WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Oct 8, 2023 – 11:39 PM EDT

PDB ID	:	6WOQ
Title	:	Structure of Hepatitis C Virus Envelope Glycoprotein E2 core from genotype 1a bound to neutralizing antibody HC1AM and non neutralizing antibody E1
Authors	:	Tzarum, N.; Wilson, I.A.; Law, M.
Deposited on	:	2020-04-25
Resolution	:	3.67 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:

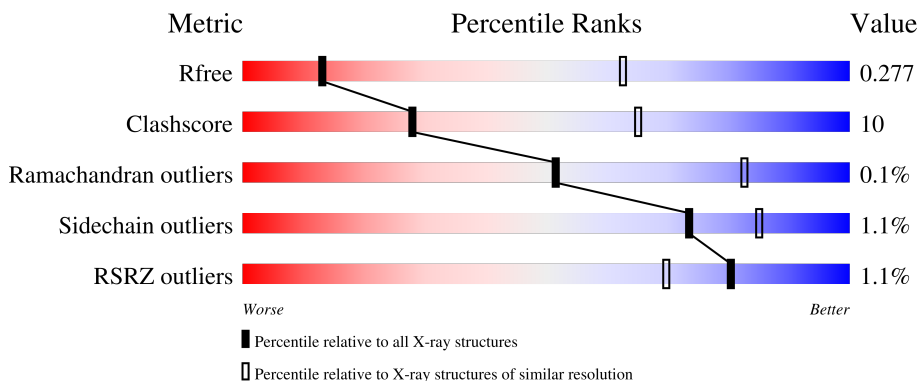|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.67 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		0.277
Clashscore		10
Ramachandran outliers		0.1%
Sidechain outliers		1.1%
RSRZ outliers		1.1%

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	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)
RSRZ outliers	127900	1441 (3.82-3.50)

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% 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	227	78% 16% 5%
1	C	227	% 68% 16% 16%
2	B	221	78% 20% ·
2	D	221	75% 23% ··
3	E	191	% 48% 24% 28%

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Mol	Chain	Length	Quality of chain
3	F	191	2% / 46% / 19% / 35%
4	G	229	73% / 19% / 7%
4	J	229	69% / 24% / 5%
5	H	215	6% / 77% / 13% / 9%
5	K	215	82% / 16%
6	I	2	50% / 50%
6	L	2	50% / 50%
6	M	2	50% / 50%
6	N	2	50% / 50%
6	O	2	100%

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
6	NAG	N	2	-	-	-	X

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 14990 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 Fab E1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total 1597	C 1011	N 264	O 314	S 8	0	0	0
1	C	191	Total 1436	C 916	N 236	O 276	S 8	0	0	0

- Molecule 2 is a protein called Fab E1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total 1676	C 1049	N 290	O 332	S 5	0	0	0
2	D	217	Total 1676	C 1049	N 290	O 332	S 5	0	0	0

- Molecule 3 is a protein called Envelope glycoprotein E2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	137	Total 1065	C 681	N 183	O 189	S 12	0	0	0
3	F	125	Total 982	C 630	N 167	O 175	S 10	0	0	0

- Molecule 4 is a protein called Fab HC1AM heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	218	Total 1627	C 1031	N 275	O 315	S 6	0	0	0
4	G	213	Total 1597	C 1015	N 267	O 309	S 6	0	0	0

- Molecule 5 is a protein called Fab HC1AM light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	212	Total 1631	C 1020	N 285	O 322	S 4	0	0	0
5	H	195	Total 1521	C 960	N 259	O 298	S 4	0	0	0

- Molecule 6 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
6	I	2	Total 28	C 16	N 2	O 10	0	0	0
6	L	2	Total 28	C 16	N 2	O 10	0	0	0
6	M	2	Total 28	C 16	N 2	O 10	0	0	0
6	N	2	Total 28	C 16	N 2	O 10	0	0	0
6	O	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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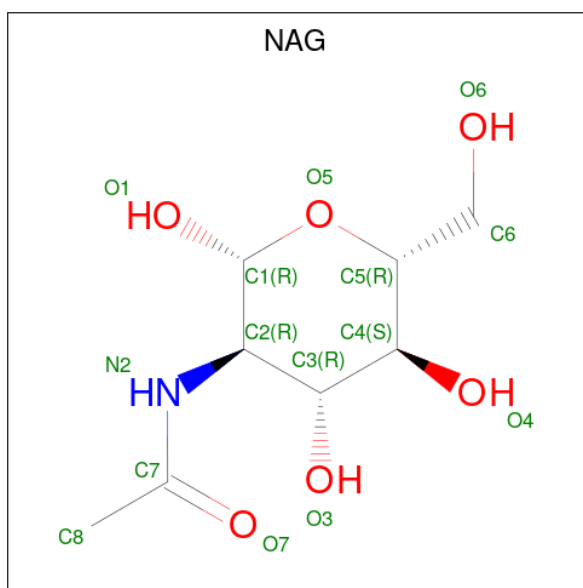
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total 14	C 8	N 1	O 5	0	0
7	F	1	Total 14	C 8	N 1	O 5	0	0
7	G	1	Total 14	C 8	N 1	O 5	0	0

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 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.
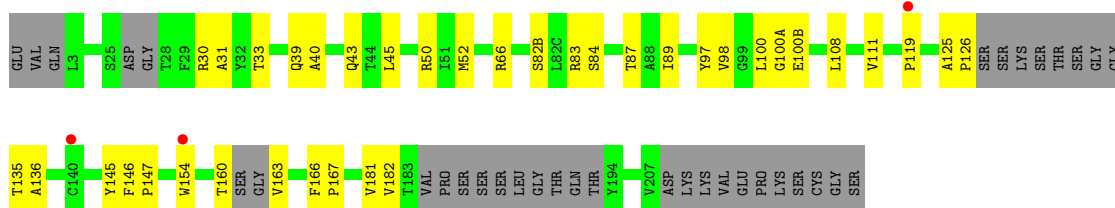
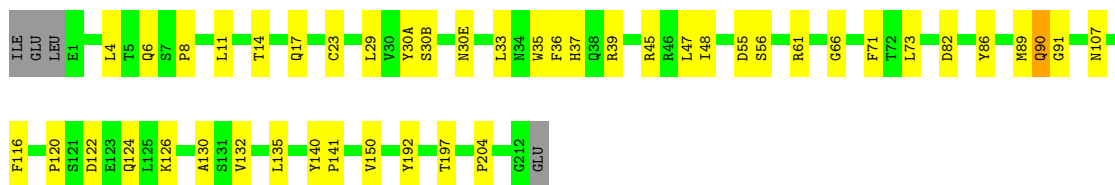• Molecule 1: Fab E1 heavy chain

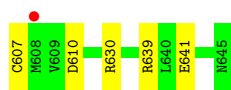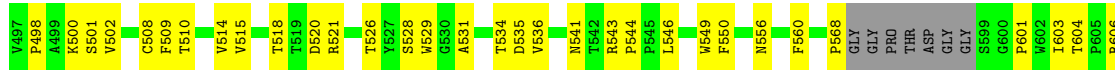Chain A:
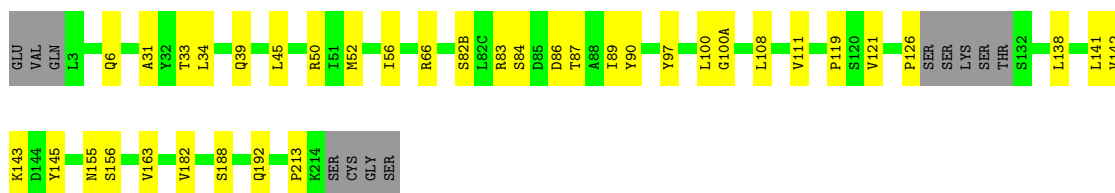
• Molecule 1: Fab E1 heavy chain

Chain C:

• Molecule 2: Fab E1 light chain

Chain B:

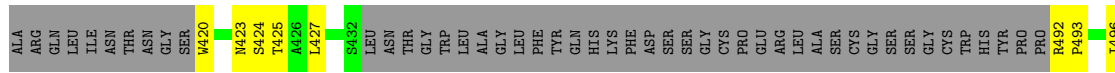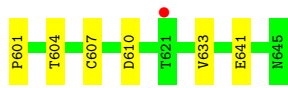• Molecule 2: Fab E1 light chain

Chain D:

F98 G101 T102 N107 P120 S121 D122 K126 S127 G128 V132 Y140 P141 K149 V150 T164 Y192 A193 T197 P204 G212 GLU

• Molecule 3: Envelope glycoprotein E2

Chain E:

%

48%   24%   28%

ALA ARG GLN LEU ILE ASN THR ASN GLY SER W420 N423 S424 T425 A426 L427 S432 LEU ASN THR GLY TRP LEU ALA GLY LEU PHE TYR GLN HIS LYS PHE ASP SER SER GLY CYS PRO GLU LEU ALA SER CYS GLY SER SER GLY CYS TRP HIS TYR PRO PRO R492 P493 I496

V497 P498 A499 K500 S501 V502 C508 F509 T510 V514 V515 T518 T519 D520 R521 T526 Y527 S528 W529 G530 A531 T534 D535 V536 N541 T542 R543 P544 P545 L546 W549 F550 N556 F560 P568 GLY GLY PRO THR ASP GLY S599 G600 P601 W602 I603 T604 P605 R606

C607 M608 V609 D610 R630 R639 L640 E641 N645

• Molecule 3: Envelope glycoprotein E2

Chain F:

2%

46%   19%   35%

ALA ARG GLN LEU ILE ASN THR ASN GLY SER TRP H421 I422 N423 S424 N428 E431 SER LEU ASN THR GLY TRP LEU ALA GLY LEU PHE TYR GLN HIS LYS PHE ASP SER SER GLY CYS PRO GLU LEU ARG LEU ALA SER CYS GLY SER SER GLY CYS TRP HIS TYR PRO PRO ARG PRO CYS

GLY I496 V497 P498 A499 V502 C503 C508 F509 T510 V514 T518 T519 D520 R521 S522 G523 T526 Y527 S528 N532 D533 T534 D535 V536 R543 P544 P545 L546 W549 W554 M555 F560 T561 K562 V563 CYS GLY ALA PRO PRO GLY GLY PRO THR ASP GLY SER G600

P601 T604 C607 D610 T621 V633 E641 N645

• Molecule 4: Fab HC1AM heavy chain

Chain J:

69%   24%   • 5%

Q1 L4 V5 Q6 S7 K19 V20 S21 C22 K23 A24 SER GLY GLY THR TYR ASN G31 E32 V33 I34 S35 W36 A40 E43 W47 L48 G49 V50 F51 I52 F54 D58 Y59 A60 Q61 K62 F63 V67 T68 I69 S70 R73 T74 T75 S76 T77 T78 Y79 M80

R83 D86 T87 K94 V95 L96 Q97 V98 G99 R100 N100A L100B V100C V100D R100E P100F L100G D101 Q105 T110 P123 P126 L138 V184 T193 Y194 K209 K210 P213 LYS SER CYS GLY SER

• Molecule 4: Fab HC1AM heavy chain

Chain G:

73%   19%   7%

Q1 L4 V5 Q6 S7 V20 S21 C22 K23 A24 SER GLY GLY THR TYR ASN GLY E32 A40 P41 GLY E43 L48 F51 I52 P52A D58 Y59 F63 I69 S70 R73 T74 T75 S76 T77 T78 Y79 R83 S84 E85 D86 T87 A93 K94 V95 L96 GLN VAL

GLY ARG N100A V100D R100E P100F L100G D101 L102 Q105 L108 V109 T110 P126 L138 E148 T193 Y194 K210 K214 SER CYS GLY SER

• Molecule 5: Fab HC1AM light chain

Chain K:

82%   16%

E1 I2 I10 R18 R27 T28 I29 S30 R30A T31 H32 L33 Q37 P40 L47 I48 Y49 G50 V51 I56 P59 D60 R61 I75 D82 Y86 H89 Q90 TYR G92 T97 F98 K103 L104 R108 T109 E123 W148 K149 E165 Q166 D167

S168 L179 A193 G212 GLU CYS

• Molecule 5: Fab HC1AM light chain

Chain H:

6%

77%   13%   ·   9%

E1 P15 GLY GLU ARG A19 T20 L21 A25 S26 R27 T28 Q37 P40 R45 L46 L47 I48 Y49 G50 VAL SER SER R54 P59 D60 R61 F62 SER GLY SER GLY S67 T74 ILE SER ARG LEU E79 D82 F83 A84 V85 Y86 H89 Q90 Y91 G92 N93 S94 P95

Q96 T97 F98 G99 Q100 GLY THR K103 L104 R108 T109 K149 N152 E165 Q166 D167 S168 S171 K190 V191 Y192 A193 N210 ARG GLY GLU CYS
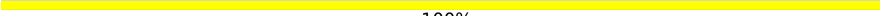
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain I:

50%   50%

NAG1 NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain L:

50%   50%

NAG1 NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain M:

50%   50%

NAG1 NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain N:

50%   50%

NAG1 NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain O:

100%

NAG1 NAG2

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	200.74Å 103.72Å 196.15Å 90.00° 113.65° 90.00°	Depositor
Resolution (Å)	34.66 – 3.67 34.66 – 3.67	Depositor EDS
% Data completeness (in resolution range)	82.2 (34.66-3.67) 82.2 (34.66-3.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 3.66Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.227 , 0.277 0.228 , 0.277	Depositor DCC
R_{free} test set	1589 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	110.9	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 61.3	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	14990	wwPDB-VP
Average B, all atoms (Å^2)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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 ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.26	0/1634	0.46	0/2224
1	C	0.25	0/1468	0.46	0/1996
2	B	0.25	0/1715	0.45	0/2331
2	D	0.28	0/1715	0.47	0/2331
3	E	0.28	0/1103	0.50	1/1514 (0.1%)
3	F	0.30	0/1015	0.50	1/1392 (0.1%)
4	G	0.25	0/1630	0.46	0/2218
4	J	0.25	0/1662	0.47	0/2264
5	H	0.25	0/1552	0.44	0/2102
5	K	0.28	0/1665	0.46	0/2257
All	All	0.26	0/15159	0.46	2/20629 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	510	THR	C-N-CD	-5.03	109.53	120.60
3	E	510	THR	C-N-CD	-5.03	109.54	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

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	1597	0	1582	22	0
1	C	1436	0	1421	22	0
2	B	1676	0	1629	25	0
2	D	1676	0	1629	43	0
3	E	1065	0	993	42	0
3	F	982	0	926	32	0
4	G	1597	0	1609	31	0
4	J	1627	0	1637	52	0
5	H	1521	0	1485	24	0
5	K	1631	0	1603	27	0
6	I	28	0	25	1	0
6	L	28	0	25	6	0
6	M	28	0	25	2	0
6	N	28	0	25	5	0
6	O	28	0	25	2	0
7	E	14	0	13	0	0
7	F	14	0	12	0	0
7	G	14	0	13	0	0
All	All	14990	0	14677	295	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 10.

The worst 5 of 295 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)
3:E:531:ALA:HB2	4:J:100(D):VAL:HG21	1.42	0.98
3:F:424:SER:O	3:F:518:THR:HG23	1.63	0.97
3:F:423:ASN:HB3	3:F:527:TYR:HB3	1.53	0.87
5:K:29:ILE:O	5:K:29:ILE:HG22	1.78	0.81
3:E:534:THR:CG2	6:L:1:NAG:HN2	1.96	0.79

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	211/227 (93%)	204 (97%)	7 (3%)	0	100	100
1	C	181/227 (80%)	174 (96%)	7 (4%)	0	100	100
2	B	215/221 (97%)	208 (97%)	7 (3%)	0	100	100
2	D	215/221 (97%)	212 (99%)	3 (1%)	0	100	100
3	E	131/191 (69%)	120 (92%)	11 (8%)	0	100	100
3	F	119/191 (62%)	109 (92%)	10 (8%)	0	100	100
4	G	205/229 (90%)	195 (95%)	10 (5%)	0	100	100
4	J	214/229 (93%)	204 (95%)	10 (5%)	0	100	100
5	H	183/215 (85%)	177 (97%)	6 (3%)	0	100	100
5	K	208/215 (97%)	200 (96%)	7 (3%)	1 (0%)	29	66
All	All	1882/2166 (87%)	1803 (96%)	78 (4%)	1 (0%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	K	51	VAL

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	179/190 (94%)	179 (100%)	0	100	100
1	C	160/190 (84%)	158 (99%)	2 (1%)	69	82
2	B	190/194 (98%)	187 (98%)	3 (2%)	62	79
2	D	190/194 (98%)	187 (98%)	3 (2%)	62	79
3	E	118/159 (74%)	118 (100%)	0	100	100
3	F	109/159 (69%)	107 (98%)	2 (2%)	59	77
4	G	183/193 (95%)	182 (100%)	1 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	J	185/193 (96%)	180 (97%)	5 (3%)	44	68
5	H	171/186 (92%)	169 (99%)	2 (1%)	71	84
5	K	183/186 (98%)	183 (100%)	0	100	100
All	All	1668/1844 (90%)	1650 (99%)	18 (1%)	73	85

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	534	THR
5	H	91	TYR
5	H	28	THR
1	C	98	VAL
3	F	422	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
5	K	90	GLN
2	D	34	ASN
5	H	90	GLN
5	H	37	GLN
5	K	89	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

10 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	$\#|Z| > 2$
6	NAG	I	1	6	14,14,15	0.55	0	17,19,21	0.59	0
6	NAG	I	2	6	14,14,15	0.35	0	17,19,21	0.45	0
6	NAG	L	1	6,3	14,14,15	0.33	0	17,19,21	0.71	0
6	NAG	L	2	6	14,14,15	0.38	0	17,19,21	0.38	0
6	NAG	M	1	6,3	14,14,15	0.37	0	17,19,21	0.90	1 (5%)
6	NAG	M	2	6	14,14,15	0.22	0	17,19,21	0.41	0
6	NAG	N	1	6	14,14,15	0.37	0	17,19,21	0.55	0
6	NAG	N	2	6	14,14,15	0.40	0	17,19,21	0.41	0
6	NAG	O	1	6,3	14,14,15	0.41	0	17,19,21	0.49	0
6	NAG	O	2	6	14,14,15	0.36	0	17,19,21	0.55	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
6	NAG	I	1	6	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
6	NAG	L	1	6,3	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1
6	NAG	M	1	6,3	-	4/6/23/26	0/1/1/1
6	NAG	M	2	6	-	1/6/23/26	0/1/1/1
6	NAG	N	1	6	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	0/6/23/26	0/1/1/1
6	NAG	O	1	6,3	-	0/6/23/26	0/1/1/1
6	NAG	O	2	6	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	1	NAG	C2-N2-C7	-2.59	119.22	122.90

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	O	2	NAG	O5-C5-C6-O6
6	M	1	NAG	C1-C2-N2-C7
6	M	2	NAG	O5-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6
6	M	1	NAG	C8-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	1	NAG	2	0
6	N	1	NAG	5	0
6	O	2	NAG	1	0
6	I	1	NAG	1	0
6	O	1	NAG	1	0
6	L	1	NAG	6	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 I

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 O

Bond lengths   Bond angles   Torsions   Rings
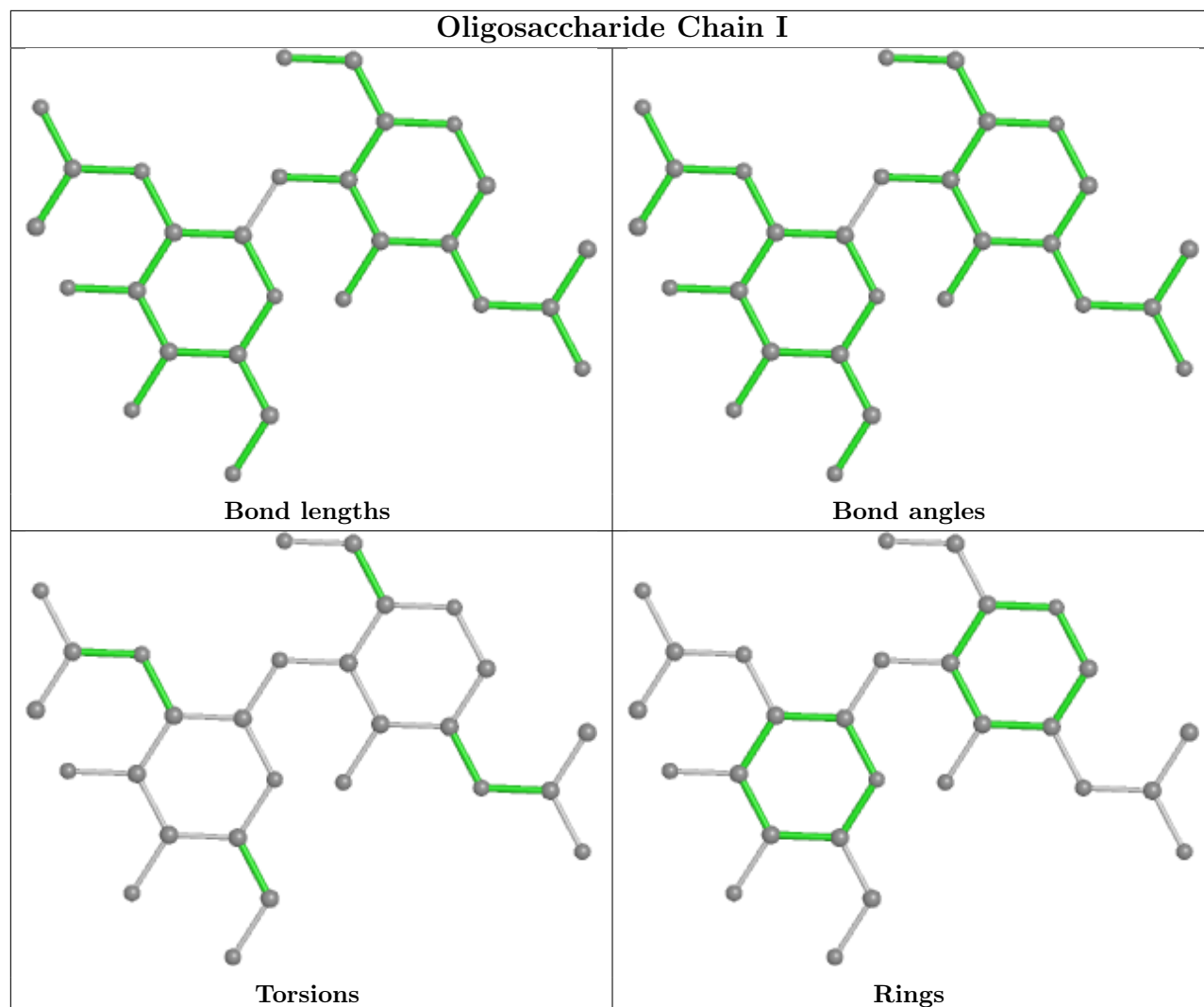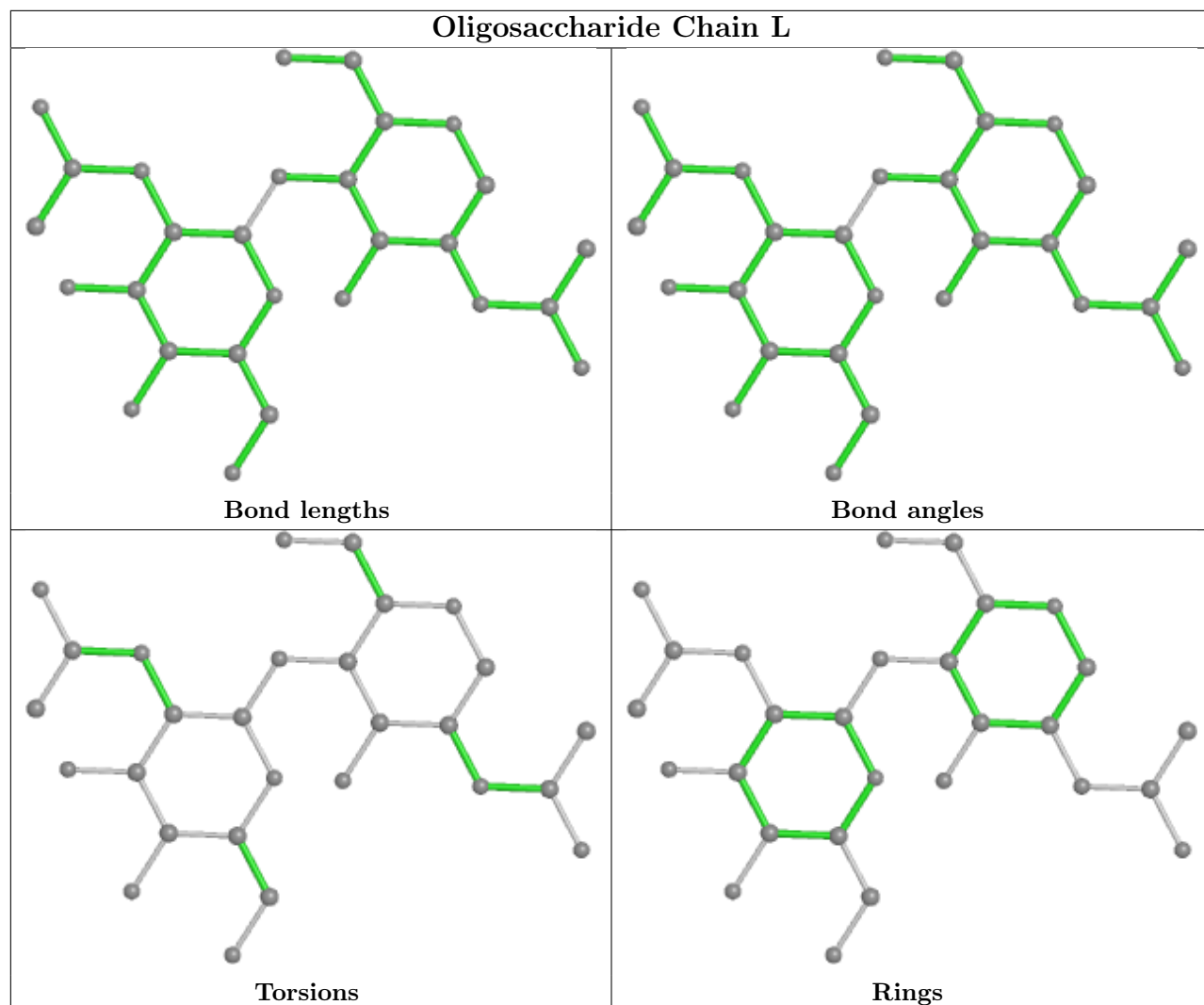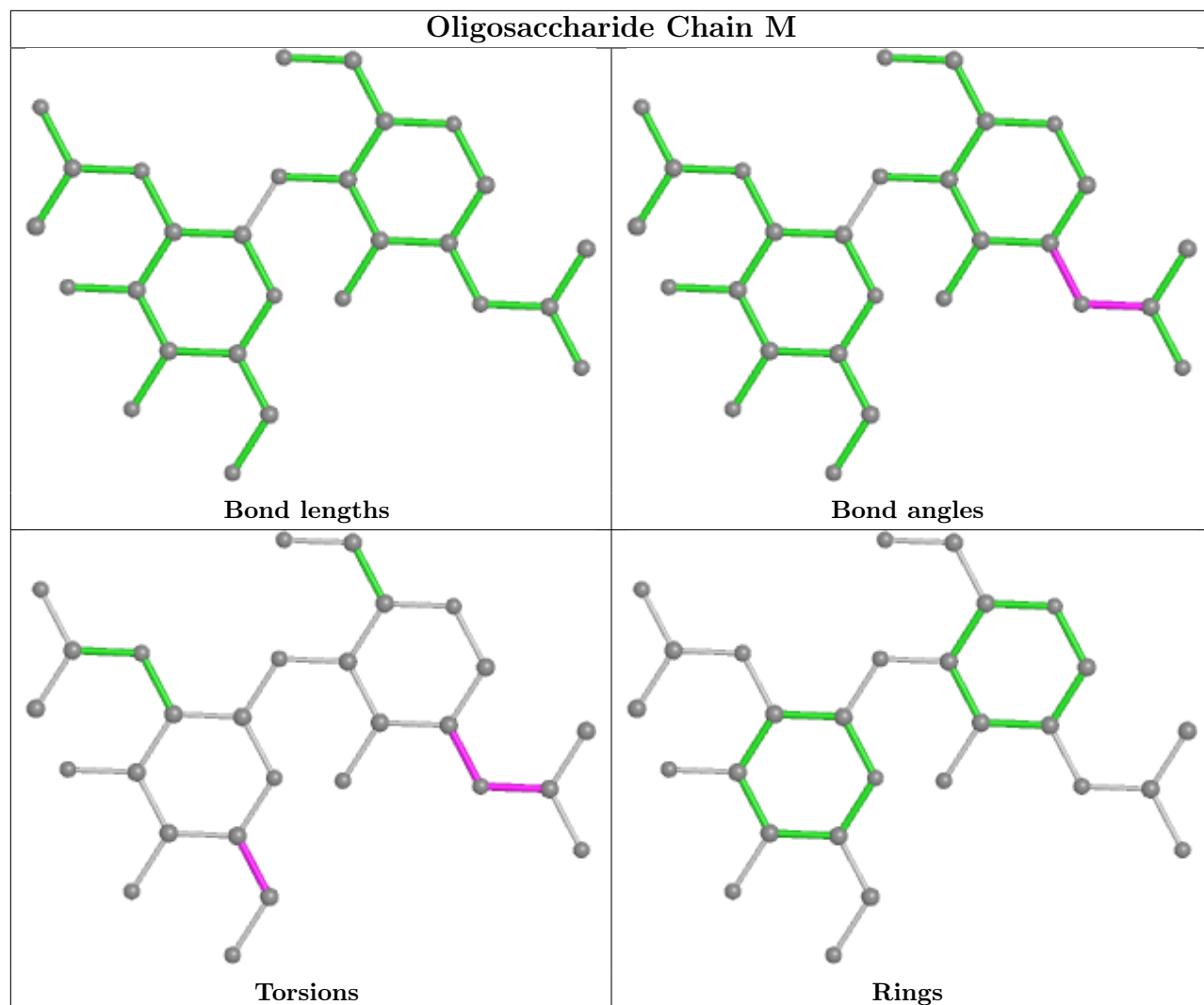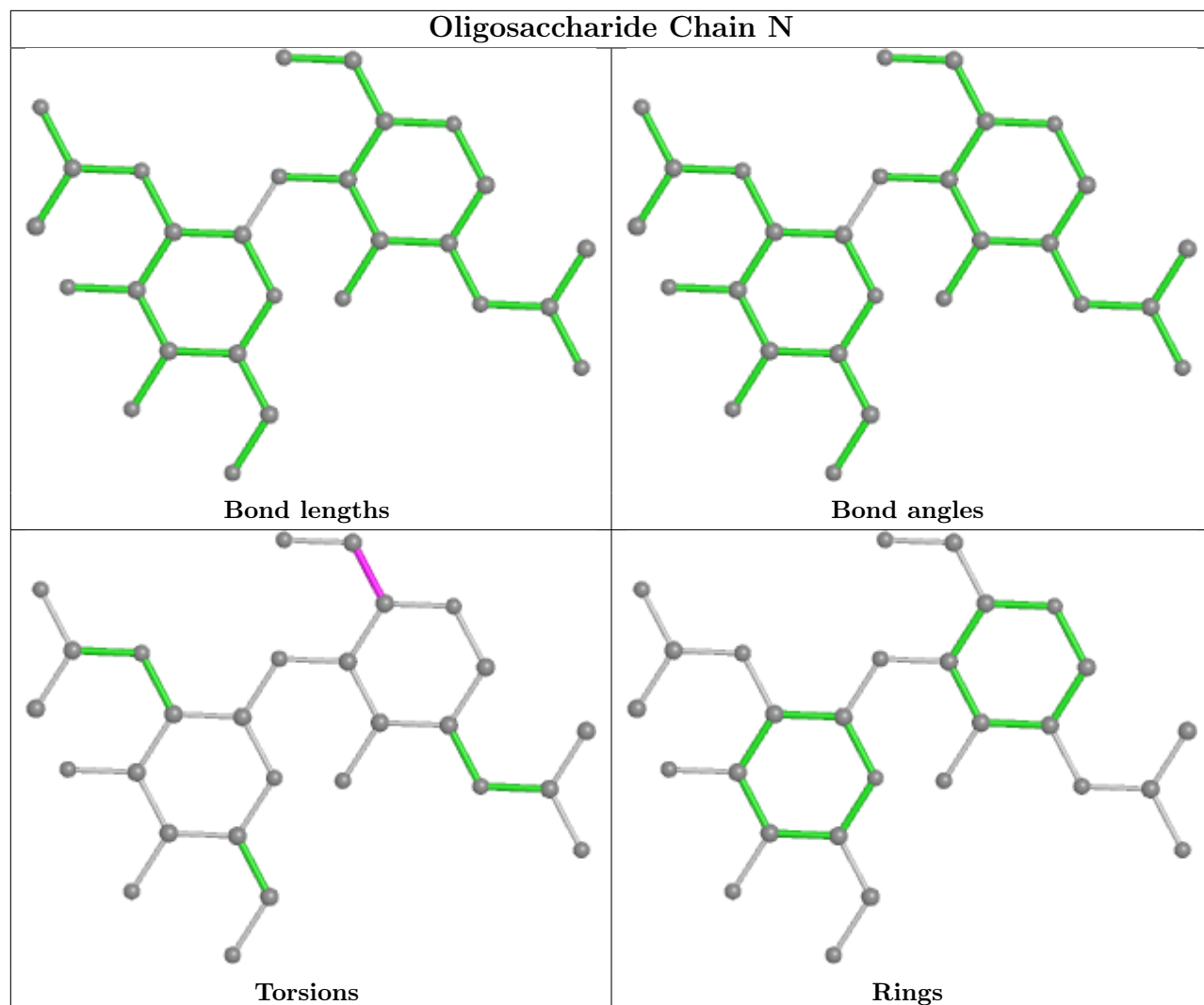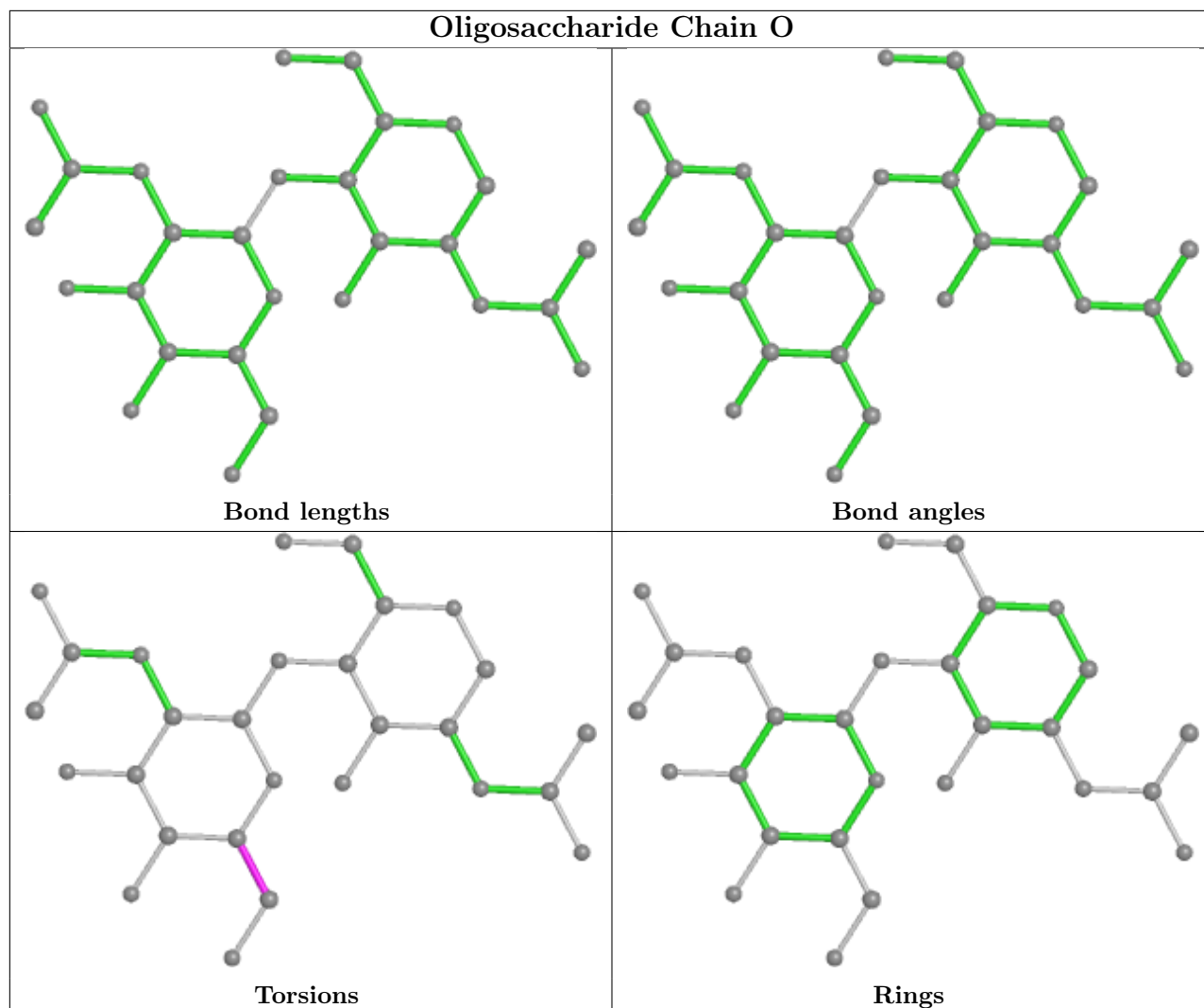
5.6 Ligand geometry ⓘ

3 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	#$|Z| > 2$
7	NAG	E	705	3	14,14,15	0.28	0	17,19,21	0.44	0
7	NAG	F	901	3	14,14,15	0.86	1 (7%)	17,19,21	0.97	1 (5%)
7	NAG	G	301	-	14,14,15	0.34	0	17,19,21	0.37	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
7	NAG	E	705	3	-	0/6/23/26	0/1/1/1
7	NAG	F	901	3	-	2/6/23/26	0/1/1/1
7	NAG	G	301	-	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	901	NAG	O5-C1	-3.13	1.38	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	901	NAG	C1-O5-C5	-3.06	108.04	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	901	NAG	C4-C5-C6-O6
7	F	901	NAG	O5-C5-C6-O6
7	G	301	NAG	C4-C5-C6-O6
7	G	301	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	215/227 (94%)	-0.22	0	100	100	52, 102, 137, 158	0
1	C	191/227 (84%)	0.06	3 (1%)	72	59	97, 144, 178, 205	0
2	B	217/221 (98%)	-0.33	0	100	100	40, 95, 134, 156	0
2	D	217/221 (98%)	0.15	1 (0%)	91	85	65, 153, 183, 218	0
3	E	137/191 (71%)	-0.01	1 (0%)	87	80	71, 120, 152, 170	0
3	F	125/191 (65%)	0.27	4 (3%)	47	34	83, 147, 170, 178	0
4	G	213/229 (93%)	-0.13	1 (0%)	91	85	89, 129, 162, 181	0
4	J	218/229 (95%)	-0.35	0	100	100	60, 101, 138, 185	0
5	H	195/215 (90%)	0.38	12 (6%)	20	13	99, 150, 189, 212	0
5	K	212/215 (98%)	-0.32	0	100	100	60, 99, 133, 158	0
All	All	1940/2166 (89%)	-0.07	22 (1%)	80	70	40, 122, 171, 218	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	119	PRO	3.6
5	H	25	ALA	3.5
5	H	191	VAL	3.4
5	H	103	LYS	3.4
5	H	192	TYR	3.3

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

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

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6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	I	2	14/15	0.77	0.26	143,182,210,216	0
6	NAG	N	2	14/15	0.77	0.44	154,182,204,208	0
6	NAG	N	1	14/15	0.79	0.25	144,167,199,205	0
6	NAG	L	2	14/15	0.79	0.37	159,172,216,232	0
6	NAG	I	1	14/15	0.83	0.23	93,141,170,172	0
6	NAG	L	1	14/15	0.87	0.18	124,142,173,199	0
6	NAG	O	2	14/15	0.88	0.28	155,163,179,199	0
6	NAG	M	2	14/15	0.90	0.28	132,153,185,189	0
6	NAG	O	1	14/15	0.92	0.26	155,175,188,192	0
6	NAG	M	1	14/15	0.93	0.21	101,130,163,163	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.
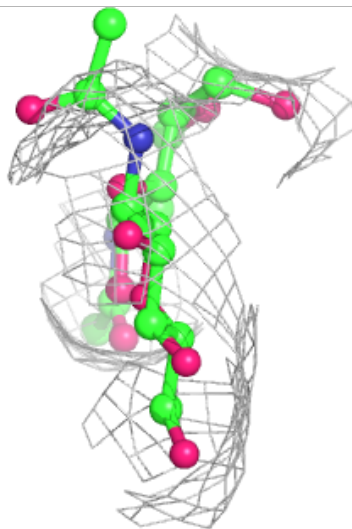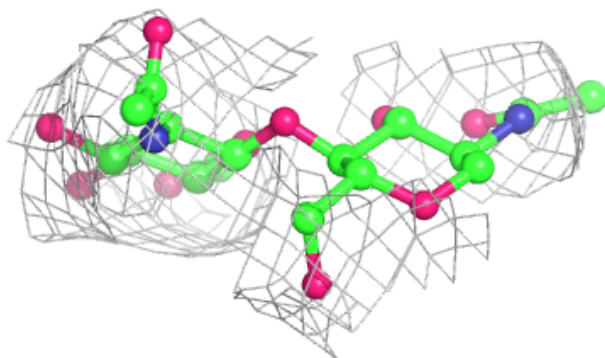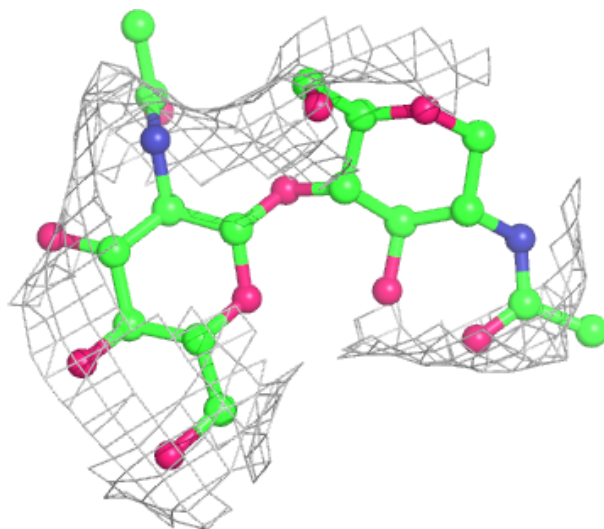
Electron density around Chain I:

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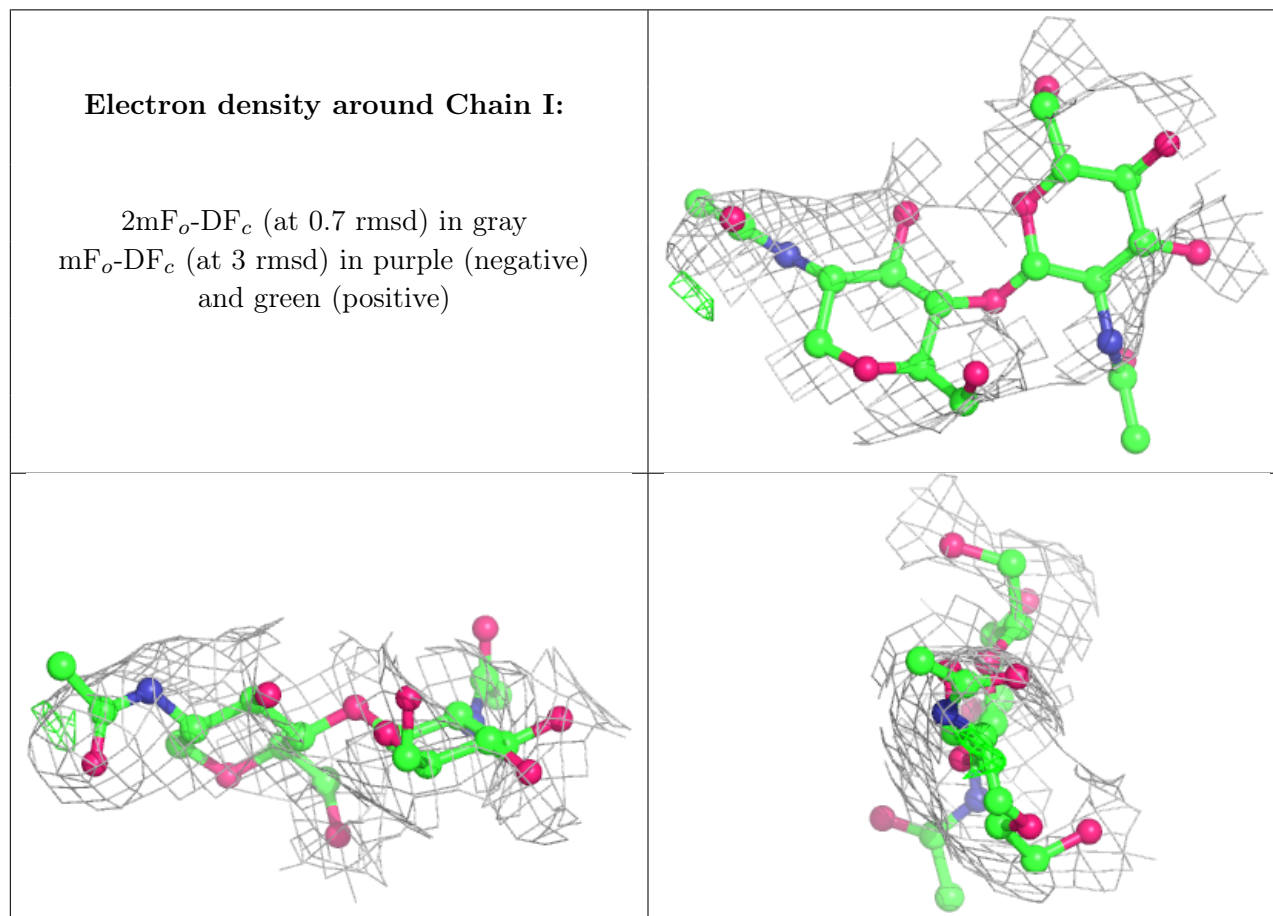
Electron density around Chain L:

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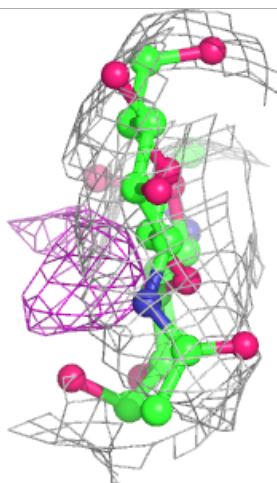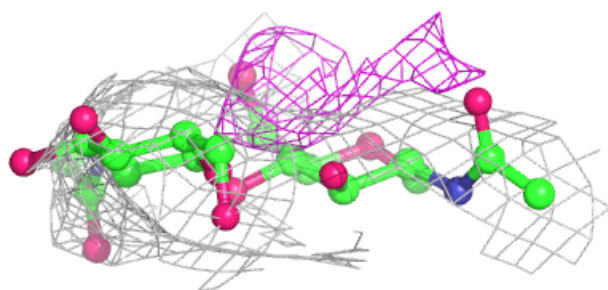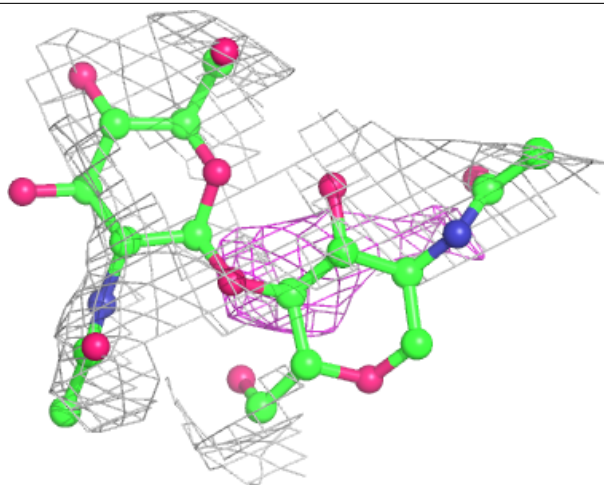and green (positive)
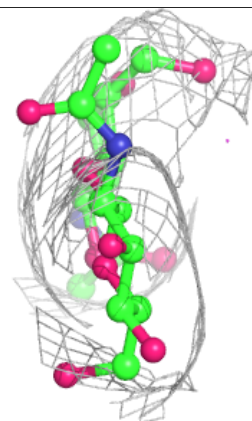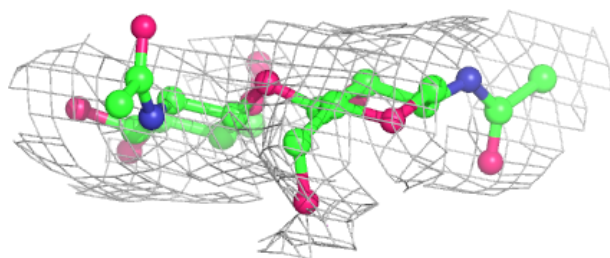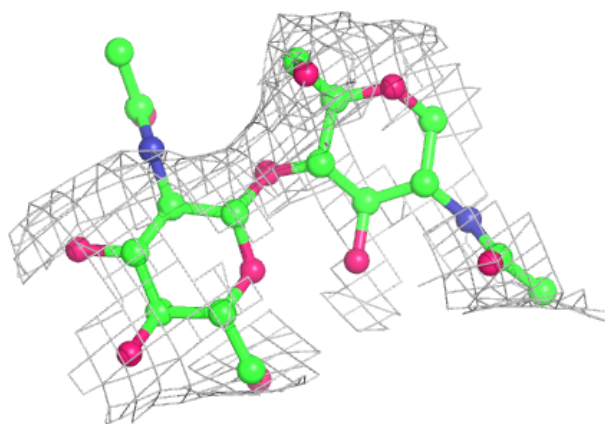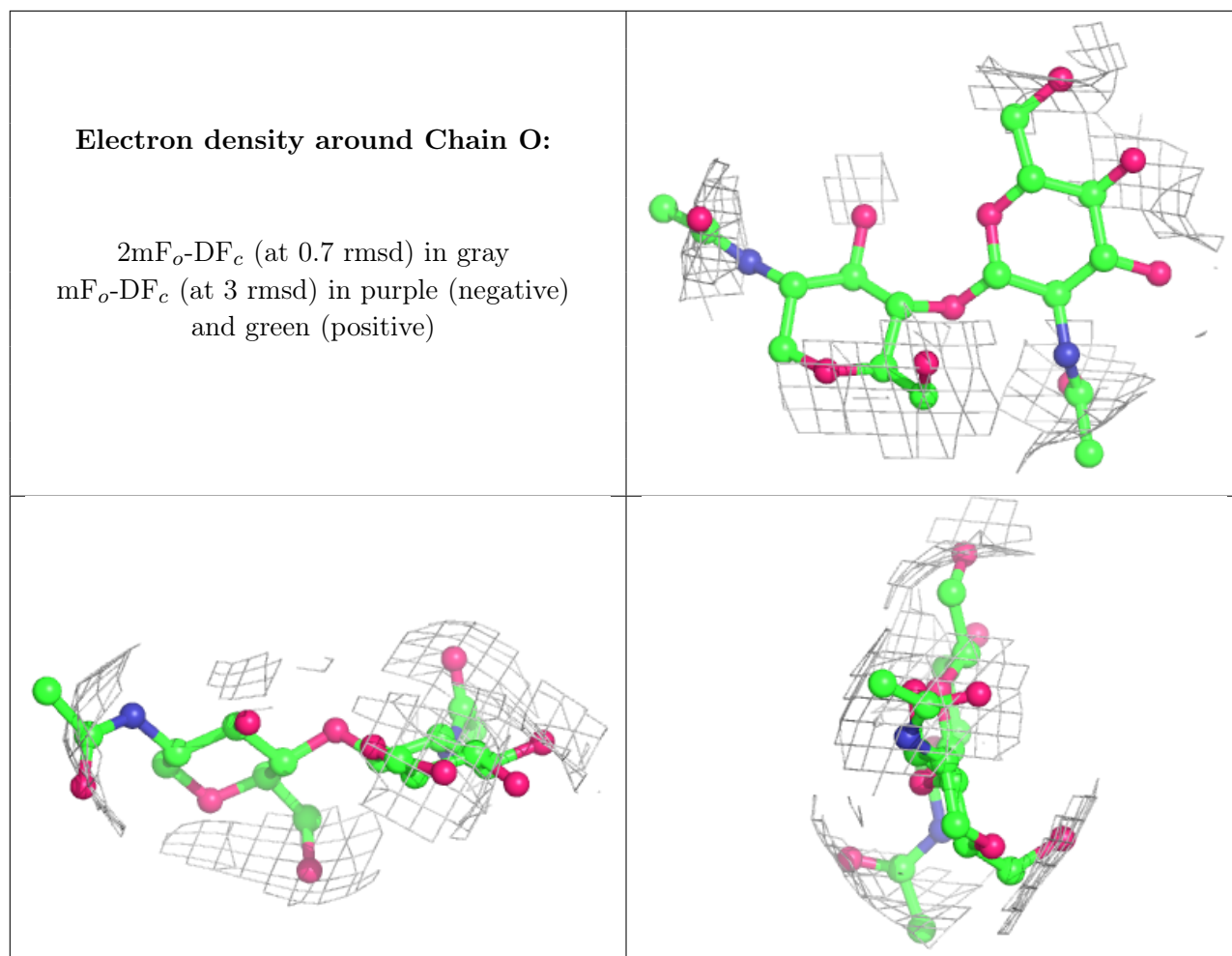
Electron density around Chain M:

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

Electron density around Chain N:

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

Electron density around Chain O:

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

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	G	301	14/15	0.80	0.32	160,174,207,210	0
7	NAG	F	901	14/15	0.86	0.24	138,169,186,188	0
7	NAG	E	705	14/15	0.87	0.28	106,126,143,163	0

6.5 Other polymers ⓘ

There are no such residues in this entry.