WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Dec 5, 2022 – 12:18 am GMT

PDB ID	:	7OL4
Title	:	Mouse contactin-1 neurofascin-155 immunoglobulin domains adhesion complex
Authors	:	Chataigner, L.M.P.; Janssen, B.J.C.
Deposited on	:	2021-05-19
Resolution	:	4.80 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 (i) 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 (i)) were used in the production of this report:

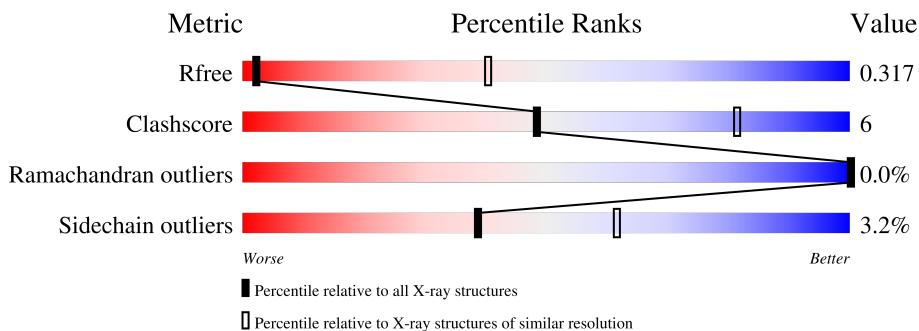|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.80 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	Percentile Ranks	Value
Rfree		0.317
Clashscore		6
Ramachandran outliers		0.0%
Sidechain outliers		3.2%

Worse *Better*

▪ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1096 (5.80-3.80)
Clashscore	141614	1170 (5.80-3.80)
Ramachandran outliers	138981	1105 (5.80-3.80)
Sidechain outliers	138945	1085 (5.80-3.80)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	592	79% · · 17% · ·
1	B	592	80% 15% · ·
2	C	617	79% 16% · 5%
2	D	617	82% 13% · ·
3	E	3	100%
3	F	3	33% 33% 33%
3	H	3	100%

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Mol	Chain	Length	Quality of chain
4	G	4	75% 25%
4	P	4	100%
5	I	4	25% 50% 25%
6	J	6	100%
7	K	6	67% 17% 17%
8	L	5	40% 20% 40%
9	M	7	43% 57%
10	N	5	40% 60%
10	R	5	40% 40% 20%
11	O	5	80% 20%
11	S	5	60% 40%
12	Q	8	25% 75%
13	T	4	75% 25%

2   Entry composition ⓘ

There are 14 unique types of molecules in this entry. The entry contains 19300 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 Contactin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	570	Total 4515	C 2879	N 759	O 852	S 25	0	0	0
1	B	568	Total 4498	C 2870	N 757	O 846	S 25	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	GLY	-	expression tag	UNP P12960
A	20	SER	-	expression tag	UNP P12960
A	433	VAL	ILE	conflict	UNP P12960
A	605	HIS	-	expression tag	UNP P12960
A	606	HIS	-	expression tag	UNP P12960
A	607	HIS	-	expression tag	UNP P12960
A	608	HIS	-	expression tag	UNP P12960
A	609	HIS	-	expression tag	UNP P12960
A	610	HIS	-	expression tag	UNP P12960
B	19	GLY	-	expression tag	UNP P12960
B	20	SER	-	expression tag	UNP P12960
B	433	VAL	ILE	conflict	UNP P12960
B	605	HIS	-	expression tag	UNP P12960
B	606	HIS	-	expression tag	UNP P12960
B	607	HIS	-	expression tag	UNP P12960
B	608	HIS	-	expression tag	UNP P12960
B	609	HIS	-	expression tag	UNP P12960
B	610	HIS	-	expression tag	UNP P12960

- Molecule 2 is a protein called Neurofascin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	587	Total 4648	C 2917	N 825	O 878	S 28	0	0	0

Continued on next page...

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	590	Total 4668	C 2927	N 828	O 885	S 28	0	0	0

- Molecule 3 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.
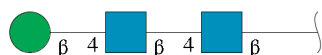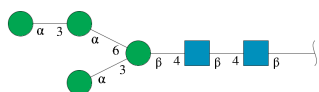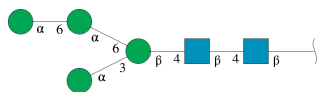

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total 39	C 22	N 2	O 15	0	0	0
3	F	3	Total 39	C 22	N 2	O 15	0	0	0
3	H	3	Total 39	C 22	N 2	O 15	0	0	0

- Molecule 4 is an oligosaccharide called 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.
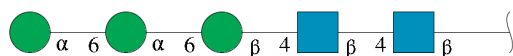

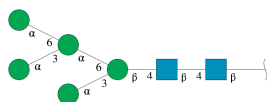| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total 50	C 28	N 2	O 20	0	0	0
4	P	4	Total 50	C 28	N 2	O 20	0	0	0

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

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

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyran ose-(1-6)-[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			
6	J	6	72	40	2	30	0	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyran ose-(1-6)-[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			
7	K	6	72	40	2	30	0	0	0

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyran ose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.

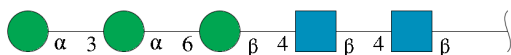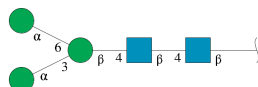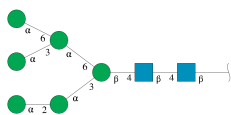| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	L	5	61	34	2	25	0	0	0

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran ose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyran ose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glu

copyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	M	7	83	46	2	35	0	0	0

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyra
  nose-(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			
10	N	5	61	34	2	25	0	0	0
10	R	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyra
  nose-(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			
11	O	5	61	34	2	25	0	0	0
11	S	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyra
  nose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopy
  ranose-(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
12	Q	8	Total 94	C 52	N 2	O 40	0	0	0

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyran ose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glu copyranose.

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

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).
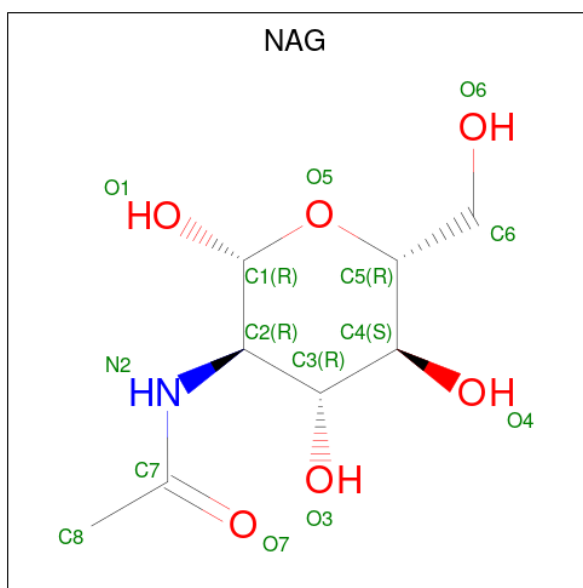
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total 14	C 8	N 1	O 5	0	0
14	B	1	Total 14	C 8	N 1	O 5	0	0

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: Contactin-1

Chain A:
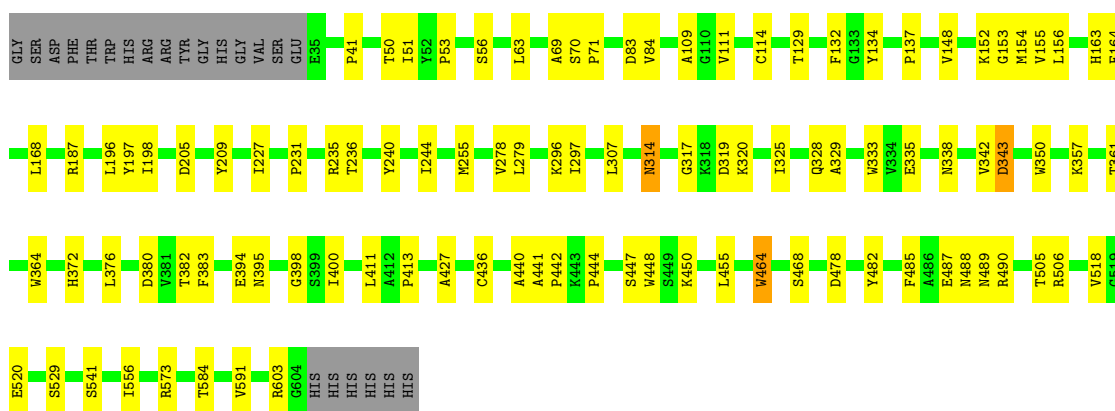
• Molecule 1: Contactin-1

Chain B:
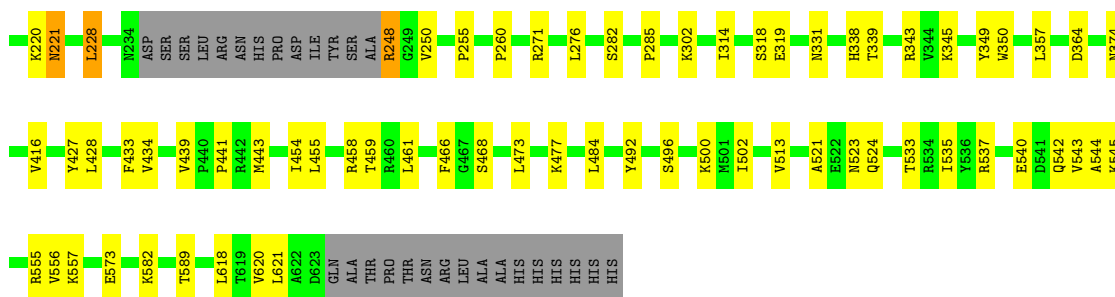

• Molecule 2: Neurofascin

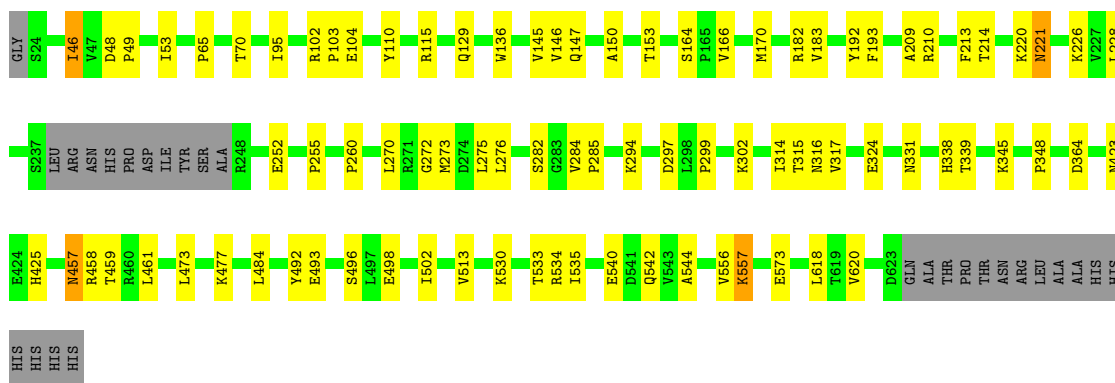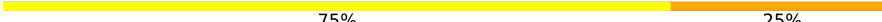Chain C:

- Molecule 2: Neurofascin

Chain D:

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

Chain E:

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

Chain F:

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

Chain H:

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

Chain G:

75%   25%

NAG1 NAG2 BMA3 MAN4

• Molecule 4: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose
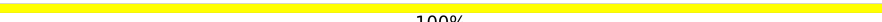
Chain P:

100%

NAG1 NAG2 BMA3 MAN4

• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

25%   50%   25%

NAG1 NAG2 BMA3 MAN4

• Molecule 6: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyran ose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetam ido-2-deoxy-beta-D-glucopyranose

Chain J:

100%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6

• Molecule 7: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyran ose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetam ido-2-deoxy-beta-D-glucopyranose

Chain K:

67%   17%   17%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6

• Molecule 8: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyrano se-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra nose

Chain L:

40%   20%   40%

NAG1 NAG2 BMA3 MAN4 MAN5

• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyran ose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-VD-glucopyranose

Chain M:

43%   57%

• Molecule 10: 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 N:

40%   60%

• Molecule 10: 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 R:

40%   40%   20%

• Molecule 11: 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
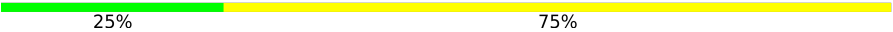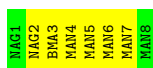
Chain O:

80%   20%

• Molecule 11: 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 S:

60%   40%

• Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 Q:

25%   75%

• Molecule 13: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	146.77Å 151.78Å 162.34Å 90.00° 111.78° 90.00°	Depositor
Resolution (Å)	75.38 – 4.80 75.89 – 4.80	Depositor EDS
% Data completeness (in resolution range)	48.0 (75.38-4.80) 48.1 (75.89-4.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 4.87Å)	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
R, R_{free}	0.288 , 0.326 0.288 , 0.317	Depositor DCC
R_{free} test set	794 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	103.8	Xtriage
Anisotropy	1.170	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< |L| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.77	EDS
Total number of atoms	19300	wwPDB-VP
Average B, all atoms (Å^2)	259.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, MAN, NAG

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	0/4628	0.51	0/6291
1	B	0.25	0/4611	0.50	0/6268
2	C	0.25	0/4754	0.52	0/6450
2	D	0.25	0/4774	0.51	0/6477
All	All	0.25	0/18767	0.51	0/25486

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	4515	0	4412	60	1
1	B	4498	0	4402	54	0
2	C	4648	0	4577	56	0
2	D	4668	0	4591	48	0
3	E	39	0	34	0	0
3	F	39	0	34	1	0
3	H	39	0	34	0	0
4	G	50	0	43	2	0
4	P	50	0	43	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	50	0	43	3	0
6	J	72	0	61	0	0
7	K	72	0	61	4	0
8	L	61	0	52	1	0
9	M	83	0	70	0	0
10	N	61	0	52	1	0
10	R	61	0	52	1	0
11	O	61	0	52	2	0
11	S	61	0	52	0	0
12	Q	94	0	79	0	0
13	T	50	0	43	2	0
14	A	14	0	13	0	0
14	B	14	0	13	0	0
All	All	19300	0	18813	230	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 6.

The worst 5 of 230 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:B:413:PRO:HD3	1:B:488:ASN:HD22	1.46	0.80
1:B:425:LEU:HB3	1:B:591:VAL:HG12	1.64	0.79
1:A:427:ALA:HB2	1:A:591:VAL:HB	1.64	0.78
1:A:413:PRO:HD3	1:A:488:ASN:HD22	1.47	0.78
11:O:1:NAG:H3	11:O:1:NAG:H83	1.71	0.71

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:A:152:LYS:NZ	1:A:380:ASP:OD2[2_656]	2.17	0.03

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	568/592 (96%)	521 (92%)	47 (8%)	0	100	100
1	B	566/592 (96%)	520 (92%)	45 (8%)	1 (0%)	47	81
2	C	583/617 (94%)	546 (94%)	37 (6%)	0	100	100
2	D	586/617 (95%)	556 (95%)	30 (5%)	0	100	100
All	All	2303/2418 (95%)	2143 (93%)	159 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	175	ASN

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	494/513 (96%)	480 (97%)	14 (3%)	43	65
1	B	492/513 (96%)	470 (96%)	22 (4%)	27	53
2	C	520/545 (95%)	506 (97%)	14 (3%)	44	66
2	D	523/545 (96%)	509 (97%)	14 (3%)	44	66
All	All	2029/2116 (96%)	1965 (97%)	64 (3%)	39	61

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	457	ASN
2	D	530	LYS
1	B	314	ASN
1	B	302	LEU
2	D	534	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	72	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5   Carbohydrates ⓘ

77 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	E	1	1,3	14,14,15	0.30	0	17,19,21	0.54	0
3	NAG	E	2	3	14,14,15	0.49	0	17,19,21	0.52	0
3	BMA	E	3	3	11,11,12	0.70	0	15,15,17	0.74	0
3	NAG	F	1	1,3	14,14,15	0.23	0	17,19,21	0.52	0
3	NAG	F	2	3	14,14,15	0.39	0	17,19,21	1.00	1 (5%)
3	BMA	F	3	3	11,11,12	0.76	0	15,15,17	0.82	0
4	NAG	G	1	4,1	14,14,15	0.27	0	17,19,21	0.44	0
4	NAG	G	2	4	14,14,15	0.42	0	17,19,21	0.91	1 (5%)
4	BMA	G	3	4	11,11,12	1.05	1 (9%)	15,15,17	1.61	1 (6%)
4	MAN	G	4	4	11,11,12	0.91	1 (9%)	15,15,17	0.98	0
3	NAG	H	1	1,3	14,14,15	0.29	0	17,19,21	0.67	0
3	NAG	H	2	3	14,14,15	0.59	0	17,19,21	0.54	0
3	BMA	H	3	3	11,11,12	0.59	0	15,15,17	0.73	0
5	NAG	I	1	5,1	14,14,15	0.59	0	17,19,21	0.83	0
5	NAG	I	2	5	14,14,15	1.63	2 (14%)	17,19,21	1.38	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	BMA	I	3	5	11,11,12	0.99	0	15,15,17	0.92	0
5	MAN	I	4	5	11,11,12	0.73	0	15,15,17	0.88	1 (6%)
6	NAG	J	1	1,6	14,14,15	1.31	1 (7%)	17,19,21	1.24	1 (5%)
6	NAG	J	2	6	14,14,15	0.80	0	17,19,21	1.57	2 (11%)
6	BMA	J	3	6	11,11,12	1.68	4 (36%)	15,15,17	1.01	1 (6%)
6	MAN	J	4	6	11,11,12	1.35	1 (9%)	15,15,17	1.31	2 (13%)
6	MAN	J	5	6	11,11,12	0.83	1 (9%)	15,15,17	0.94	1 (6%)
6	MAN	J	6	6	11,11,12	0.92	1 (9%)	15,15,17	0.87	1 (6%)
7	NAG	K	1	7,1	14,14,15	0.22	0	17,19,21	0.37	0
7	NAG	K	2	7	14,14,15	0.55	0	17,19,21	1.13	1 (5%)
7	BMA	K	3	7	11,11,12	0.65	0	15,15,17	0.87	0
7	MAN	K	4	7	11,11,12	0.78	0	15,15,17	0.81	0
7	MAN	K	5	7	11,11,12	0.71	0	15,15,17	0.83	0
7	MAN	K	6	7	11,11,12	0.69	0	15,15,17	0.80	0
8	NAG	L	1	8,1	14,14,15	0.30	0	17,19,21	0.60	0
8	NAG	L	2	8	14,14,15	0.29	0	17,19,21	0.66	1 (5%)
8	BMA	L	3	8	11,11,12	0.68	0	15,15,17	0.68	0
8	MAN	L	4	8	11,11,12	0.63	0	15,15,17	1.02	1 (6%)
8	MAN	L	5	8	11,11,12	0.91	1 (9%)	15,15,17	0.98	0
9	NAG	M	1	9,2	14,14,15	0.20	0	17,19,21	0.32	0
9	NAG	M	2	9	14,14,15	0.56	0	17,19,21	0.76	1 (5%)
9	BMA	M	3	9	11,11,12	1.24	2 (18%)	15,15,17	0.77	0
9	MAN	M	4	9	11,11,12	0.58	0	15,15,17	0.85	1 (6%)
9	MAN	M	5	9	11,11,12	0.70	0	15,15,17	0.76	0
9	MAN	M	6	9	11,11,12	0.78	0	15,15,17	0.85	1 (6%)
9	MAN	M	7	9	11,11,12	0.70	0	15,15,17	0.70	0
10	NAG	N	1	10,2	14,14,15	0.24	0	17,19,21	0.43	0
10	NAG	N	2	10	14,14,15	0.42	0	17,19,21	0.81	1 (5%)
10	BMA	N	3	10	11,11,12	0.75	0	15,15,17	0.73	0
10	MAN	N	4	10	11,11,12	0.72	0	15,15,17	0.82	1 (6%)
10	MAN	N	5	10	11,11,12	0.67	0	15,15,17	0.83	0
11	NAG	O	1	11,2	14,14,15	0.96	1 (7%)	17,19,21	1.22	1 (5%)
11	NAG	O	2	11	14,14,15	0.45	0	17,19,21	0.79	1 (5%)
11	BMA	O	3	11	11,11,12	1.05	0	15,15,17	1.09	1 (6%)
11	MAN	O	4	11	11,11,12	0.94	1 (9%)	15,15,17	1.10	2 (13%)
11	MAN	O	5	11	11,11,12	0.98	0	15,15,17	1.01	1 (6%)
4	NAG	P	1	4,2	14,14,15	0.91	1 (7%)	17,19,21	0.51	0
4	NAG	P	2	4	14,14,15	0.49	0	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	BMA	P	3	4	11,11,12	0.50	0	15,15,17	0.59	0
4	MAN	P	4	4	11,11,12	0.70	0	15,15,17	0.76	0
12	NAG	Q	1	12,2	14,14,15	0.31	0	17,19,21	0.41	0
12	NAG	Q	2	12	14,14,15	0.75	1 (7%)	17,19,21	0.85	1 (5%)
12	BMA	Q	3	12	11,11,12	2.15	3 (27%)	15,15,17	1.48	3 (20%)
12	MAN	Q	4	12	11,11,12	1.02	0	15,15,17	1.30	1 (6%)
12	MAN	Q	5	12	11,11,12	0.74	0	15,15,17	1.03	1 (6%)
12	MAN	Q	6	12	11,11,12	1.18	1 (9%)	15,15,17	1.45	4 (26%)
12	MAN	Q	7	12	11,11,12	0.82	1 (9%)	15,15,17	0.81	1 (6%)
12	MAN	Q	8	12	11,11,12	0.76	0	15,15,17	0.94	0
10	NAG	R	1	10,2	14,14,15	0.20	0	17,19,21	0.78	1 (5%)
10	NAG	R	2	10	14,14,15	0.51	0	17,19,21	0.49	0
10	BMA	R	3	10	11,11,12	0.55	0	15,15,17	0.81	0
10	MAN	R	4	10	11,11,12	0.88	0	15,15,17	1.02	1 (6%)
10	MAN	R	5	10	11,11,12	0.65	0	15,15,17	0.86	0
11	NAG	S	1	11,2	14,14,15	0.31	0	17,19,21	0.48	0
11	NAG	S	2	11	14,14,15	0.56	0	17,19,21	0.65	1 (5%)
11	BMA	S	3	11	11,11,12	0.71	0	15,15,17	0.70	0
11	MAN	S	4	11	11,11,12	0.68	0	15,15,17	0.75	0
11	MAN	S	5	11	11,11,12	0.62	0	15,15,17	0.80	1 (6%)
13	NAG	T	1	2,13	14,14,15	1.07	2 (14%)	17,19,21	1.26	3 (17%)
13	NAG	T	2	13	14,14,15	0.79	0	17,19,21	0.94	2 (11%)
13	BMA	T	3	13	11,11,12	0.93	0	15,15,17	1.15	1 (6%)
13	MAN	T	4	13	11,11,12	0.95	1 (9%)	15,15,17	0.93	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
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	1/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	G	3	4	-	1/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	BMA	H	3	3	-	1/2/19/22	0/1/1/1
5	NAG	I	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	I	2	5	-	5/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
5	MAN	I	4	5	-	0/2/19/22	0/1/1/1
6	NAG	J	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
6	BMA	J	3	6	-	2/2/19/22	0/1/1/1
6	MAN	J	4	6	-	0/2/19/22	0/1/1/1
6	MAN	J	5	6	-	0/2/19/22	0/1/1/1
6	MAN	J	6	6	-	0/2/19/22	0/1/1/1
7	NAG	K	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	K	2	7	-	3/6/23/26	0/1/1/1
7	BMA	K	3	7	-	0/2/19/22	0/1/1/1
7	MAN	K	4	7	-	2/2/19/22	0/1/1/1
7	MAN	K	5	7	-	0/2/19/22	0/1/1/1
7	MAN	K	6	7	-	0/2/19/22	0/1/1/1
8	NAG	L	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	L	2	8	-	1/6/23/26	0/1/1/1
8	BMA	L	3	8	-	2/2/19/22	0/1/1/1
8	MAN	L	4	8	-	2/2/19/22	0/1/1/1
8	MAN	L	5	8	-	1/2/19/22	0/1/1/1
9	NAG	M	1	9,2	-	1/6/23/26	0/1/1/1
9	NAG	M	2	9	-	0/6/23/26	0/1/1/1
9	BMA	M	3	9	-	0/2/19/22	0/1/1/1
9	MAN	M	4	9	-	0/2/19/22	0/1/1/1
9	MAN	M	5	9	-	0/2/19/22	0/1/1/1
9	MAN	M	6	9	-	0/2/19/22	0/1/1/1
9	MAN	M	7	9	-	0/2/19/22	0/1/1/1
10	NAG	N	1	10,2	-	0/6/23/26	0/1/1/1
10	NAG	N	2	10	-	0/6/23/26	0/1/1/1
10	BMA	N	3	10	-	2/2/19/22	0/1/1/1
10	MAN	N	4	10	-	0/2/19/22	0/1/1/1
10	MAN	N	5	10	-	1/2/19/22	0/1/1/1
11	NAG	O	1	11,2	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	O	2	11	-	2/6/23/26	0/1/1/1
11	BMA	O	3	11	-	0/2/19/22	0/1/1/1
11	MAN	O	4	11	-	1/2/19/22	0/1/1/1
11	MAN	O	5	11	-	0/2/19/22	0/1/1/1
4	NAG	P	1	4,2	-	1/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	BMA	P	3	4	-	0/2/19/22	0/1/1/1
4	MAN	P	4	4	-	1/2/19/22	0/1/1/1
12	NAG	Q	1	12,2	-	0/6/23/26	0/1/1/1
12	NAG	Q	2	12	-	1/6/23/26	0/1/1/1
12	BMA	Q	3	12	-	0/2/19/22	0/1/1/1
12	MAN	Q	4	12	-	1/2/19/22	0/1/1/1
12	MAN	Q	5	12	-	0/2/19/22	0/1/1/1
12	MAN	Q	6	12	-	2/2/19/22	0/1/1/1
12	MAN	Q	7	12	-	0/2/19/22	0/1/1/1
12	MAN	Q	8	12	-	0/2/19/22	0/1/1/1
10	NAG	R	1	10,2	-	0/6/23/26	0/1/1/1
10	NAG	R	2	10	-	1/6/23/26	0/1/1/1
10	BMA	R	3	10	-	1/2/19/22	0/1/1/1
10	MAN	R	4	10	-	0/2/19/22	0/1/1/1
10	MAN	R	5	10	-	0/2/19/22	0/1/1/1
11	NAG	S	1	11,2	-	0/6/23/26	0/1/1/1
11	NAG	S	2	11	-	0/6/23/26	0/1/1/1
11	BMA	S	3	11	-	0/2/19/22	0/1/1/1
11	MAN	S	4	11	-	0/2/19/22	0/1/1/1
11	MAN	S	5	11	-	0/2/19/22	0/1/1/1
13	NAG	T	1	2,13	-	2/6/23/26	0/1/1/1
13	NAG	T	2	13	-	3/6/23/26	0/1/1/1
13	BMA	T	3	13	-	1/2/19/22	0/1/1/1
13	MAN	T	4	13	-	1/2/19/22	0/1/1/1

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	2	NAG	C1-C2	4.71	1.59	1.52
12	Q	3	BMA	O5-C1	-4.41	1.36	1.43
6	J	1	NAG	O5-C1	-4.16	1.37	1.43
5	I	2	NAG	O5-C1	3.74	1.49	1.43
12	Q	3	BMA	C2-C3	3.72	1.58	1.52

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	3	BMA	O5-C5-C6	5.59	115.97	107.20
6	J	2	NAG	C1-O5-C5	5.07	119.06	112.19
5	I	2	NAG	C2-N2-C7	4.44	129.22	122.90
11	O	1	NAG	C2-N2-C7	4.04	128.66	122.90
7	K	2	NAG	C2-N2-C7	3.78	128.29	122.90

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	T	2	NAG	O5-C5-C6-O6
4	P	2	NAG	C1-C2-N2-C7
6	J	3	BMA	O5-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
13	T	2	NAG	C4-C5-C6-O6

There are no ring outliers.

18 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	3	BMA	1	0
8	L	5	MAN	1	0
3	F	2	NAG	1	0
13	T	1	NAG	2	0
4	G	2	NAG	1	0
5	I	2	NAG	3	0
4	G	1	NAG	1	0
8	L	2	NAG	1	0
7	K	1	NAG	2	0
4	P	4	MAN	1	0
4	P	2	NAG	2	0
5	I	1	NAG	2	0
3	F	1	NAG	1	0
7	K	2	NAG	3	0
10	R	3	BMA	1	0
10	R	4	MAN	1	0
11	O	1	NAG	2	0
10	N	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.

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain P

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain J

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain K

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain L

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain M

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain N

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain R

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain O

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain S

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain Q

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain T

Bond lengths	Bond angles
Torsions	Rings

5.6 Ligand geometry ⓘ

2 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	#$|Z| > 2$
14	NAG	A	701	1	14,14,15	0.22	0	17,19,21	0.82	0
14	NAG	B	701	1	14,14,15	0.20	0	17,19,21	0.51	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
14	NAG	A	701	1	-	3/6/23/26	0/1/1/1
14	NAG	B	701	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	701	NAG	C4-C5-C6-O6
14	A	701	NAG	O5-C5-C6-O6
14	A	701	NAG	C3-C2-N2-C7

There are no ring outliers.

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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand NAG A 701

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG B 701

Bond lengths

Bond angles

Torsions

Rings
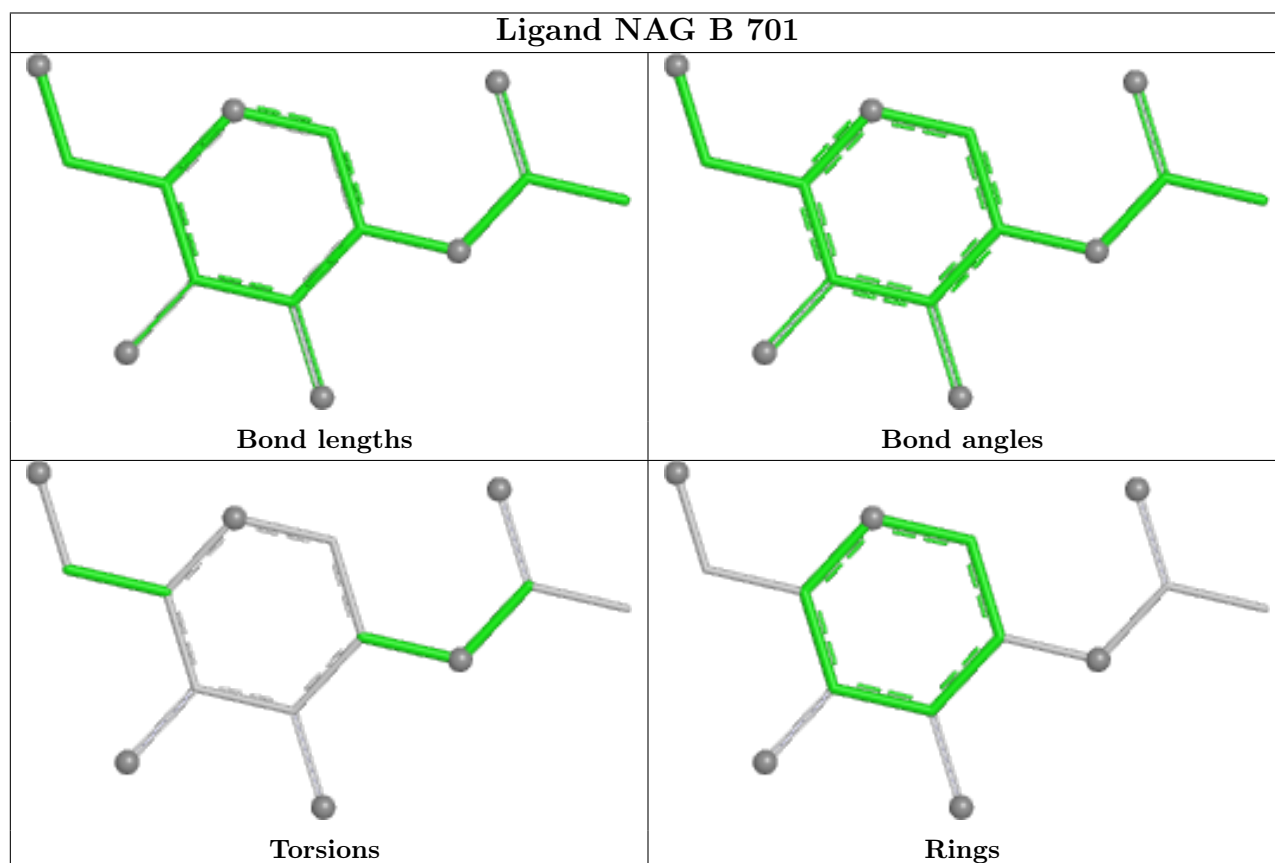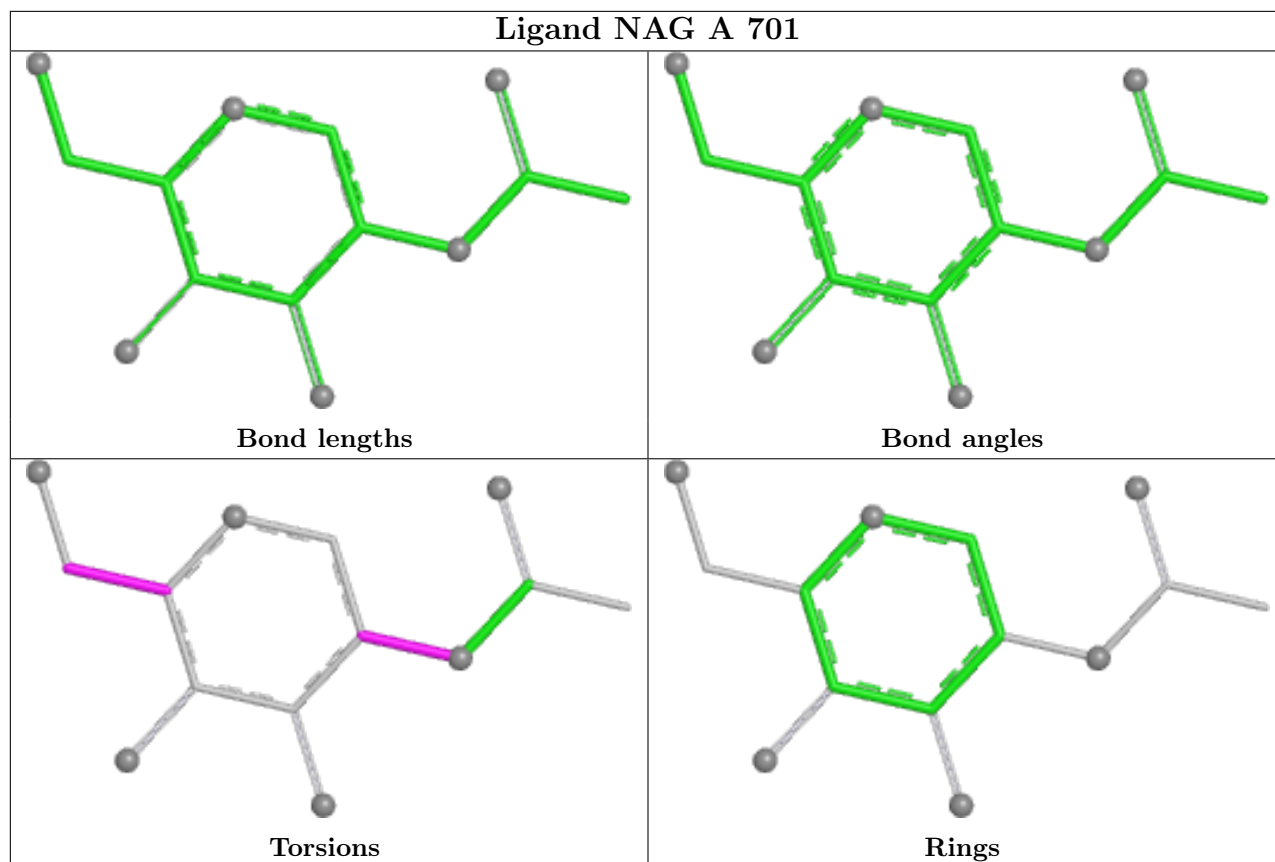
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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 E:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
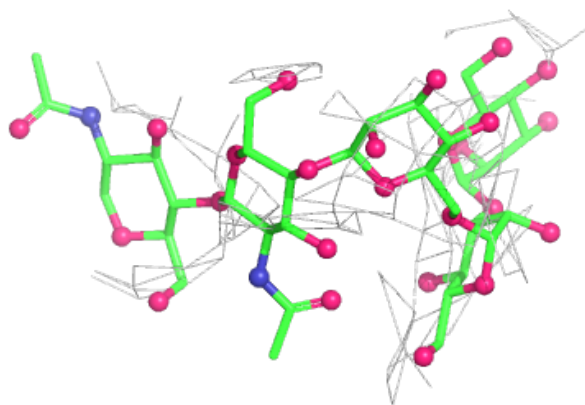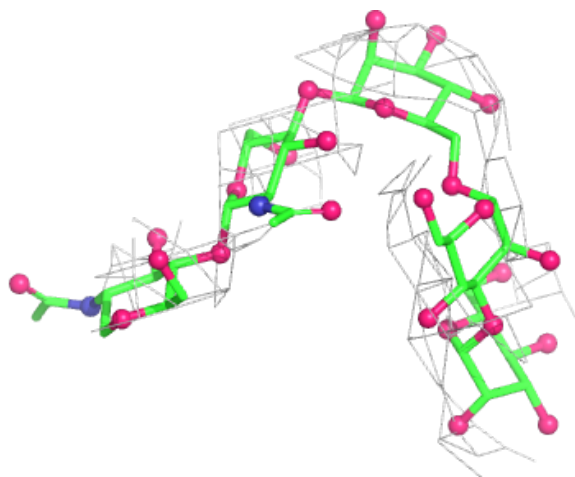$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
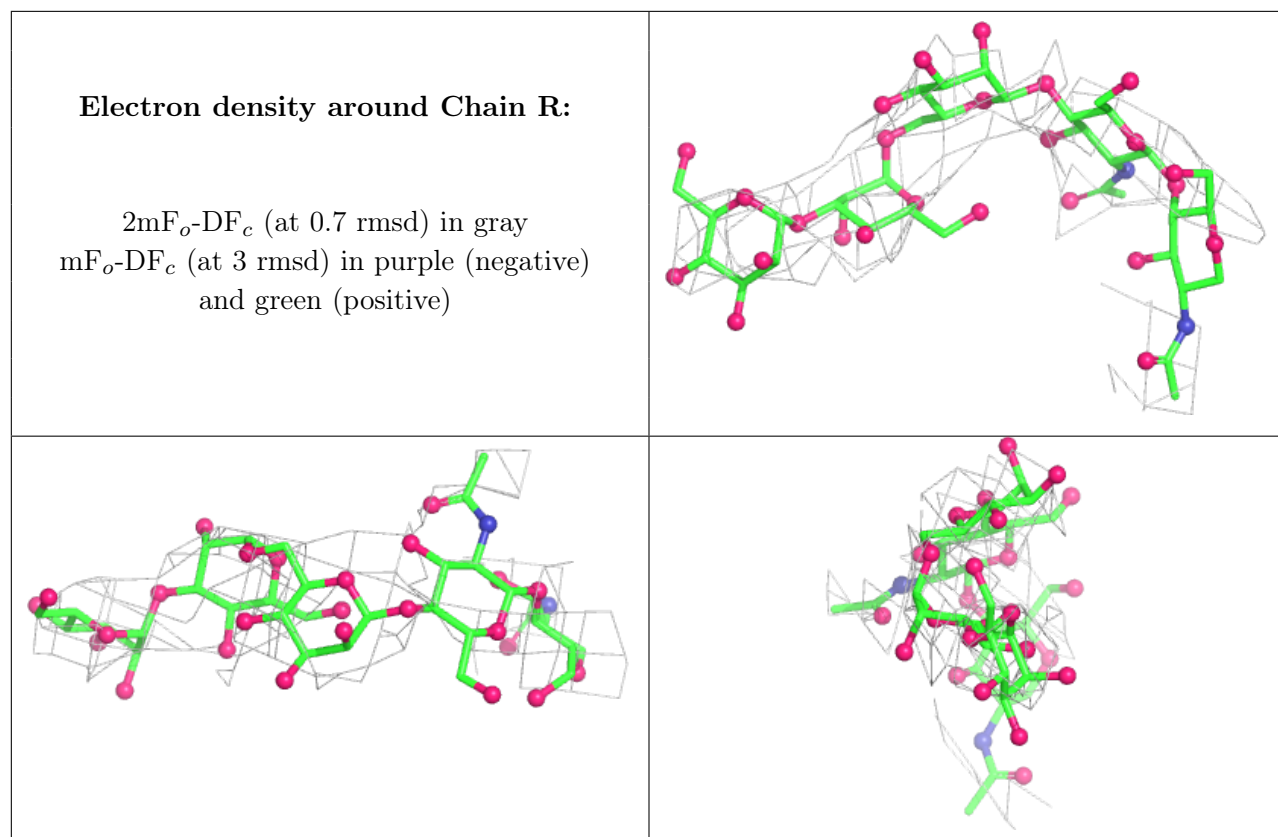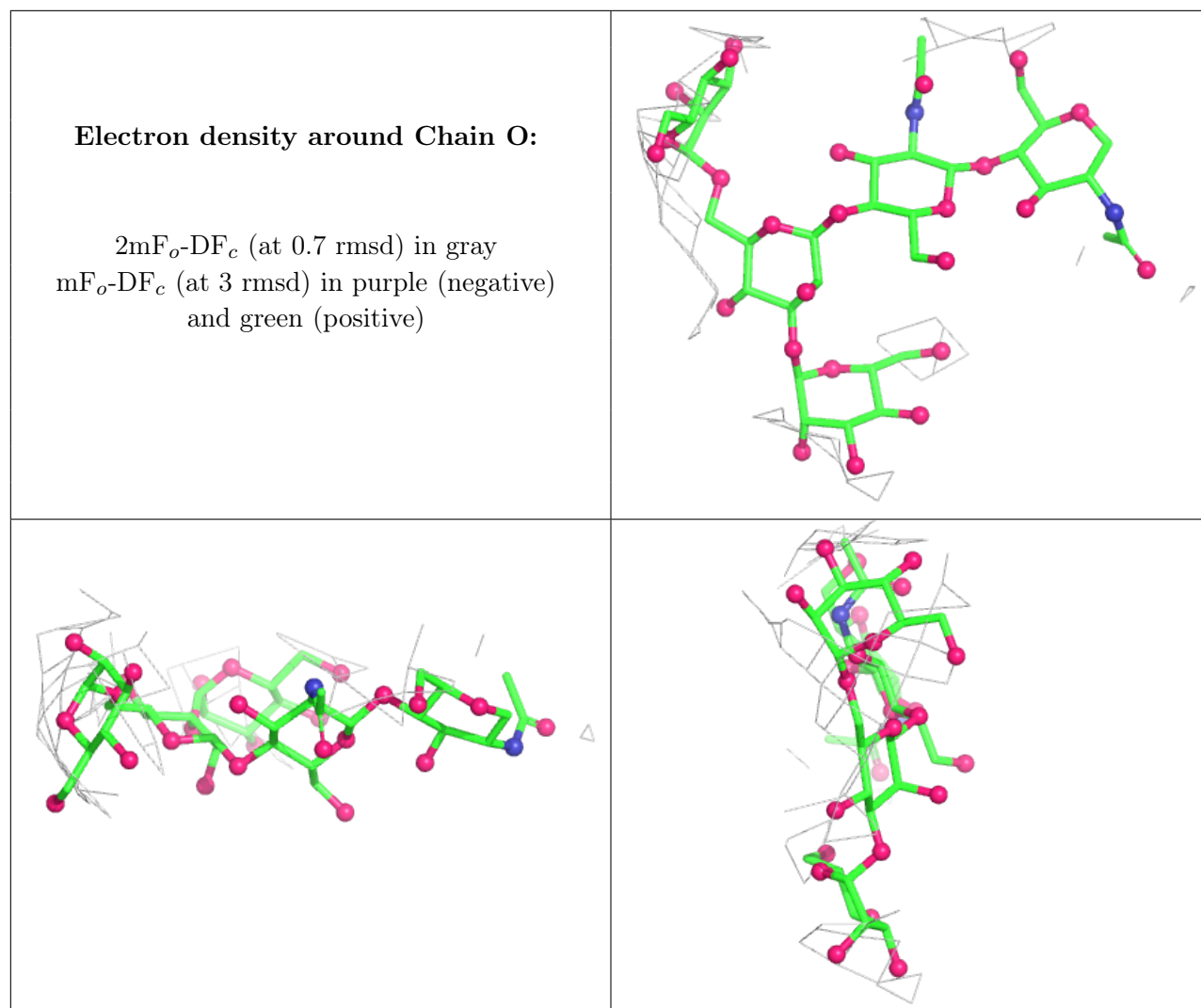and green (positive)
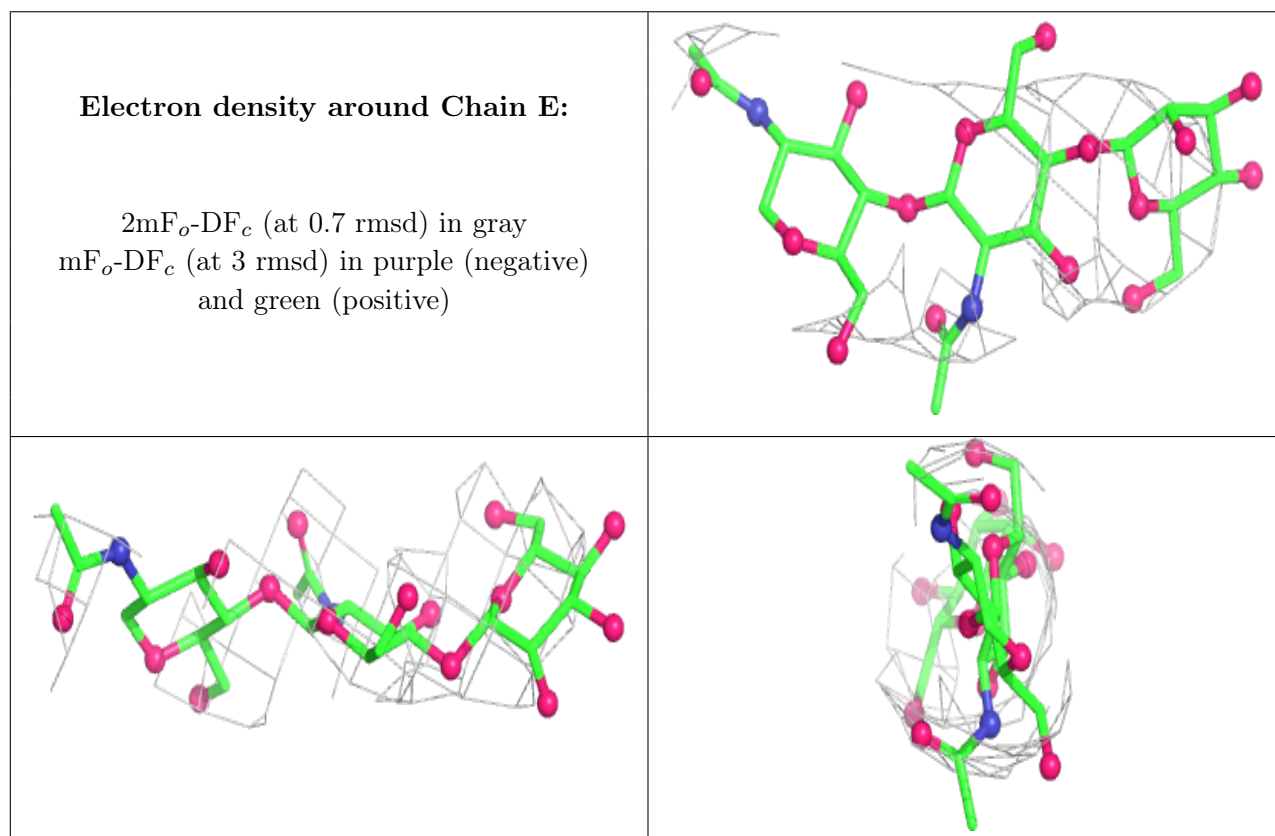
Electron density around Chain F:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
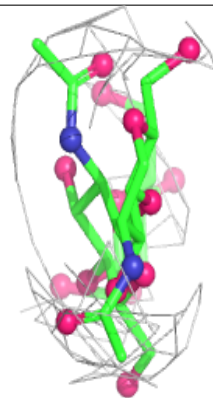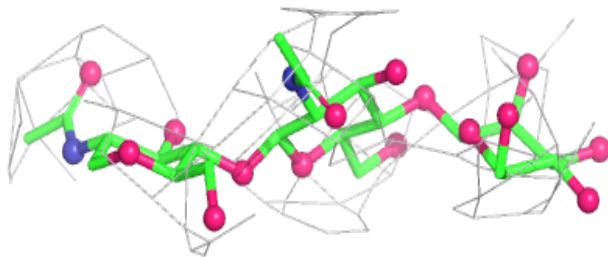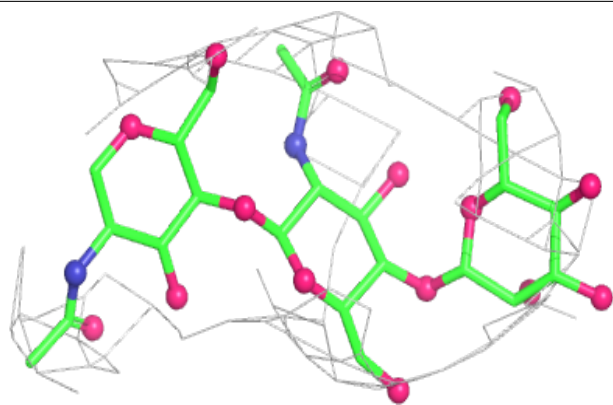
Electron density around Chain H:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
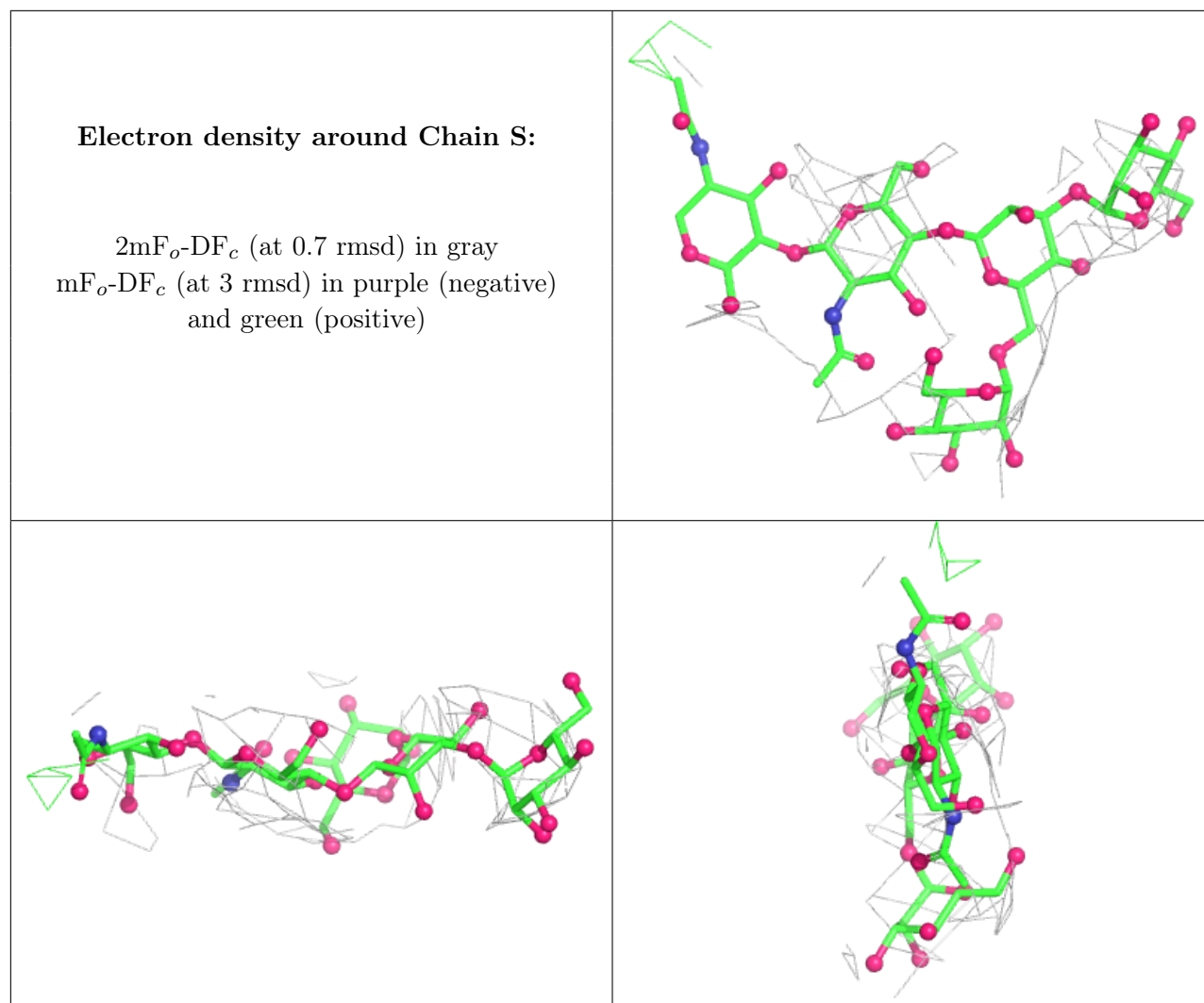$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
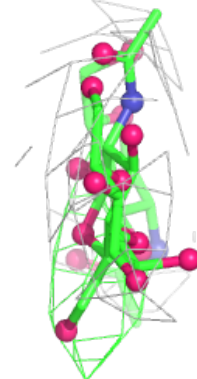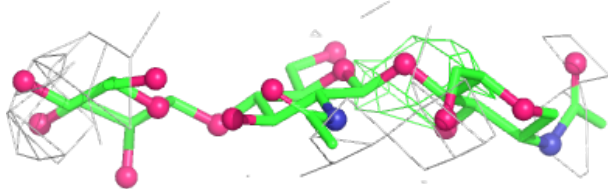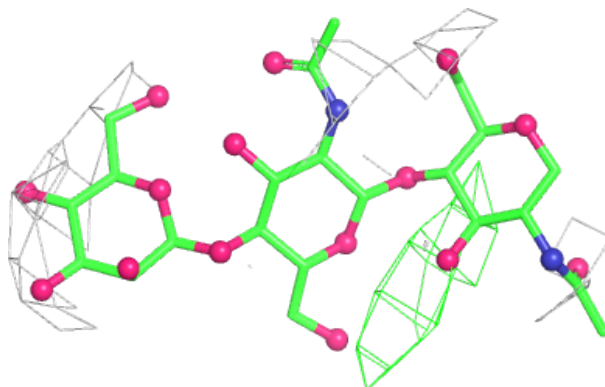
Electron density around Chain G:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
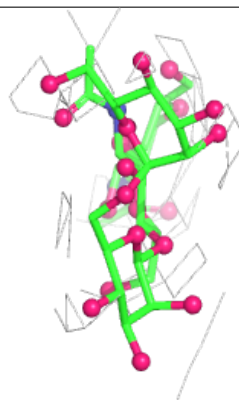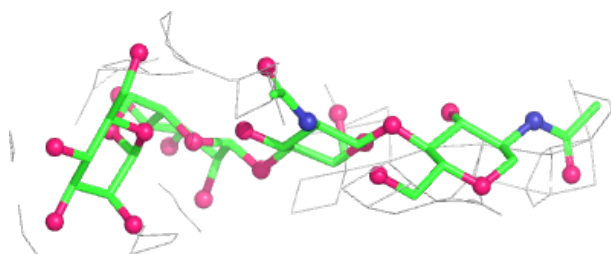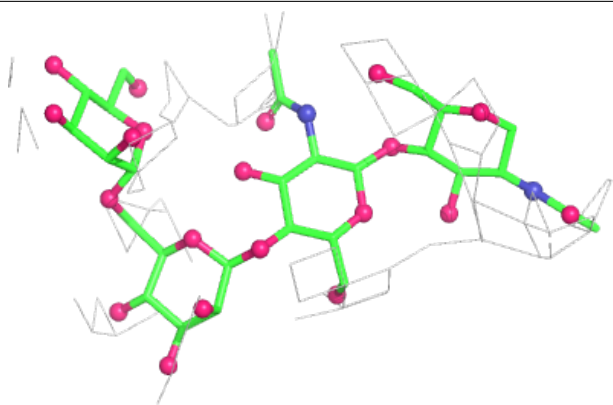
Electron density around Chain P:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
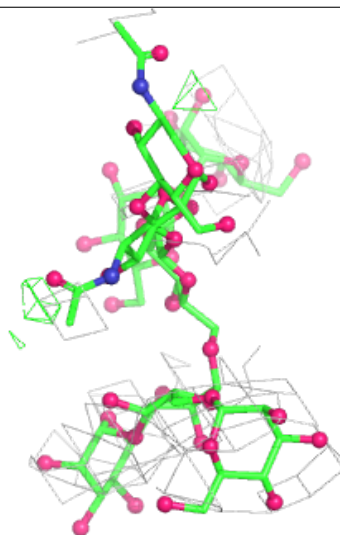and green (positive)

Electron density around Chain I:

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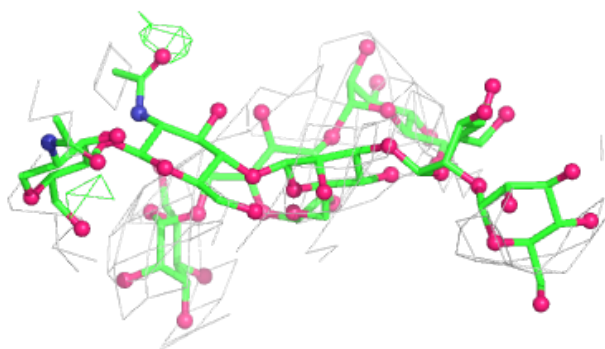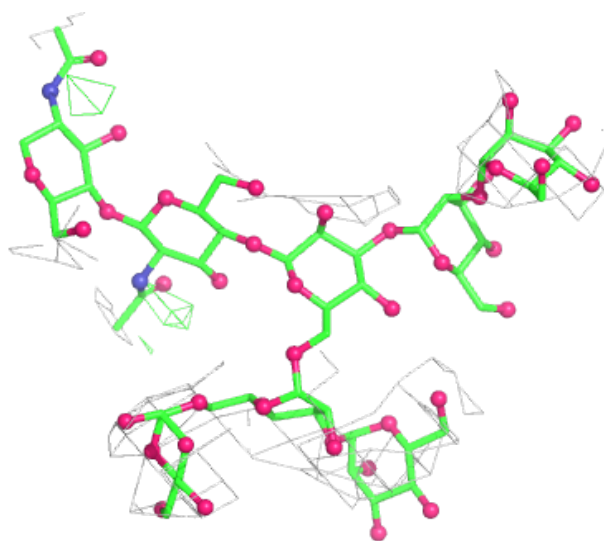and green (positive)

Electron density around Chain J:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
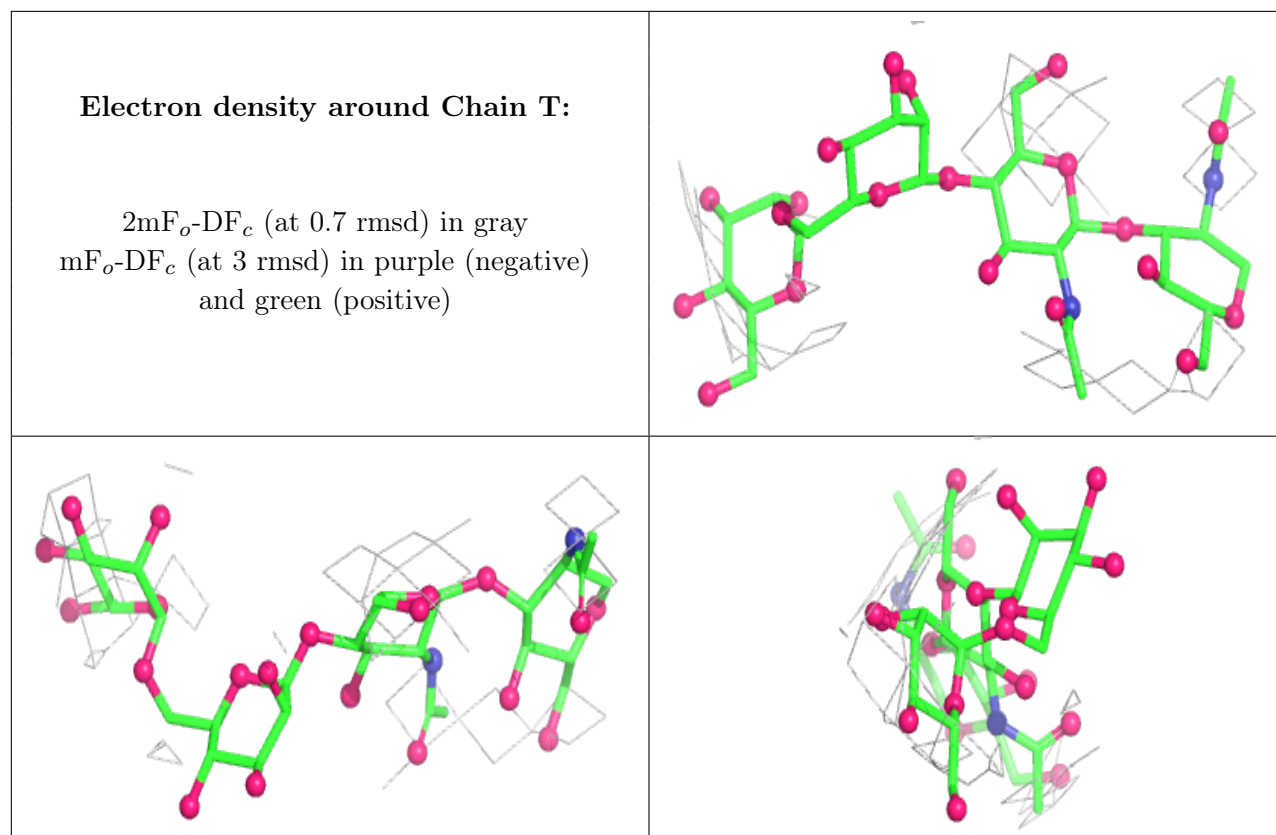mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
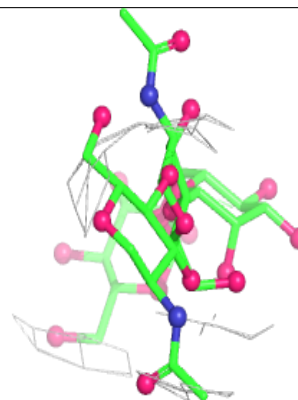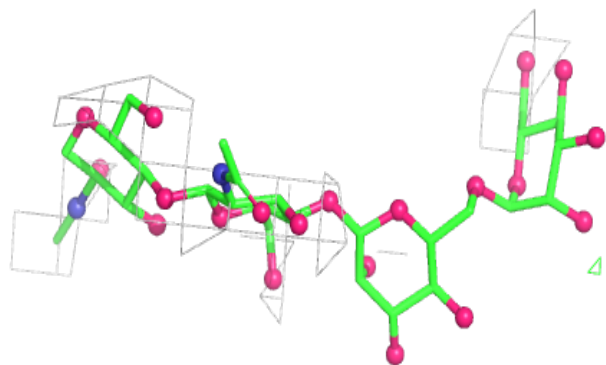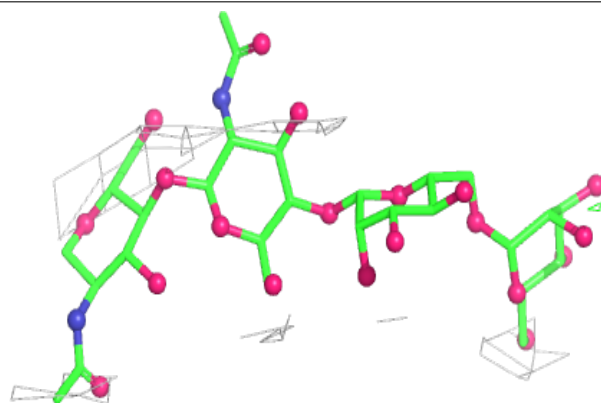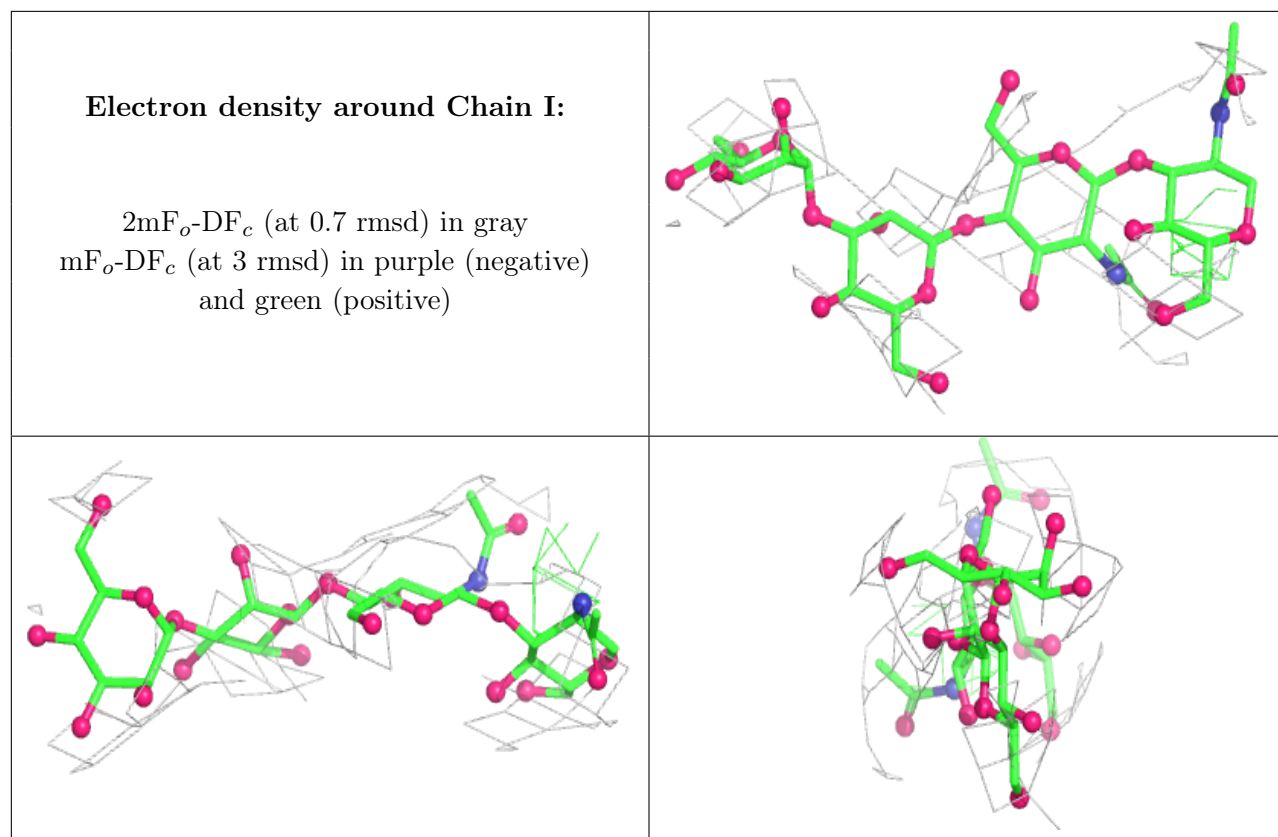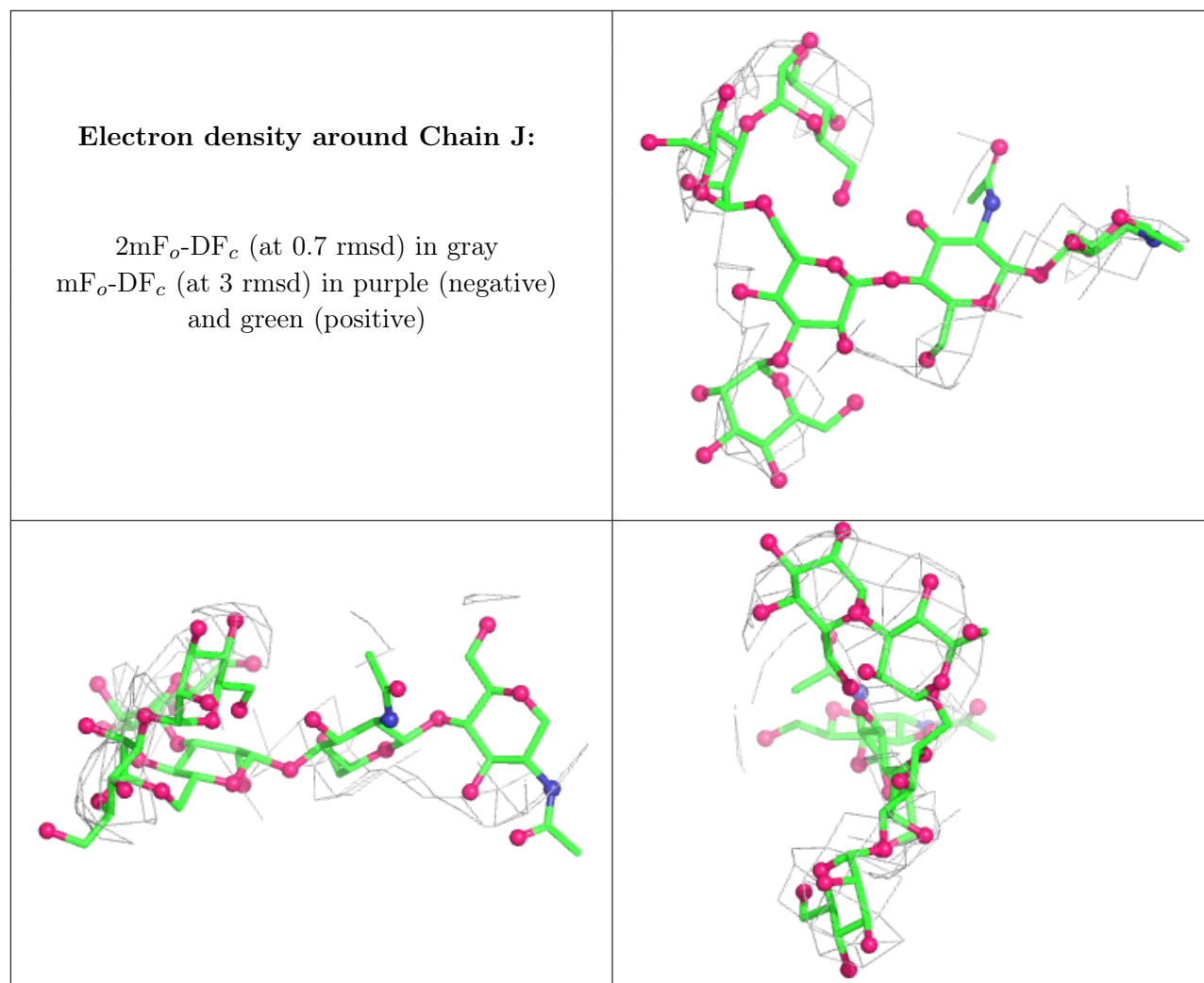
Electron density around Chain K:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
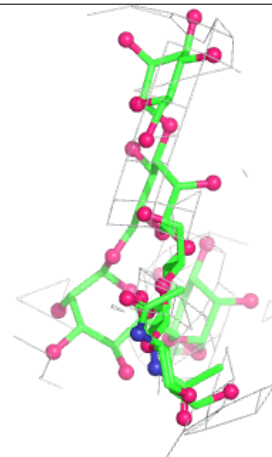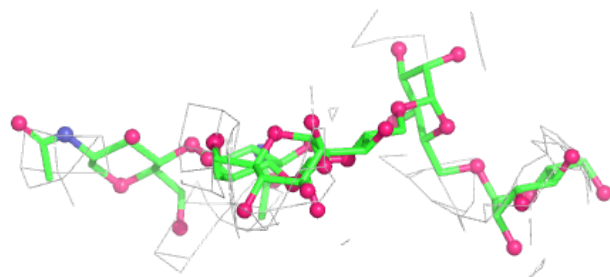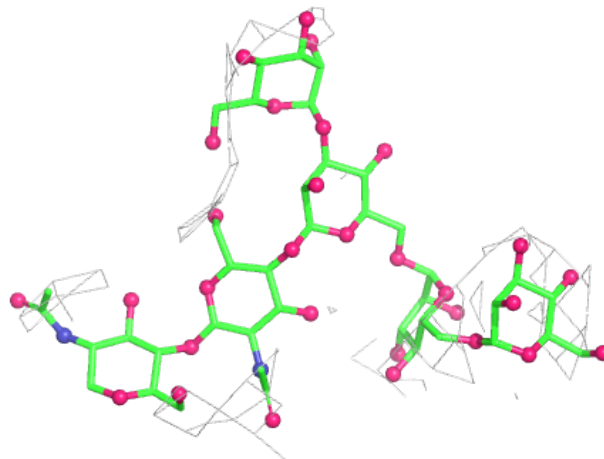
Electron density around Chain L:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
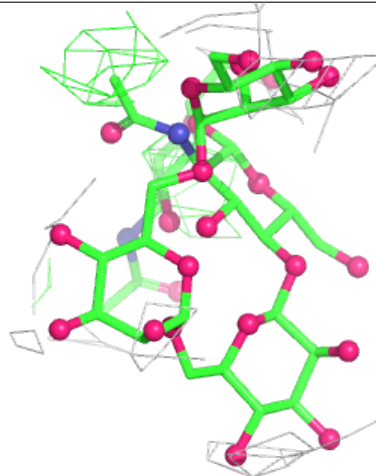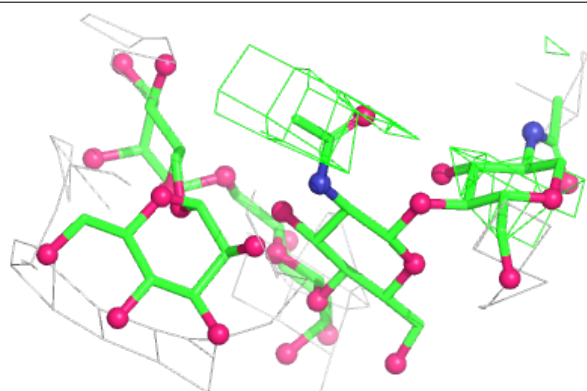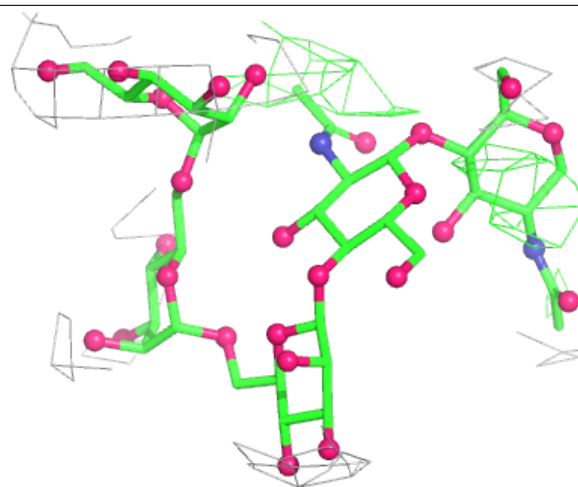
Electron density around Chain M:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
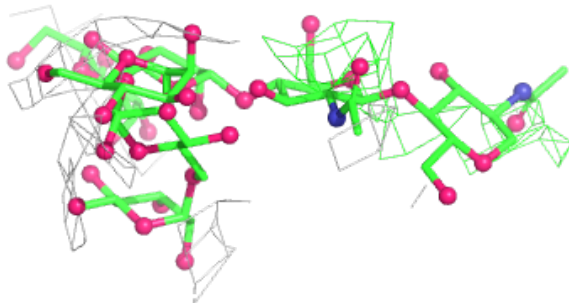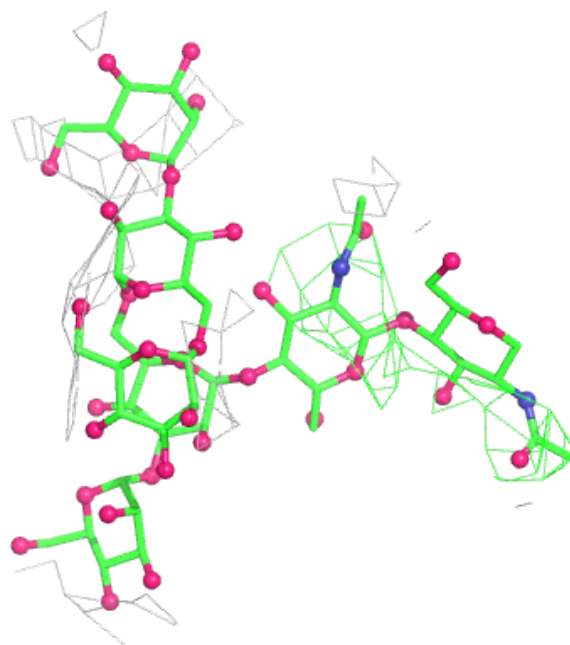
Electron density around Chain N:

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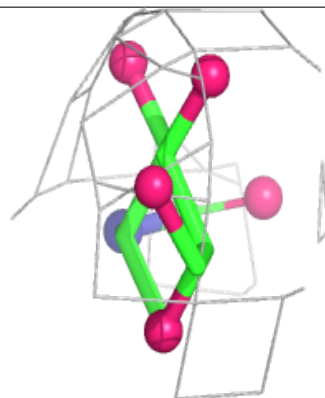mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around Chain R:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

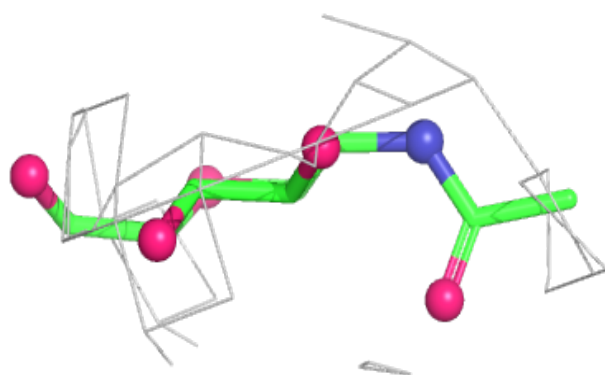**Electron density around Chain O:**

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

Electron density around Chain S:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
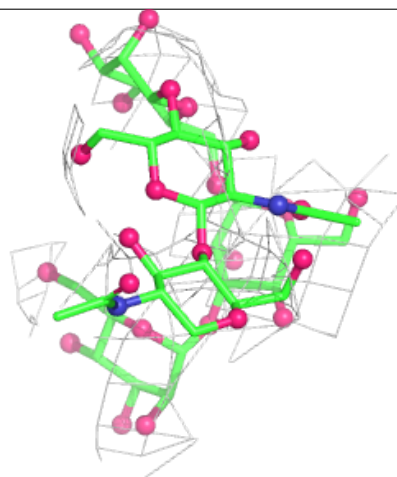
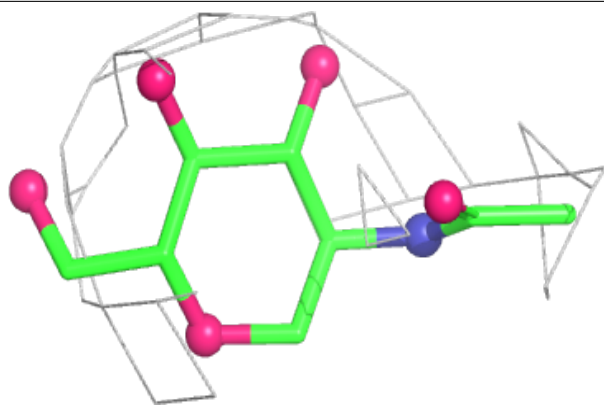**Electron density around Chain Q:**

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

Electron density around Chain T:

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

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.
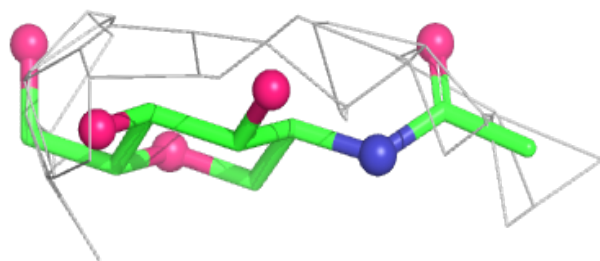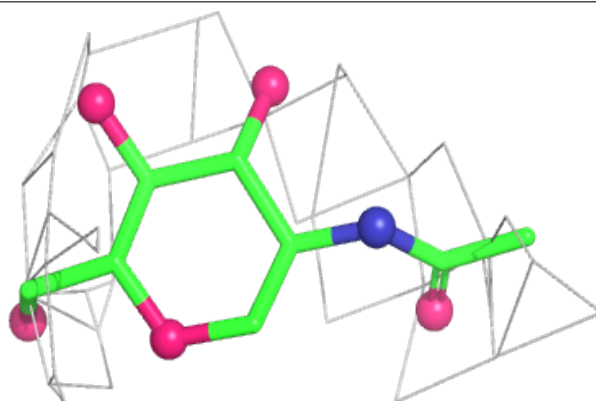
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAG A 701:

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

Electron density around NAG B 701:

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

6.5 Other polymers ⓘ

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