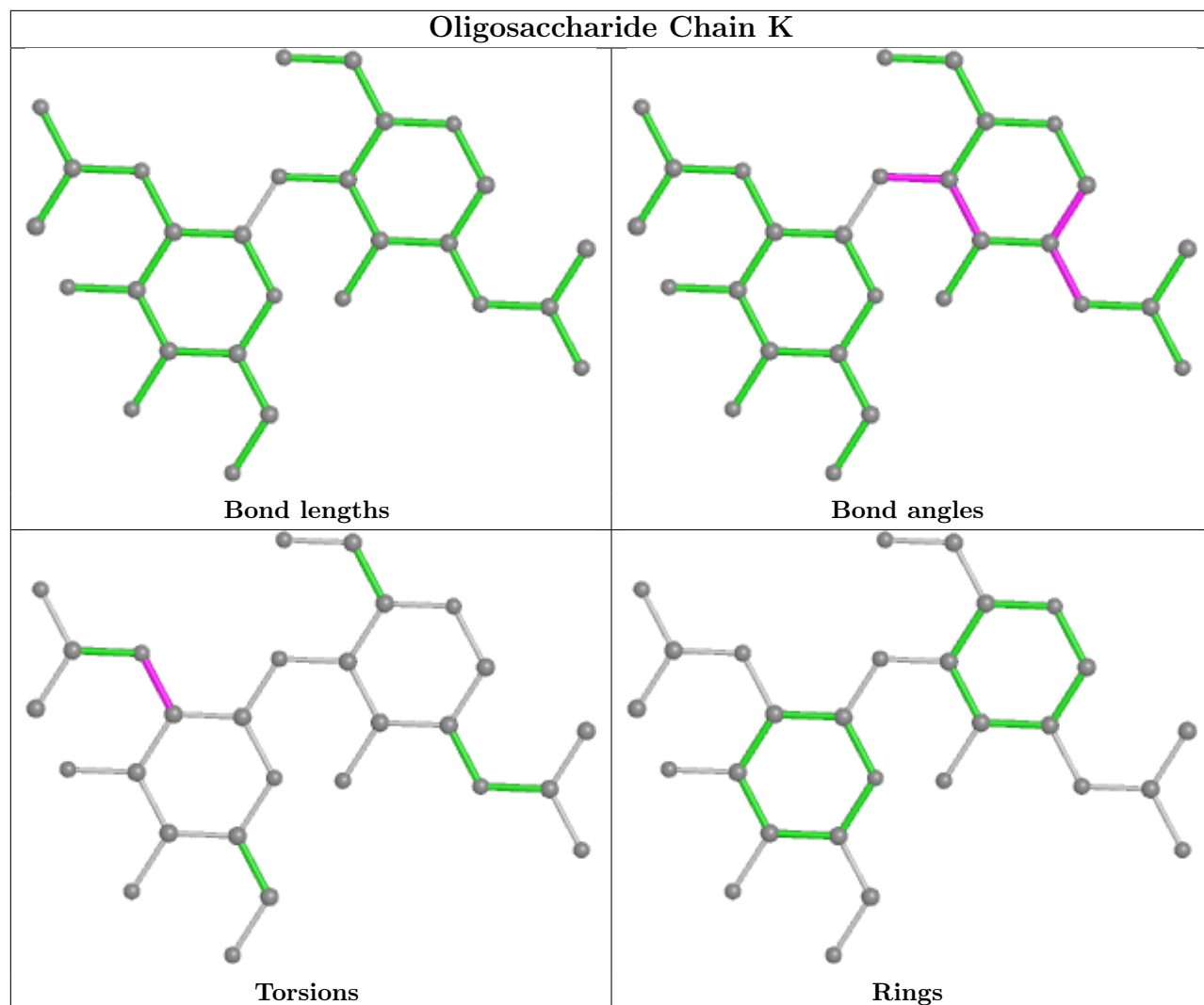
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	2	NAG	1	0
5	K	1	NAG	1	0
5	H	1	NAG	1	0

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

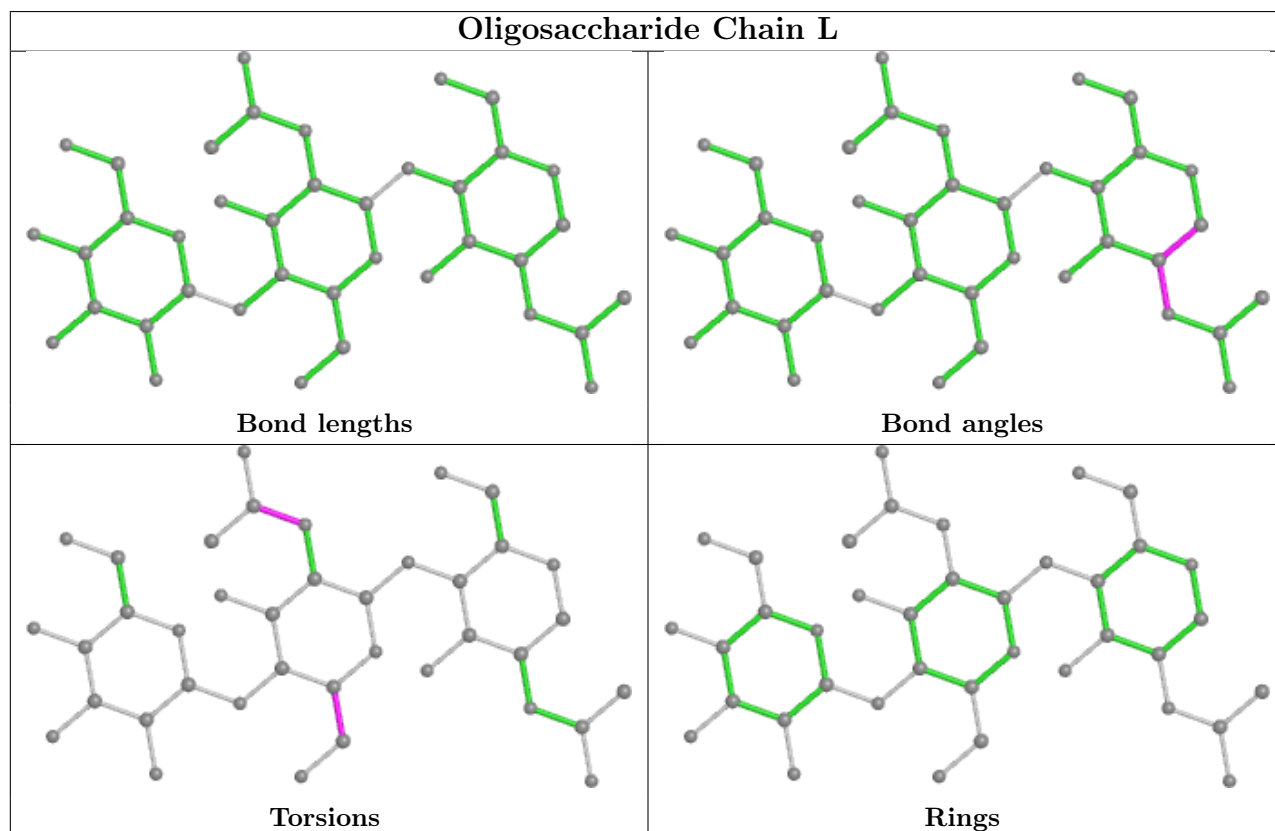
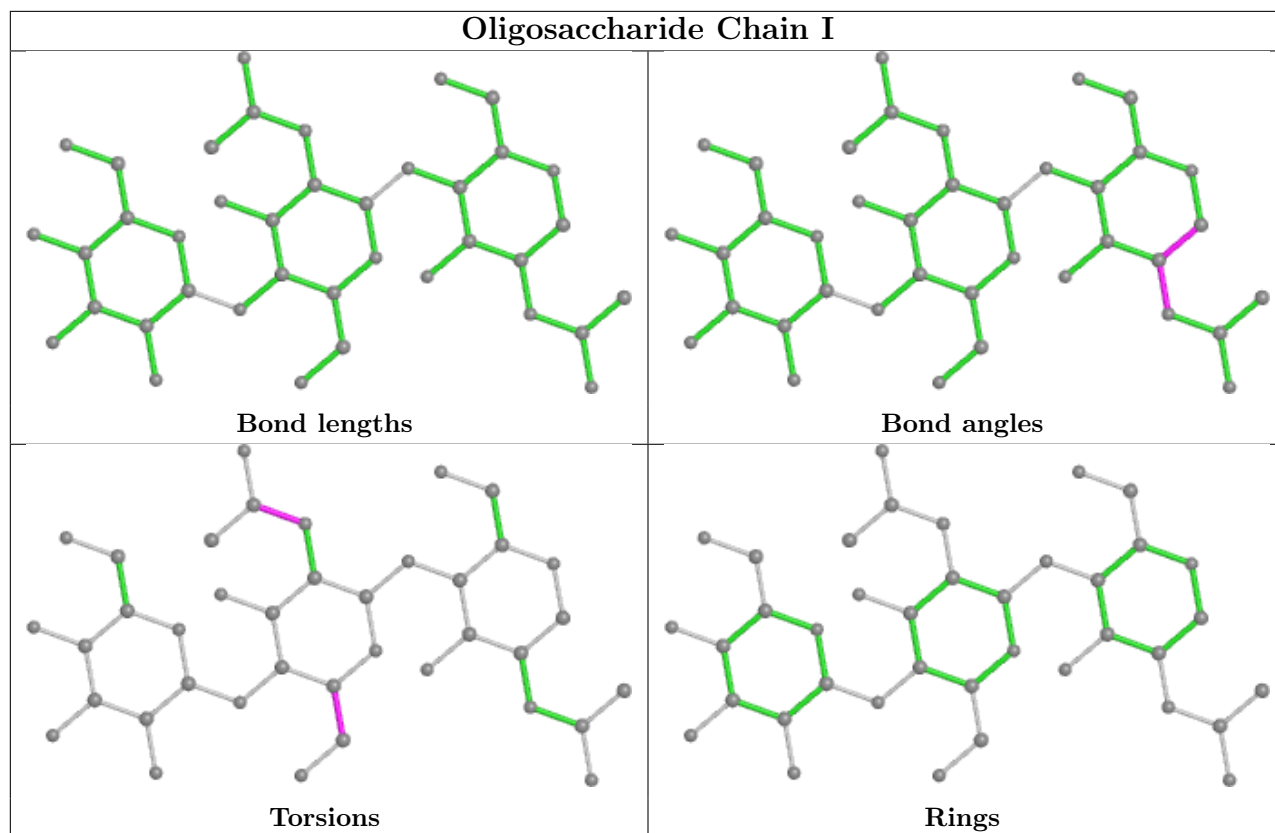












## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

### 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	257/267 (96%)	-0.61	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	18, 30, 52, 61	0
1	D	258/267 (96%)	-0.57	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	18, 30, 51, 73	0
2	B	259/262 (98%)	-0.58	1 (0%) <span style="border: 1px solid blue; padding: 2px;">92</span> <span style="border: 1px solid blue; padding: 2px;">95</span>	18, 32, 54, 69	0
2	E	260/262 (99%)	-0.59	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	18, 32, 57, 82	0
3	C	109/130 (83%)	1.10	19 (17%) <span style="border: 1px solid red; padding: 2px;">1</span> <span style="border: 1px solid red; padding: 2px;">1</span>	43, 78, 106, 123	0
3	F	109/130 (83%)	1.05	21 (19%) <span style="border: 1px solid red; padding: 2px;">1</span> <span style="border: 1px solid red; padding: 2px;">1</span>	44, 77, 106, 124	0
All	All	1252/1318 (94%)	-0.30	41 (3%) <span style="border: 1px solid gray; padding: 2px;">46</span> <span style="border: 1px solid gray; padding: 2px;">53</span>	18, 33, 89, 124	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	13	GLN	7.6
3	C	75	TYR	6.0
3	F	91	THR	5.0
3	C	13	GLN	4.7
3	C	87	LYS	4.6
3	F	87	LYS	4.6
3	C	3	GLN	4.5
3	F	120	VAL	4.5
3	F	75	TYR	3.9
3	F	95	TYR	3.8
3	C	11	LEU	3.6
3	C	23	ALA	3.5
3	C	91	THR	3.5
3	C	118	VAL	3.2
3	F	12	VAL	3.2
3	C	44	GLU	3.1
3	F	93	VAL	3.1
3	C	88	PRO	3.1
3	F	88	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
3	F	11	LEU	2.9
3	C	5	ALA	2.9
3	C	12	VAL	2.8
3	C	117	LEU	2.7
3	C	15	GLY	2.7
3	F	45	ARG	2.6
3	C	116	THR	2.6
3	F	89	GLU	2.6
3	F	25	SER	2.4
3	F	19	ARG	2.4
3	F	117	LEU	2.4
3	F	3	GLN	2.3
3	F	64	VAL	2.2
3	F	17	SER	2.2
3	C	119	THR	2.2
3	C	9	GLY	2.2
2	B	140	PHE	2.1
3	F	77	ASN	2.1
3	F	15	GLY	2.1
3	C	95	TYR	2.1
3	F	4	LEU	2.0
3	C	77	ASN	2.0

## 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.

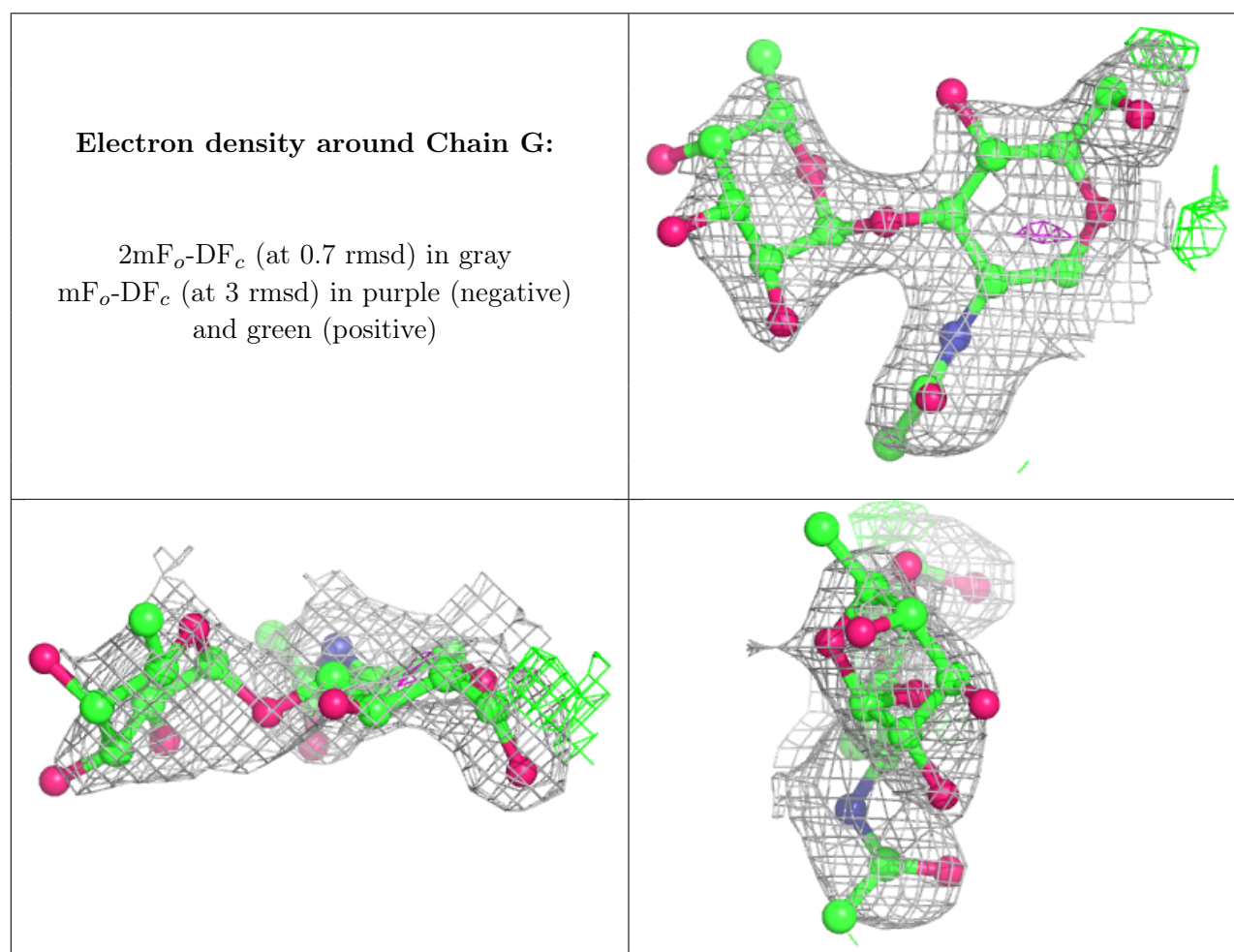
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	BMA	I	3	11/12	0.75	0.27	84,90,93,94	0
6	BMA	L	3	11/12	0.76	0.26	83,87,91,92	0
4	NAG	G	1	14/15	0.78	0.26	52,62,67,68	0
5	NAG	K	2	14/15	0.84	0.20	53,64,72,74	0
4	FUC	G	2	10/11	0.84	0.28	68,71,73,73	0
4	NAG	J	1	14/15	0.84	0.26	49,58,64,65	0

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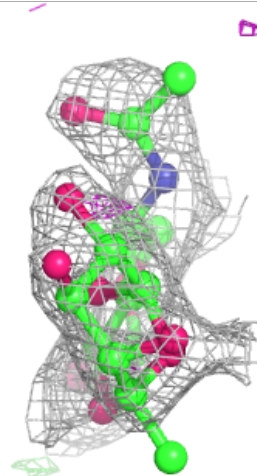
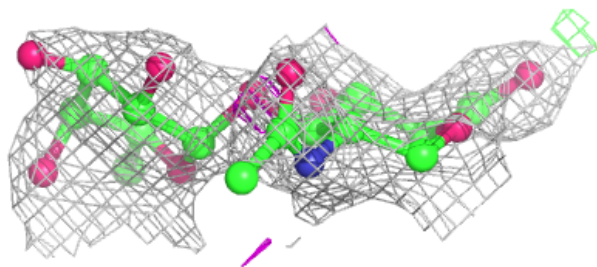
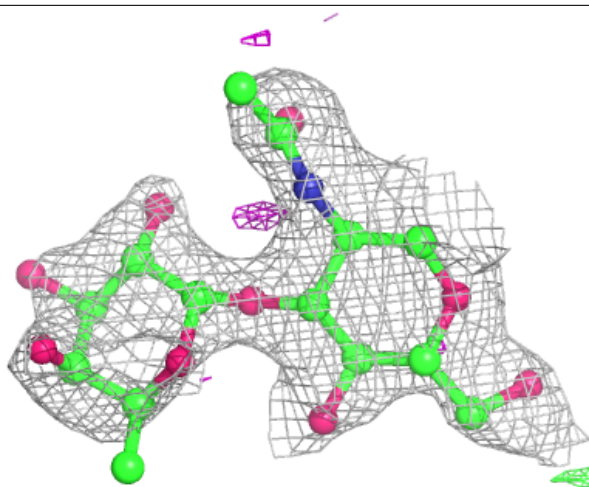
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	H	2	14/15	0.86	0.21	57,69,75,75	0
4	FUC	J	2	10/11	0.87	0.21	67,69,71,73	0
6	NAG	L	2	14/15	0.88	0.17	42,57,68,75	0
6	NAG	I	2	14/15	0.89	0.16	41,55,64,74	0
6	NAG	L	1	14/15	0.95	0.10	34,36,41,47	0
5	NAG	H	1	14/15	0.95	0.10	26,33,42,56	0
6	NAG	I	1	14/15	0.95	0.10	30,35,43,45	0
5	NAG	K	1	14/15	0.96	0.11	26,33,39,50	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.



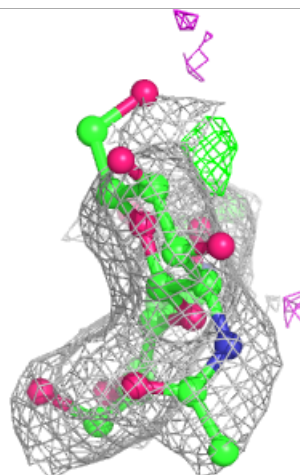
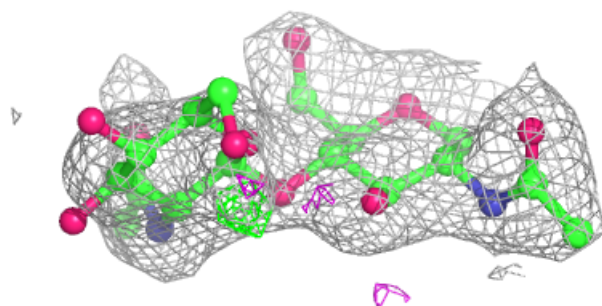
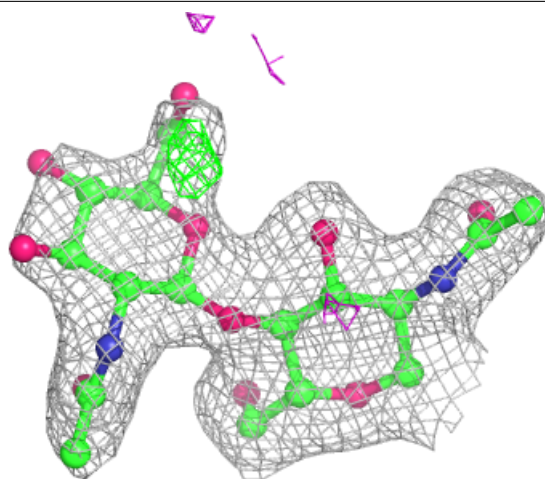
**Electron density around Chain J:**

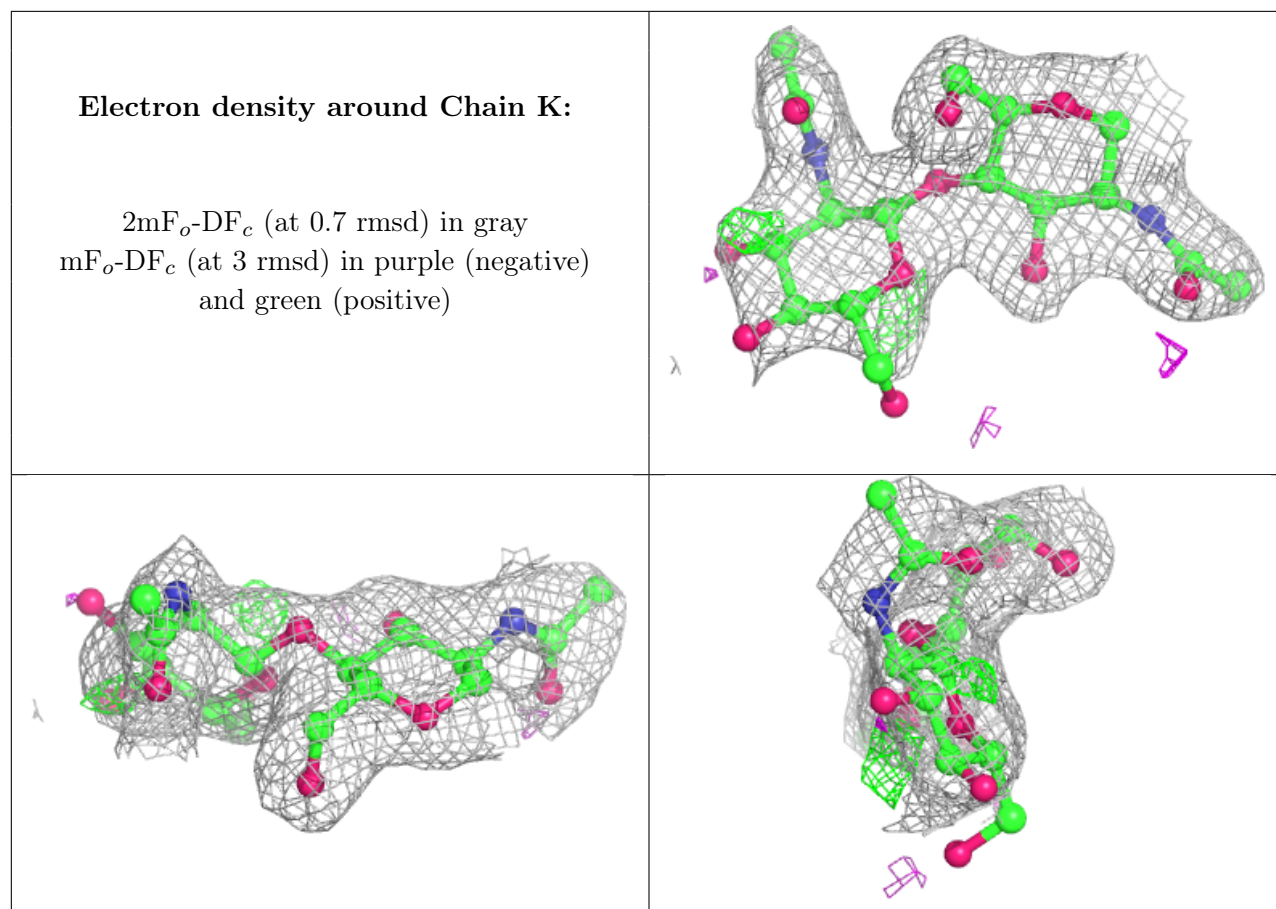
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



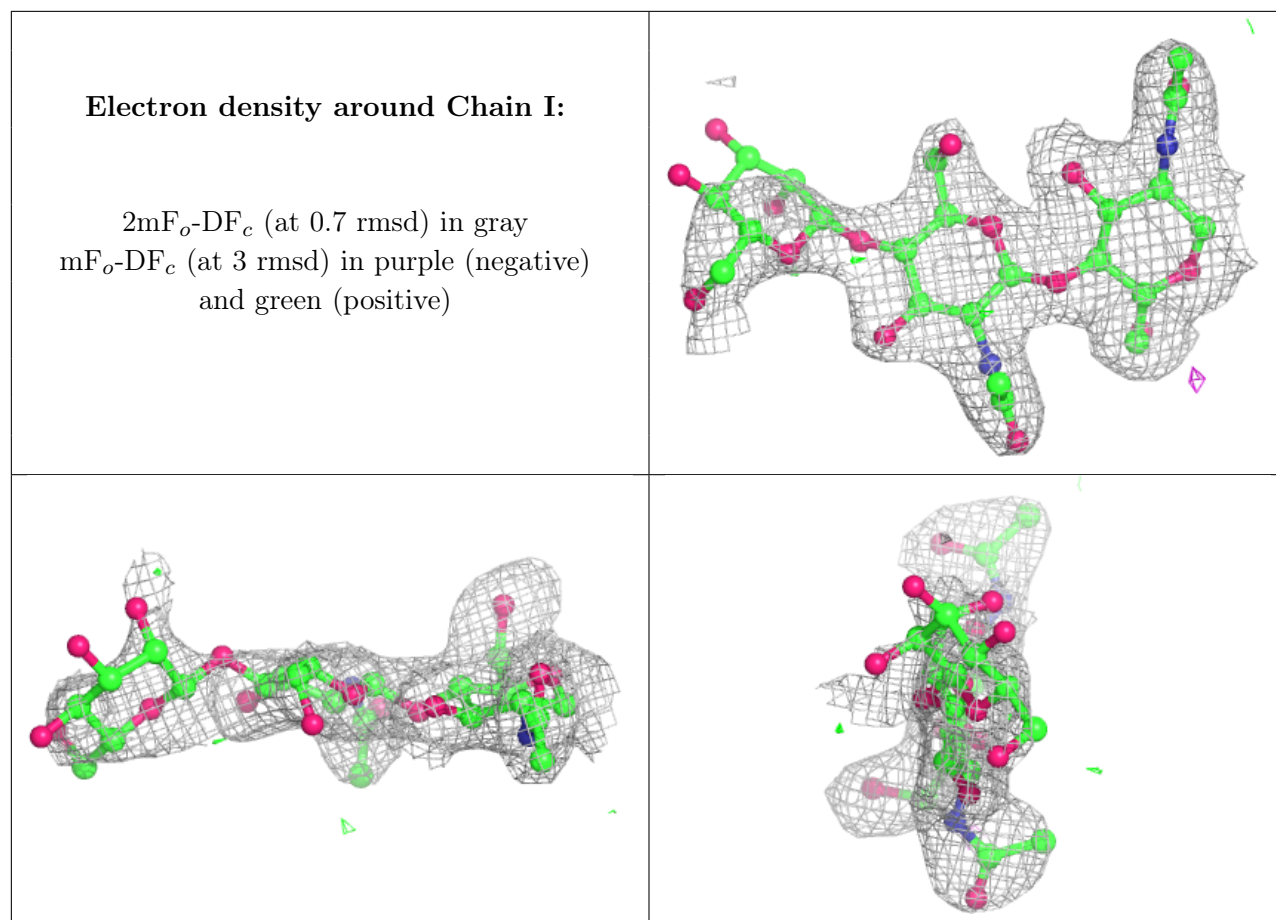
**Electron density around Chain H:**

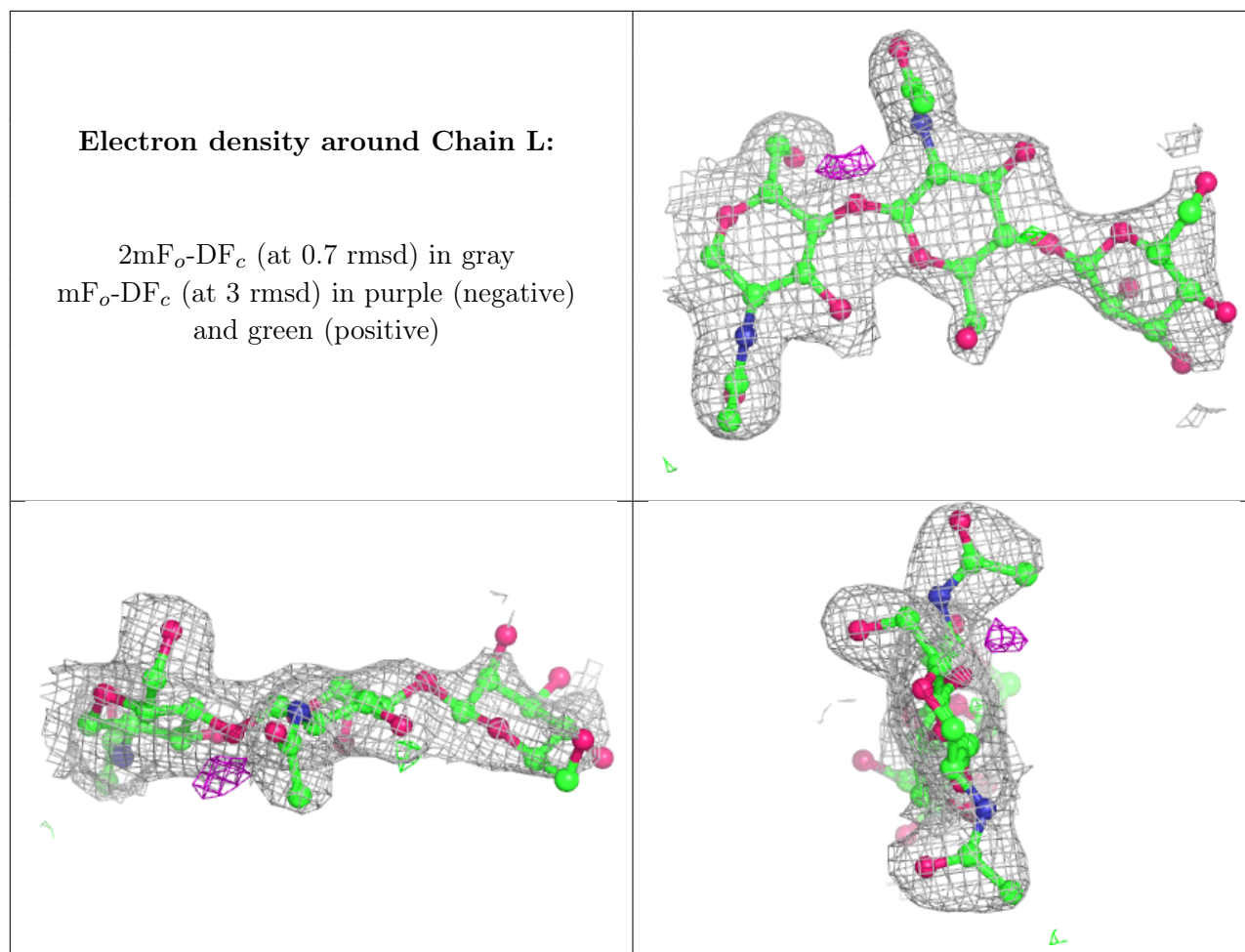
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)











## 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
7	ZN	A	303	1/1	0.78	0.07	99,99,99,99	0
8	CL	D	305	1/1	0.85	0.13	64,64,64,64	0
7	ZN	D	304	1/1	0.91	0.04	96,96,96,96	0
7	ZN	B	301	1/1	0.94	0.04	69,69,69,69	0
8	CL	B	302	1/1	0.95	0.07	50,50,50,50	0
7	ZN	E	301	1/1	0.95	0.04	76,76,76,76	0
7	ZN	D	303	1/1	0.97	0.06	45,45,45,45	0
8	CL	E	302	1/1	0.97	0.08	37,37,37,37	0
7	ZN	A	301	1/1	0.98	0.07	55,55,55,55	0
7	ZN	D	301	1/1	0.98	0.11	32,32,32,32	0
7	ZN	A	302	1/1	0.99	0.09	43,43,43,43	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	ZN	D	302	1/1	0.99	0.09	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.