



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 5, 2022 – 03:06 am GMT

PDB ID : 7OK5
Title : Crystal structure of mouse neurofascin 155 immunoglobulin domains
Authors : Chataigner, L.M.P.; Janssen, B.J.C.
Deposited on : 2021-05-17
Resolution : 2.97 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

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>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.31.3
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

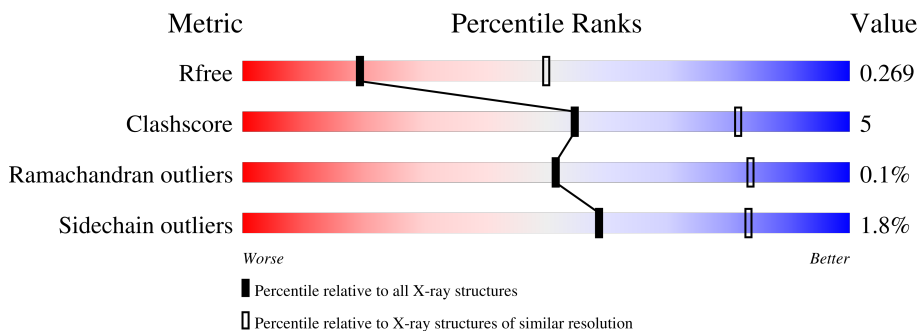
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	617	79% (green), 15% (yellow), 6% (grey)
1	B	617	80% (green), 13% (yellow), 6% (grey)
2	C	7	29% (green), 71% (yellow)
2	F	7	14% (green), 86% (yellow)
3	D	4	75% (green), 25% (yellow)
4	E	3	100% (green)
4	H	3	100% (green)

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Mol	Chain	Length	Quality of chain
5	G	5	 60% 40%

2 Entry composition [i](#)

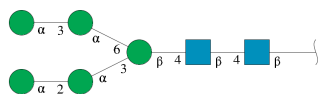
There are 5 unique types of molecules in this entry. The entry contains 9546 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Neurofascin 155.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	579	Total 4585	C 2880	N 812	O 865	S 28	0	0	0
1	A	582	Total 4606	C 2891	N 816	O 871	S 28	0	0	0

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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
			Total	C	N	O			
2	C	7	Total 83	C 46	N 2	O 35	0	0	0
2	F	7	Total 83	C 46	N 2	O 35	0	0	0

- Molecule 3 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.



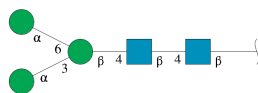
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	4	Total 50	C 28	N 2	O 20	0	0	0

- Molecule 4 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
			Total	C	N	O			
4	E	3	39	22	2	15	0	0	0
4	H	3	39	22	2	15	0	0	0

- 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.

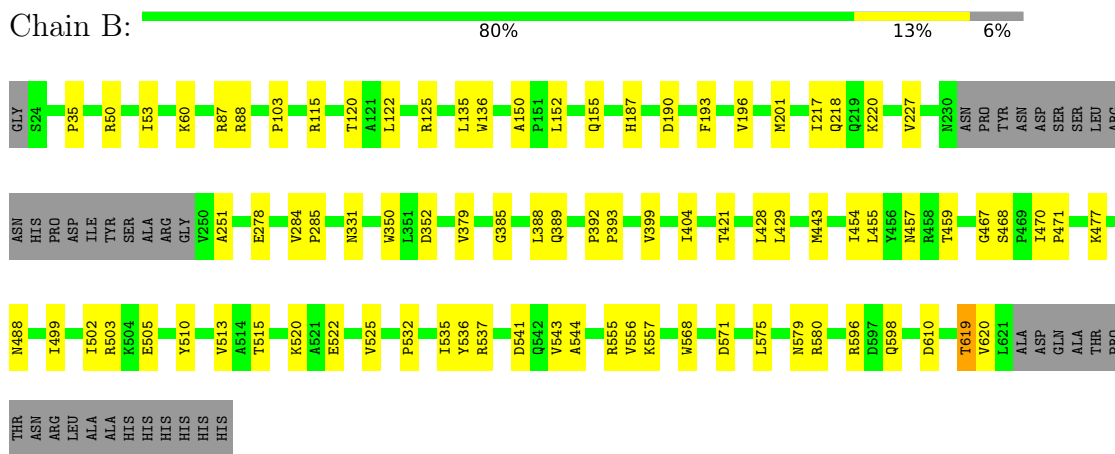


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	G	5	61	34	2	25	0	0	0

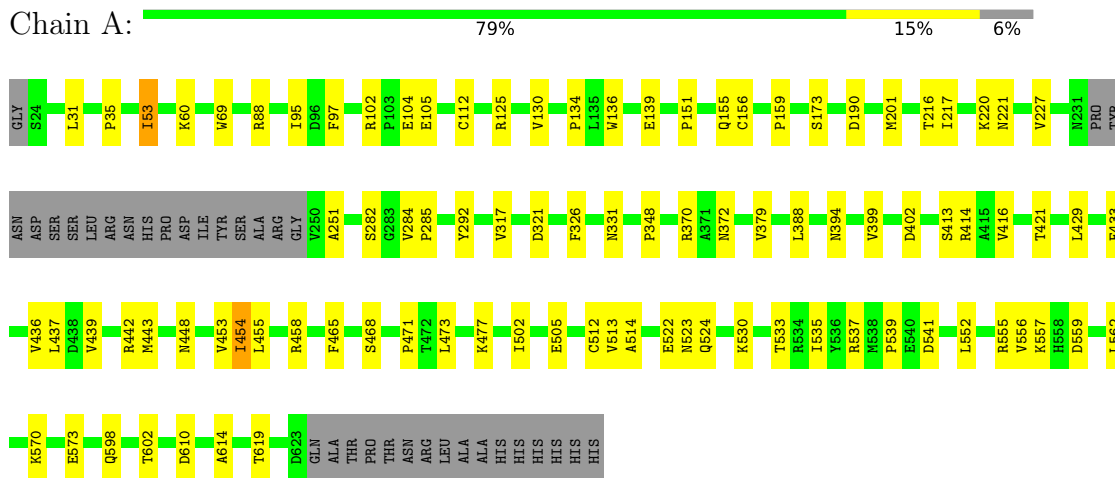
3 Residue-property plots

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. 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. 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: Neurofascin 155




- Molecule 1: Neurofascin 155



- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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



- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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 F:  14% 86%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 3: 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

Chain D:  75% 25%

MAG1
MAG2
BMA3
MAN4

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

Chain E:  100%

MAG1
MAG2
BMA3

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

Chain H:  100%

MAG1
MAG2
BMA3

- 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 G:  60% 40%

MAG1
MAG2
BMA3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.60Å 96.27Å 238.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.92 – 2.97 74.92 – 2.97	Depositor EDS
% Data completeness (in resolution range)	99.4 (74.92-2.97) 99.6 (74.92-2.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.96Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.221 , 0.269 0.222 , 0.269	Depositor DCC
R_{free} test set	1881 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	83.8	Xtrriage
Anisotropy	0.626	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9546	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: NAG, BMA, MAN

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	0.25	0/4710	0.45	0/6390
1	B	0.25	0/4689	0.44	0/6361
All	All	0.25	0/9399	0.45	0/12751

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	4606	0	4540	55	1
1	B	4585	0	4525	46	1
2	C	83	0	70	2	0
2	F	83	0	70	3	0
3	D	50	0	43	0	0
4	E	39	0	34	0	0
4	H	39	0	34	0	0
5	G	61	0	52	0	0
All	All	9546	0	9368	99	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (99) 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:A:477:LYS:NZ	1:A:505:GLU:O	2.18	0.77
1:A:388:LEU:HD21	1:A:399:VAL:HG11	1.69	0.74
1:A:379:VAL:HG22	1:A:421:THR:HG22	1.75	0.67
1:B:35:PRO:HA	1:B:60:LYS:O	1.94	0.67
1:A:53:ILE:HG23	1:A:95:ILE:HB	1.78	0.65
1:B:537:ARG:HB2	1:B:555:ARG:HB2	1.81	0.62
1:B:379:VAL:HG22	1:B:421:THR:HG22	1.82	0.61
1:A:414:ARG:HD3	1:A:436:VAL:H	1.64	0.61
1:A:454:ILE:HG21	1:A:610:ASP:HB2	1.81	0.61
1:A:535:ILE:HG12	1:A:556:VAL:HG22	1.81	0.61
1:A:513:VAL:HG22	1:A:522:GLU:HG2	1.85	0.58
1:B:477:LYS:NZ	1:B:505:GLU:O	2.36	0.58
1:B:535:ILE:HG12	1:B:556:VAL:HG22	1.85	0.58
1:B:50:ARG:NH1	1:A:136:TRP:O	2.31	0.57
1:A:348:PRO:HA	1:A:372:ASN:O	2.04	0.57
1:A:439:VAL:H	1:A:468:SER:HB2	1.70	0.56
1:A:35:PRO:HA	1:A:60:LYS:O	2.05	0.56
1:A:537:ARG:HB2	1:A:555:ARG:HB2	1.89	0.55
1:B:454:ILE:HG21	1:B:610:ASP:HB2	1.89	0.54
1:B:217:ILE:HB	1:A:217:ILE:HB	1.90	0.54
1:B:568:TRP:H	1:B:575:LEU:HD23	1.72	0.54
1:A:439:VAL:H	1:A:468:SER:CB	2.21	0.53
1:B:187:HIS:N	1:B:278:GLU:OE2	2.33	0.53
1:B:513:VAL:HG22	1:B:522:GLU:HG2	1.89	0.53
1:B:537:ARG:HE	1:B:555:ARG:HD2	1.73	0.53
1:B:53:ILE:HD11	1:B:103:PRO:HB3	1.91	0.53
1:A:125:ARG:NH1	2:F:1:NAG:O3	2.41	0.52
1:B:125:ARG:NH1	2:C:1:NAG:O3	2.43	0.52
1:A:473:LEU:HD12	1:A:514:ALA:HB2	1.92	0.52
1:A:416:VAL:HG22	1:A:433:PHE:HB3	1.91	0.52
1:B:122:LEU:HD11	1:B:385:GLY:HA2	1.93	0.51
1:B:543:VAL:HG13	1:B:619:THR:HG22	1.92	0.51
1:A:437:LEU:O	1:A:468:SER:OG	2.27	0.50
1:A:539:PRO:HB3	1:A:552:LEU:HB3	1.93	0.50
1:B:455:LEU:HB2	1:B:532:PRO:HD3	1.94	0.50
1:B:136:TRP:CE2	1:B:220:LYS:HB2	2.47	0.50
1:A:53:ILE:HD13	1:A:95:ILE:HD12	1.94	0.50
1:B:399:VAL:HG12	1:B:404:ILE:HG12	1.94	0.50
2:F:1:NAG:H61	2:F:2:NAG:HN2	1.77	0.49
1:A:151:PRO:HB3	1:A:282:SER:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:PRO:HD2	1:A:331:ASN:HD21	1.78	0.49
1:A:598:GLN:HG3	1:A:619:THR:HA	1.94	0.49
1:B:459:THR:HG22	1:B:499:ILE:HB	1.94	0.49
1:B:598:GLN:HG3	1:B:619:THR:HA	1.95	0.48
1:B:285:PRO:HB2	1:B:331:ASN:HD21	1.78	0.48
1:B:135:LEU:HD23	1:B:218:GLN:NE2	2.29	0.48
1:B:510:TYR:HB2	1:B:525:VAL:HG13	1.95	0.47
1:A:53:ILE:HG22	1:A:97:PHE:HE1	1.79	0.47
1:A:134:PRO:HG2	1:A:159:PRO:HB2	1.96	0.47
1:A:317:VAL:HA	1:A:321:ASP:OD2	2.14	0.47
1:A:443:MET:HB3	1:A:443:MET:HE3	1.87	0.47
1:B:544:ALA:O	1:B:620:VAL:HA	2.15	0.46
1:B:201:MET:SD	1:B:227:VAL:HG22	2.55	0.46
1:B:537:ARG:NE	1:B:555:ARG:HD2	2.31	0.46
1:B:155:GLN:HA	1:B:190:ASP:OD2	2.16	0.46
1:A:31:LEU:HD11	1:A:442:ARG:HH21	1.80	0.46
1:B:443:MET:HB3	1:B:443:MET:HE2	1.78	0.45
1:B:454:ILE:HG13	1:B:457:ASN:HB2	1.98	0.45
1:A:559:ASP:HB3	1:A:562:LEU:HD12	1.98	0.45
1:A:155:GLN:O	1:A:220:LYS:NZ	2.50	0.45
1:B:115:ARG:HG3	1:B:120:THR:OG1	2.17	0.45
1:A:465:PHE:CD1	1:A:471:PRO:HG2	2.52	0.45
1:B:152:LEU:HB3	1:B:193:PHE:HB2	1.98	0.44
1:A:53:ILE:HG22	1:A:97:PHE:CE1	2.53	0.44
1:A:429:LEU:HG	2:F:1:NAG:H82	1.99	0.44
1:A:292:TYR:HB2	1:A:326:PHE:CE1	2.53	0.44
1:B:467:GLY:HA3	1:B:471:PRO:HG3	2.00	0.44
1:B:536:TYR:CE2	1:B:557:LYS:HG3	2.53	0.44
1:A:537:ARG:NE	1:A:555:ARG:HD2	2.33	0.44
1:B:392:PRO:HA	1:B:393:PRO:HD3	1.93	0.43
1:A:512:CYS:SG	1:A:523:ASN:HB3	2.59	0.43
1:B:459:THR:HB	1:B:502:ILE:HD11	2.01	0.43
1:B:218:GLN:HE21	1:B:218:GLN:HA	1.83	0.43
1:B:579:ASN:O	1:B:580:ARG:HG2	2.17	0.43
1:A:102:ARG:O	1:A:105:GLU:HG2	2.19	0.43
1:A:251:ALA:O	1:A:284:VAL:HG21	2.19	0.42
1:A:453:VAL:HG11	1:A:502:ILE:HD13	2.01	0.42
1:A:602:THR:HA	1:A:614:ALA:O	2.19	0.42
1:A:370:ARG:HG2	1:A:402:ASP:OD2	2.20	0.42
1:A:448:ASN:HA	1:A:524:GLN:O	2.19	0.42
1:A:533:THR:HA	1:A:557:LYS:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:TRP:CH2	1:A:112:CYS:HB2	2.55	0.42
1:B:218:GLN:NE2	1:A:216:THR:OG1	2.50	0.42
1:B:285:PRO:O	1:B:331:ASN:ND2	2.53	0.42
1:A:156:CYS:N	1:A:190:ASP:OD2	2.44	0.42
1:B:350:TRP:CE2	1:B:428:LEU:HD13	2.55	0.41
1:B:429:LEU:HG	2:C:1:NAG:H82	2.02	0.41
1:A:201:MET:SD	1:A:227:VAL:HG22	2.59	0.41
1:A:104:GLU:HA	1:A:130:VAL:HG11	2.02	0.41
1:A:394:ASN:ND2	1:A:413:SER:HB3	2.35	0.41
1:A:455:LEU:O	1:A:502:ILE:HB	2.21	0.41
1:A:570:LYS:NZ	1:A:598:GLN:O	2.49	0.41
1:A:139:GLU:OE2	1:A:220:LYS:HE3	2.21	0.41
1:B:150:ALA:O	1:B:196:VAL:HG23	2.21	0.41
1:A:139:GLU:O	1:A:221:ASN:ND2	2.51	0.41
1:B:135:LEU:HD23	1:B:218:GLN:HE22	1.86	0.41
1:B:251:ALA:O	1:B:284:VAL:HG21	2.21	0.40
1:B:470:ILE:HA	1:B:471:PRO:HD3	1.93	0.40
1:A:155:GLN:HA	1:A:190:ASP:OD2	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ARG:NH2	1:A:173:SER:O[3_545]	2.19	0.01

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	578/617 (94%)	565 (98%)	13 (2%)	0	100 100
1	B	575/617 (93%)	556 (97%)	18 (3%)	1 (0%)	47 80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1153/1234 (93%)	1121 (97%)	31 (3%)	1 (0%)	51 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	571	ASP

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	516/545 (95%)	509 (99%)	7 (1%)	67 86
1	B	514/545 (94%)	502 (98%)	12 (2%)	50 79
All	All	1030/1090 (94%)	1011 (98%)	19 (2%)	59 83

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	87	ARG
1	B	352	ASP
1	B	388	LEU
1	B	389	GLN
1	B	468	SER
1	B	488	ASN
1	B	503	ARG
1	B	515	THR
1	B	520	LYS
1	B	541	ASP
1	B	596	ARG
1	B	619	THR
1	A	53	ILE
1	A	88	ARG
1	A	454	ILE
1	A	458	ARG
1	A	530	LYS

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Mol	Chain	Res	Type
1	A	541	ASP
1	A	573	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	218	GLN
1	B	331	ASN
1	B	598	GLN
1	A	147	GLN
1	A	218	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](#)

29 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	1	1,2	14,14,15	0.22	0	17,19,21	0.39	0
2	NAG	C	2	2	14,14,15	0.19	0	17,19,21	0.44	0
2	BMA	C	3	2	11,11,12	0.51	0	15,15,17	0.74	0
2	MAN	C	4	2	11,11,12	0.60	0	15,15,17	1.02	2 (13%)
2	MAN	C	5	2	11,11,12	0.60	0	15,15,17	1.08	2 (13%)
2	MAN	C	6	2	11,11,12	0.85	1 (9%)	15,15,17	1.23	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	C	7	2	11,11,12	0.72	0	15,15,17	0.91	1 (6%)
3	NAG	D	1	1,3	14,14,15	0.26	0	17,19,21	0.55	0
3	NAG	D	2	3	14,14,15	0.33	0	17,19,21	0.39	0
3	BMA	D	3	3	11,11,12	0.53	0	15,15,17	0.74	0
3	MAN	D	4	3	11,11,12	0.64	0	15,15,17	1.11	2 (13%)
4	NAG	E	1	1,4	14,14,15	0.22	0	17,19,21	0.38	0
4	NAG	E	2	4	14,14,15	0.21	0	17,19,21	0.44	0
4	BMA	E	3	4	11,11,12	0.51	0	15,15,17	0.74	0
2	NAG	F	1	1,2	14,14,15	0.26	0	17,19,21	0.41	0
2	NAG	F	2	2	14,14,15	0.34	0	17,19,21	0.46	0
2	BMA	F	3	2	11,11,12	0.48	0	15,15,17	0.72	0
2	MAN	F	4	2	11,11,12	0.58	0	15,15,17	1.00	1 (6%)
2	MAN	F	5	2	11,11,12	0.58	0	15,15,17	1.02	2 (13%)
2	MAN	F	6	2	11,11,12	0.78	0	15,15,17	0.90	1 (6%)
2	MAN	F	7	2	11,11,12	0.72	0	15,15,17	0.89	1 (6%)
5	NAG	G	1	1,5	14,14,15	0.39	0	17,19,21	0.49	0
5	NAG	G	2	5	14,14,15	0.23	0	17,19,21	0.37	0
5	BMA	G	3	5	11,11,12	0.74	0	15,15,17	0.80	0
5	MAN	G	4	5	11,11,12	0.84	1 (9%)	15,15,17	1.41	2 (13%)
5	MAN	G	5	5	11,11,12	0.85	0	15,15,17	1.05	2 (13%)
4	NAG	H	1	1,4	14,14,15	0.24	0	17,19,21	0.38	0
4	NAG	H	2	4	14,14,15	0.22	0	17,19,21	0.41	0
4	BMA	H	3	4	11,11,12	0.55	0	15,15,17	0.80	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	MAN	C	6	2	-	0/2/19/22	0/1/1/1
2	MAN	C	7	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
2	MAN	F	4	2	-	0/2/19/22	0/1/1/1
2	MAN	F	5	2	-	1/2/19/22	0/1/1/1
2	MAN	F	6	2	-	0/2/19/22	0/1/1/1
2	MAN	F	7	2	-	0/2/19/22	0/1/1/1
5	NAG	G	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	1/1/1/1
5	MAN	G	5	5	-	0/2/19/22	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	-	1/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	4	MAN	C1-C2	2.01	1.56	1.52
2	C	6	MAN	C1-C2	2.00	1.56	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	4	MAN	C1-O5-C5	4.38	118.12	112.19
3	D	4	MAN	C1-O5-C5	3.07	116.35	112.19
2	C	5	MAN	C1-O5-C5	3.02	116.28	112.19
2	F	5	MAN	C1-O5-C5	2.75	115.92	112.19
2	F	4	MAN	C1-O5-C5	2.75	115.92	112.19
2	C	4	MAN	C1-O5-C5	2.72	115.88	112.19
2	C	6	MAN	C1-C2-C3	2.69	112.97	109.67
3	D	4	MAN	O2-C2-C3	-2.31	105.50	110.14
2	C	5	MAN	O2-C2-C3	-2.28	105.57	110.14
2	C	4	MAN	O2-C2-C3	-2.24	105.65	110.14
2	C	7	MAN	O2-C2-C3	-2.23	105.67	110.14
2	C	6	MAN	O2-C2-C3	-2.19	105.75	110.14
2	F	5	MAN	O2-C2-C3	-2.17	105.80	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	4	MAN	O2-C2-C3	-2.13	105.87	110.14
2	F	7	MAN	O2-C2-C3	-2.12	105.88	110.14
5	G	5	MAN	C1-O5-C5	2.12	115.06	112.19
5	G	5	MAN	O2-C2-C3	-2.10	105.93	110.14
2	F	6	MAN	O2-C2-C3	-2.10	105.94	110.14
2	C	6	MAN	C1-O5-C5	2.06	114.98	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
3	D	4	MAN	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
4	H	3	BMA	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C1-C2-N2-C7
3	D	1	NAG	C3-C2-N2-C7
2	F	5	MAN	O5-C5-C6-O6

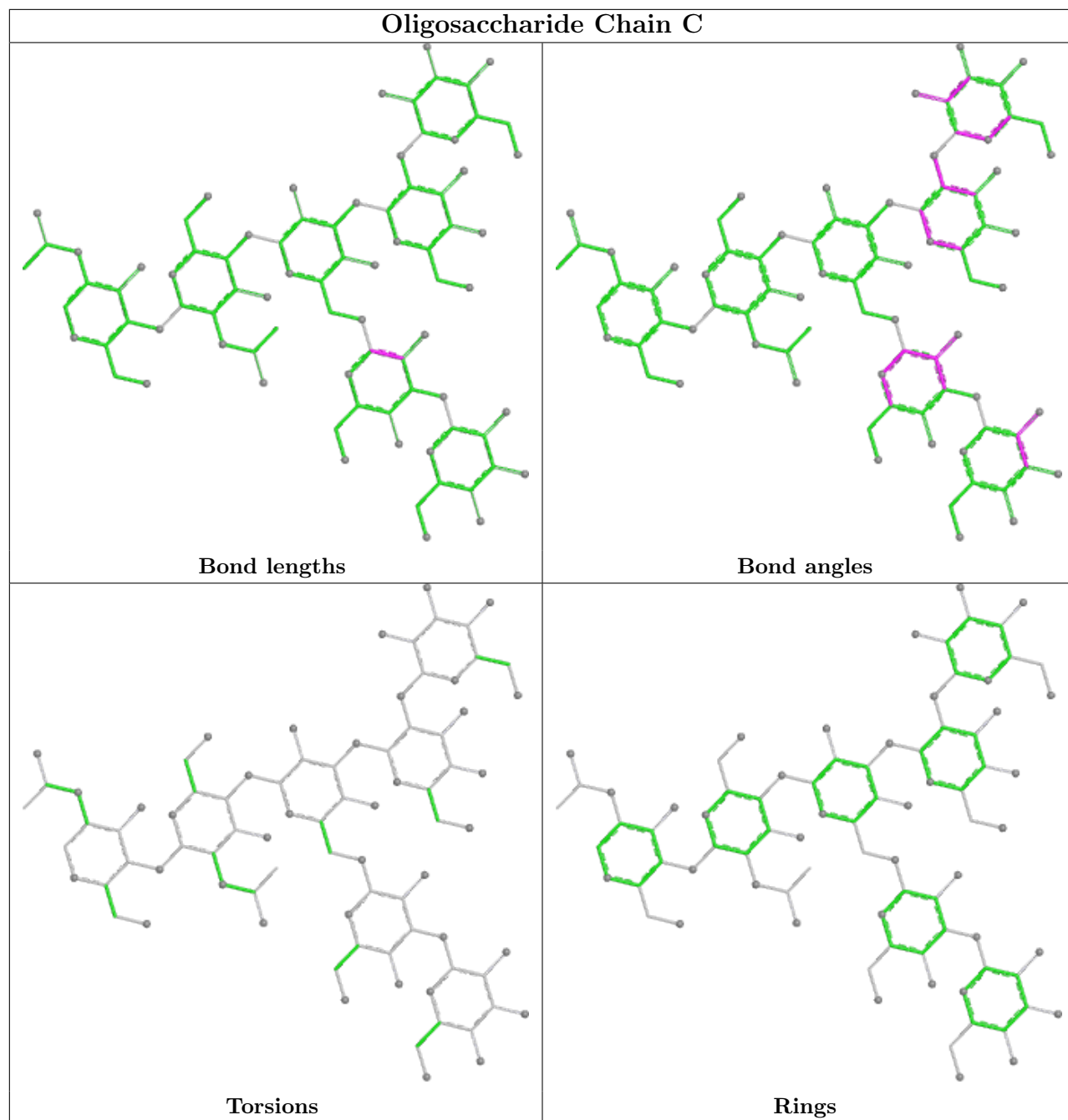
All (1) ring outliers are listed below:

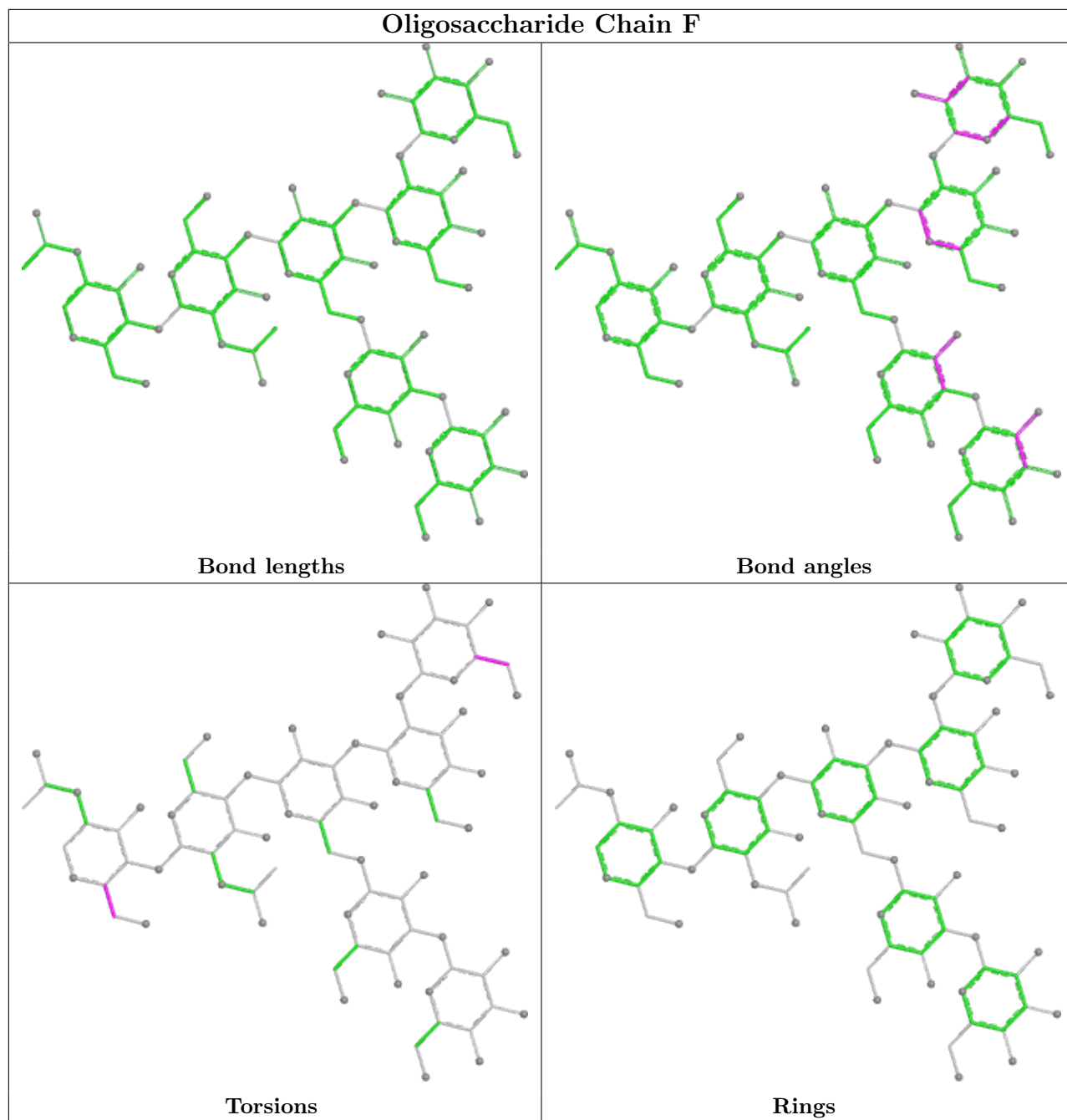
Mol	Chain	Res	Type	Atoms
5	G	4	MAN	C1-C2-C3-C4-C5-O5

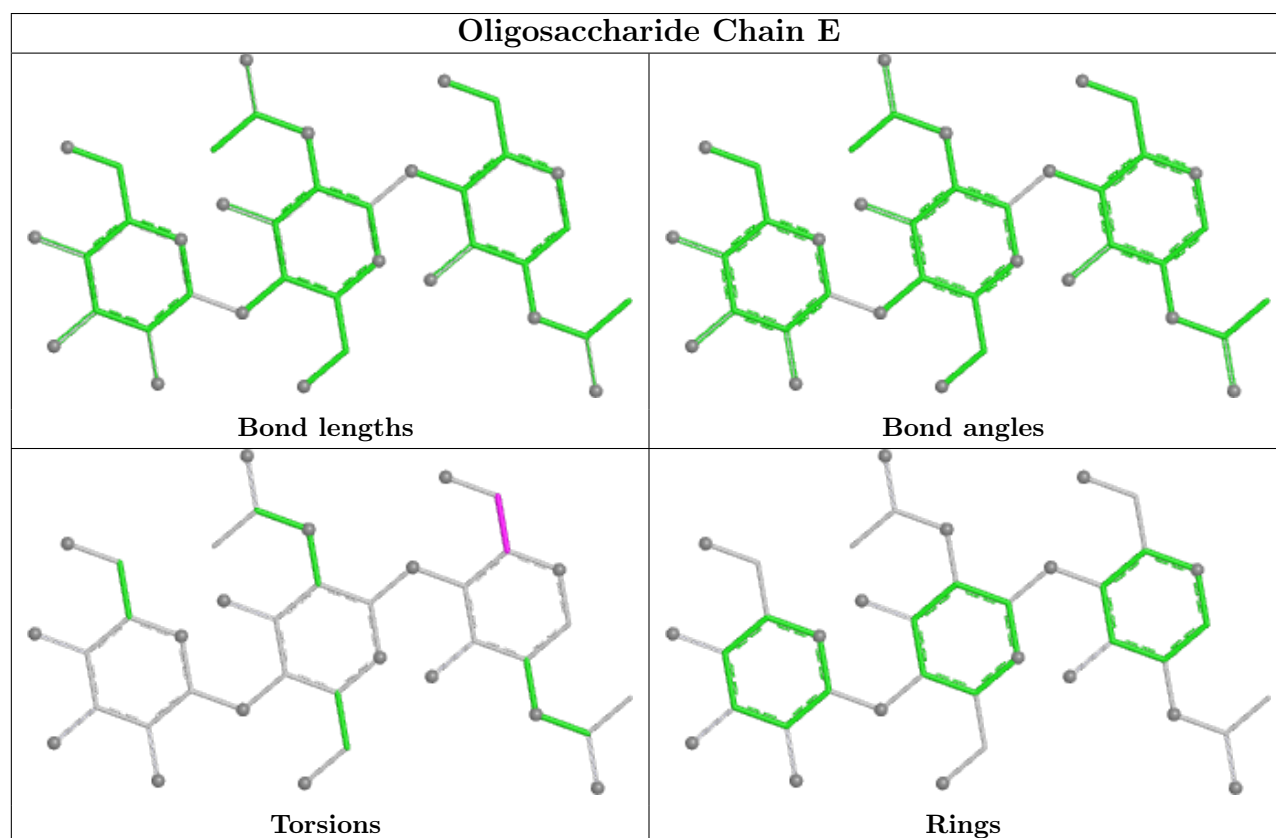
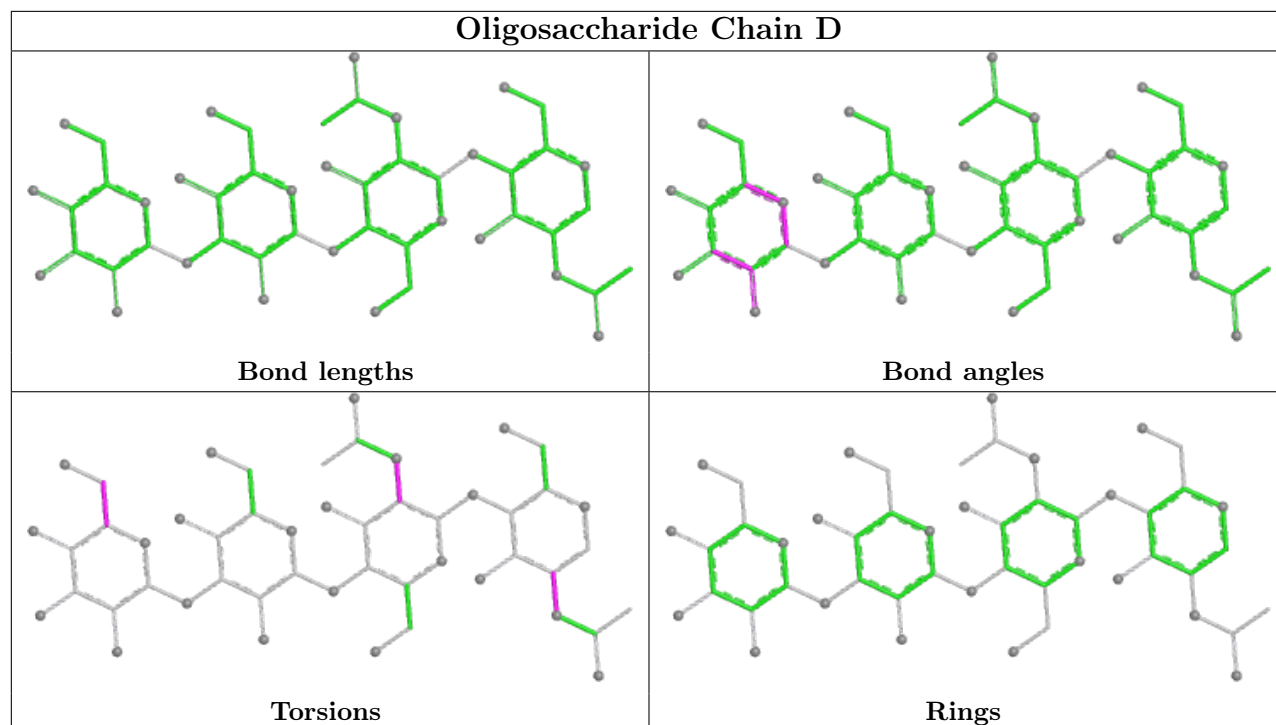
3 monomers are involved in 5 short contacts:

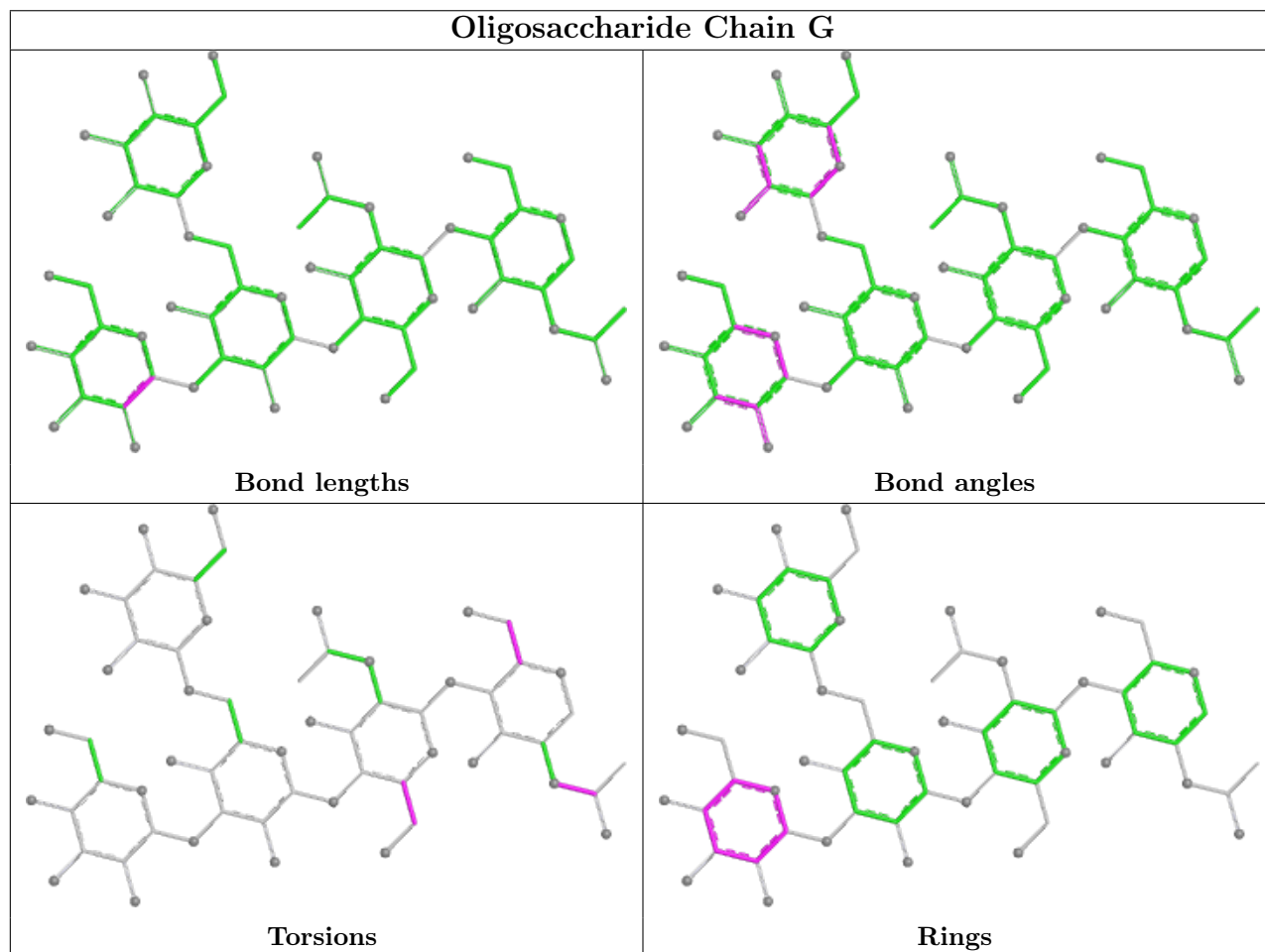
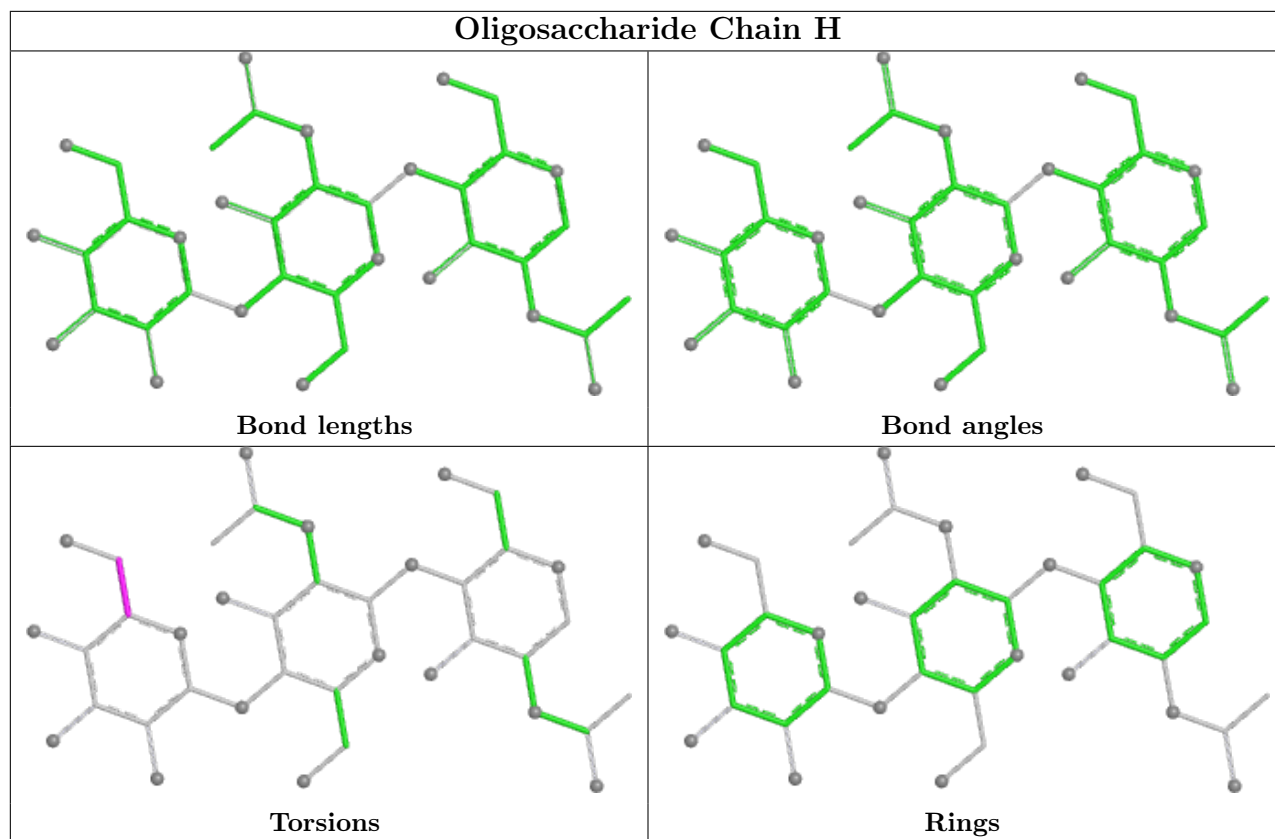
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	NAG	1	0
2	C	1	NAG	2	0
2	F	1	NAG	3	0

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









5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

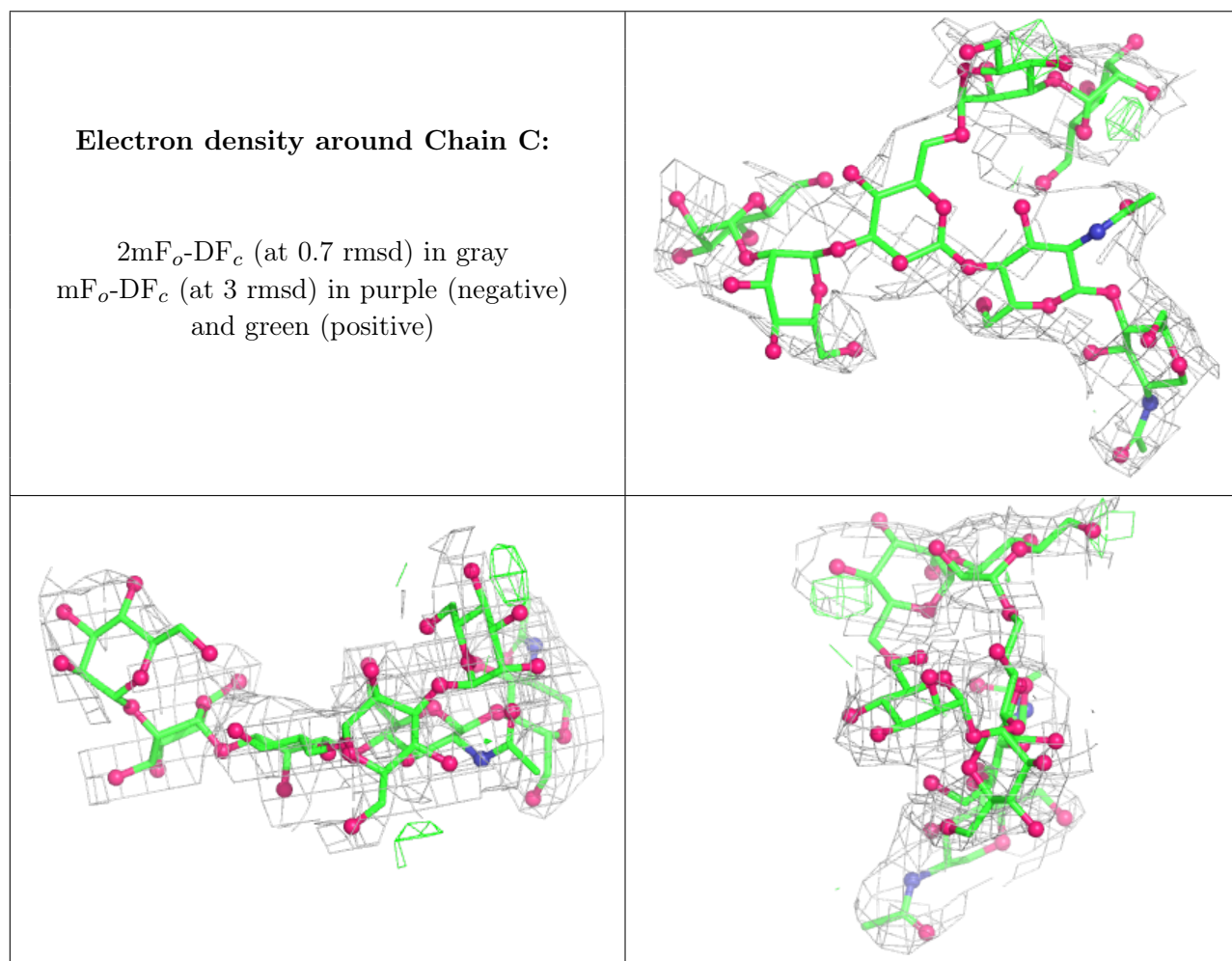
6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

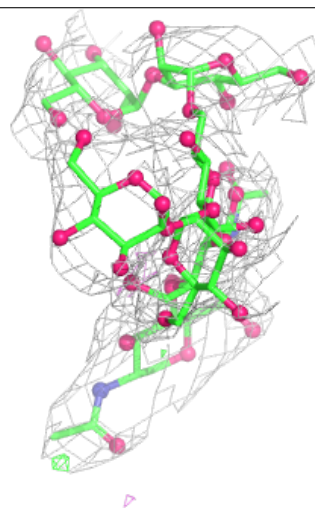
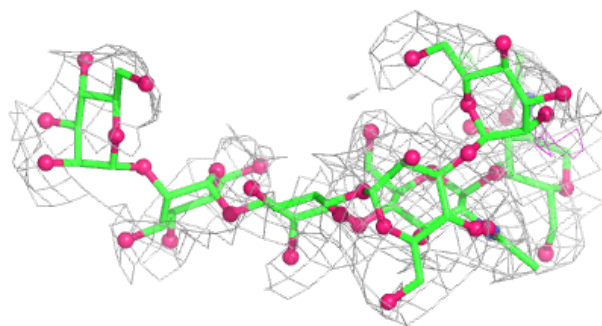
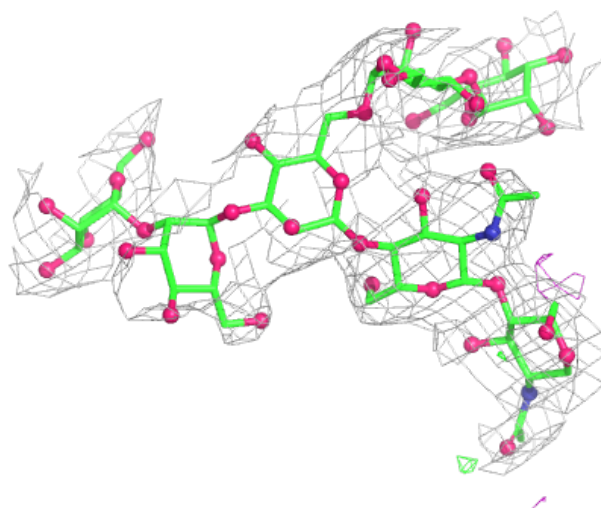
Unable to reproduce the depositors R factor - this section is therefore empty.

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.



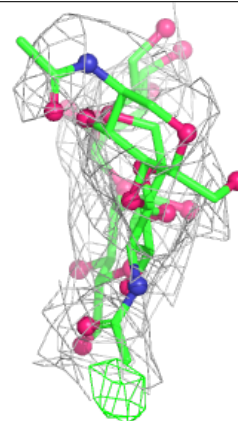
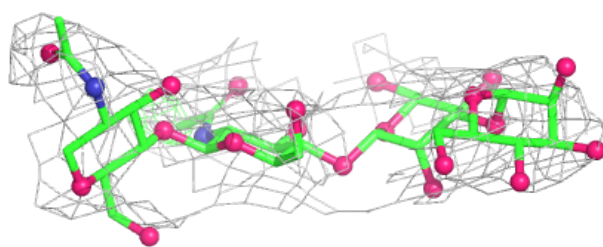
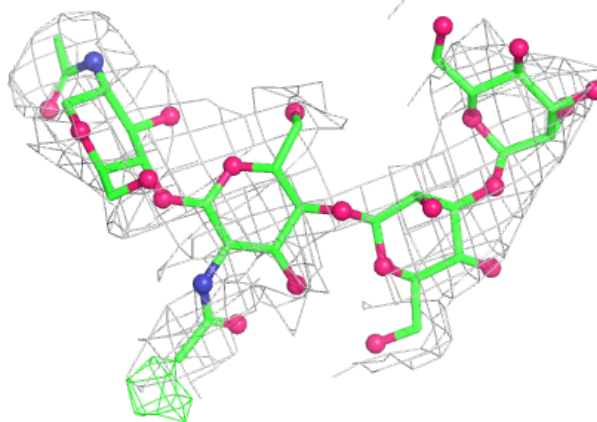
Electron density around Chain F:

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

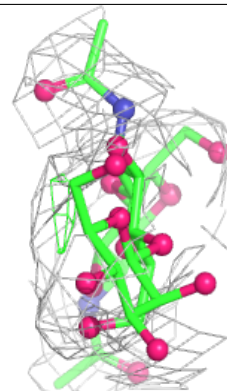
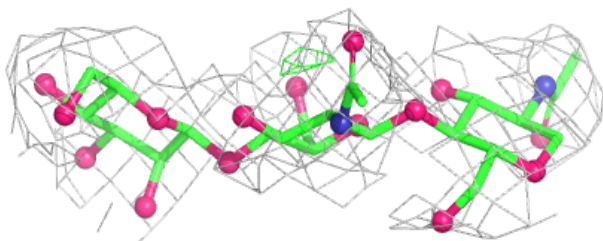
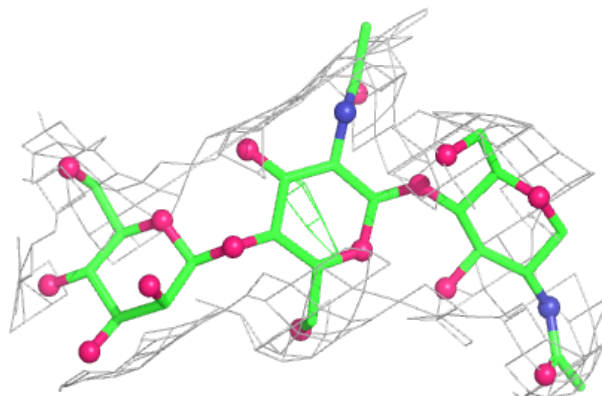


Electron density around Chain D:

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

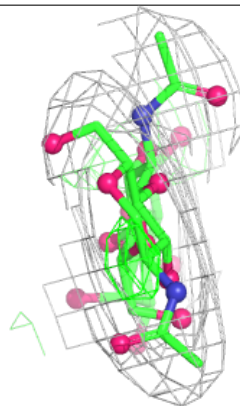
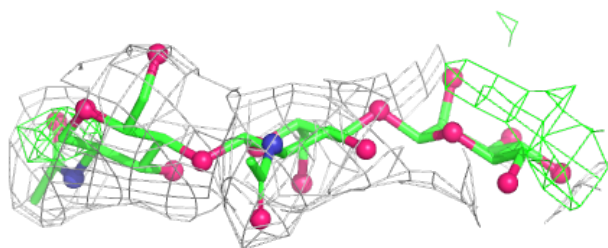
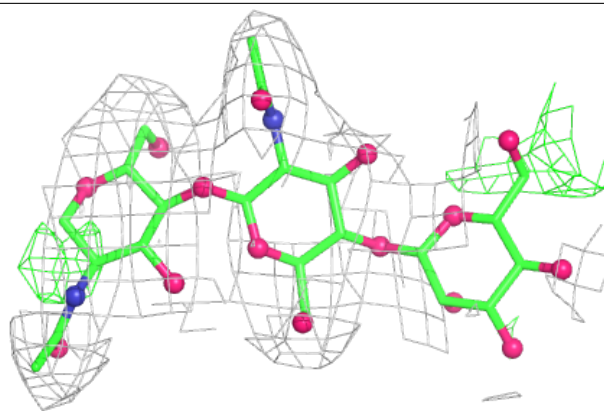
**Electron density around Chain E:**

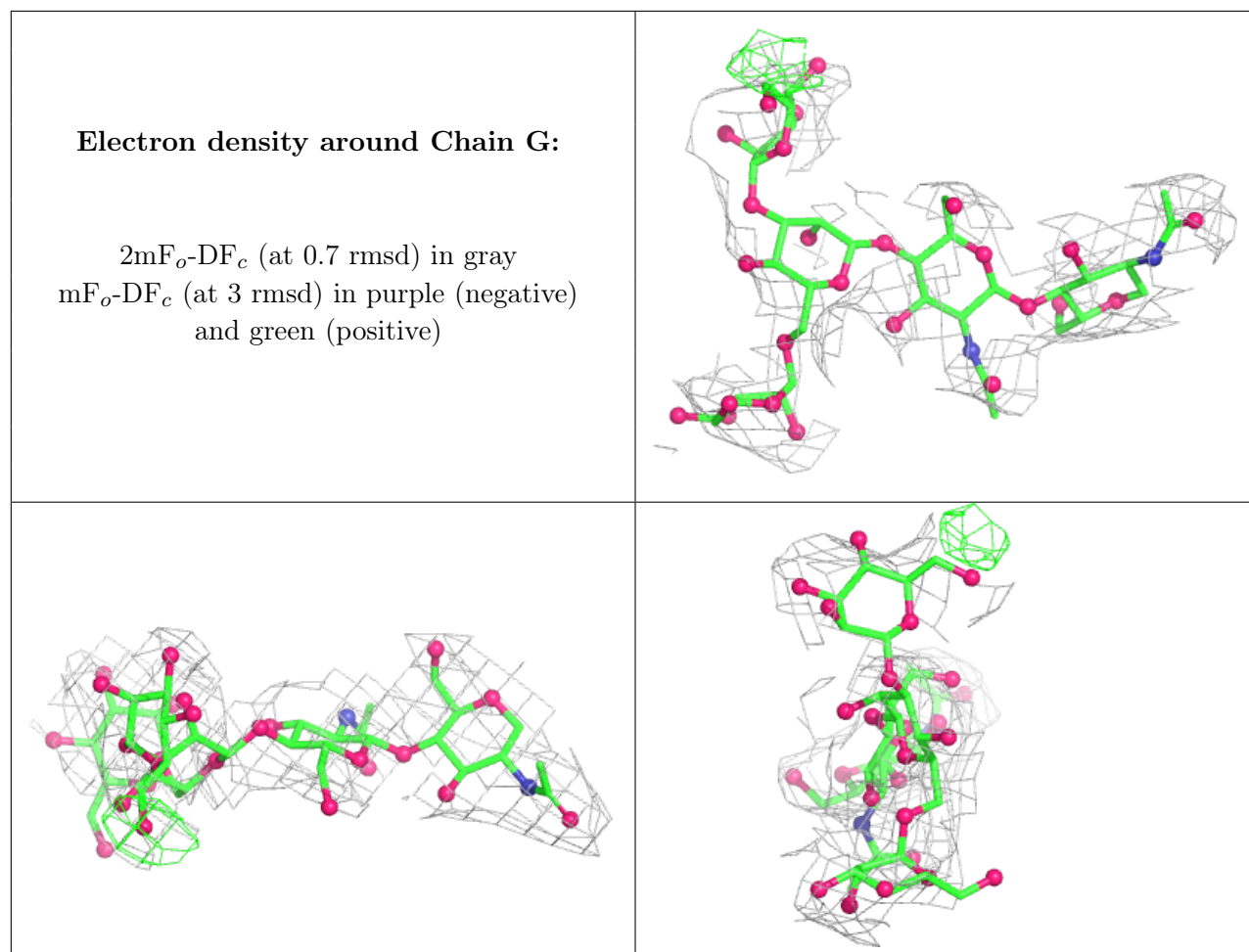
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.