W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Oct 8, 2023 – 04:18 PM EDT

PDB ID	:	6MAM
Title	:	Cleaved Ebola GP in complex with a broadly neutralizing human antibody, ADI-15946
Authors	:	West, B.R.; Moyer, C.L.; Fusco, M.L.; Saphire, E.O.
Deposited on	:	2018-08-28
Resolution	:	4.10 Å(reported)

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

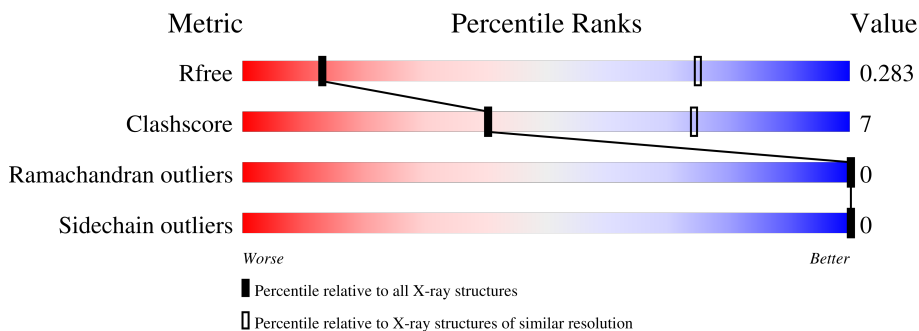|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 4.10 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		0.283
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		0

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	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	242	74% 20% 7%
1	C	242	75% 21% •
1	E	242	74% 23% •
2	B	216	88% 12%
2	D	216	79% 21%
2	F	216	77% 23%
3	G	234	57% 10% 33%

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Mol	Chain	Length	Quality of chain
3	I	234	58% 9% 33%
3	K	234	60% 6% 33%
4	H	110	86% 12% ·
4	J	110	86% 13% ·
4	L	110	85% 11% 5%
5	M	5	40% 60%
5	O	5	20% 80%
6	N	4	50% 50%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 16530 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 ADI-15946 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total 1706	C 1083	N 282	O 334	S 7	0	0	0
1	C	233	Total 1763	C 1117	N 290	O 348	S 8	0	0	0
1	E	235	Total 1774	C 1121	N 291	O 354	S 8	0	0	0

- Molecule 2 is a protein called ADI-15946 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total 1668	C 1045	N 286	O 333	S 4	0	0	0
2	D	215	Total 1668	C 1045	N 286	O 333	S 4	0	0	0
2	F	216	Total 1675	C 1048	N 287	O 335	S 5	0	0	0

- Molecule 3 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	157	Total 1199	C 761	N 210	O 223	S 5	0	0	0
3	I	156	Total 1190	C 756	N 208	O 221	S 5	0	0	0
3	K	156	Total 1190	C 756	N 208	O 221	S 5	0	0	0

- Molecule 4 is a protein called Envelope glycoprotein.

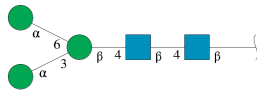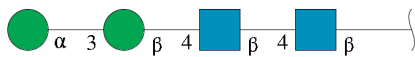| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	108	Total 846	C 540	N 147	O 153	S 6	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	109	Total 851	C 543	N 148	O 154	S 6	0	0	0
4	L	105	Total 828	C 530	N 144	O 148	S 6	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
5	M	5	Total 61	C 34	N 2	O 25	0	0	0
5	O	5	Total 61	C 34	N 2	O 25	0	0	0

- Molecule 6 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.
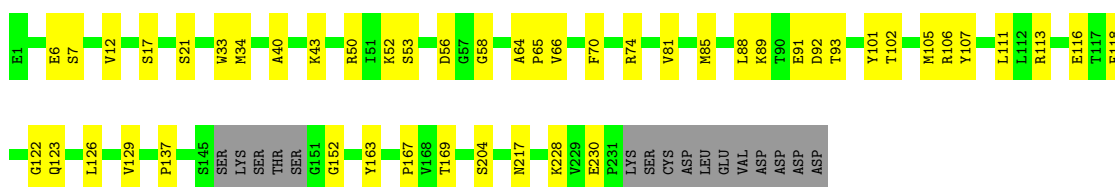

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	N	4	Total 50	C 28	N 2	O 20	0	0	0

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: ADI-15946 Fab Heavy Chain

Chain A:
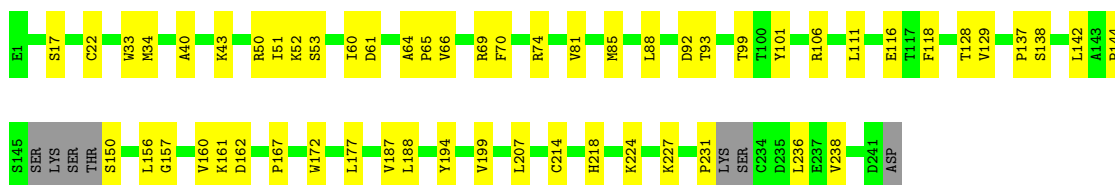
74% 20% 7%

• Molecule 1: ADI-15946 Fab Heavy Chain

Chain C:

75% 21% •

• Molecule 1: ADI-15946 Fab Heavy Chain

Chain E:

74% 23% •

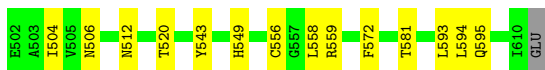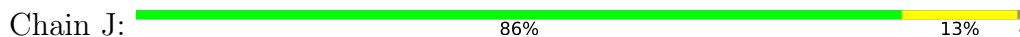• Molecule 2: ADI-15946 Fab Light Chain

Chain B:

88% 12%

• Molecule 2: ADI-15946 Fab Light Chain

Chain D:

D1 R18 V19 T20 I29 Y32 L33 N34 W35 K45 L46 L47 I48 L54 V58 L73 T74 C88 Q89 Q90 S91 Y92 P95 T99 R110 T111 V112 A113 P122 S133 V134 L138 Y142 P143 Q162 D169 S170 L181 D187 Y188 E189

K190 H191 Y194 V198 T199 P206 N212 R213 G214 E215 CYS

• Molecule 2: ADI-15946 Fab Light Chain

Chain F:

D1 Q6 A13 R18 V19 T20 Y32 L33 N34 W35 I48 Y49 N53 F71 S72 L73 T74 Q90 S91 Y92 G96 T99 Q102 K109 R110 A113 S116 V117 F118 P121 P122 S133 V134 L137 L138 N139 Y142 P143 R144 S161 Q162

V165 D169 S170 K171 D172 L181 Y188 Y194 V198 T199 R204 S205 P206 F211 E215 C216

• Molecule 3: Envelope glycoprotein

Chain G:

S32 I33 P34 V37 I38 T42 L43 Q44 V45 S46 D47 K50 L51 V52 R64 E71 W86 E100 E103 E106 N107 L111 P126 I129 R130 D163 R164 Q188 ALA LYS LYS ASP PHE PHE SER SER HIS PRO LEU ARG GLU PRO VAL ASN ALA THR

GLU ASP PRO SER SER GLY TYR TYR SER THR THR ILE ARG TYR GLN ALA THR GLY PHE GLY ASN THR HIS HIS GLN ASP THR GLY GLU GLU SER ALA SER SER GLY LYS LEU GLY LEU ILE THR ASN THR ILE ALA GLY VAL ALA GLY LEU ILE THR GLY ARG ARG THR ARG ARG

• Molecule 3: Envelope glycoprotein

Chain I:

S32 V37 I38 T42 L43 Q44 V45 S46 D47 K50 E71 E103 N107 P126 I129 R130 G131 F132 K155 L161 Y162 D163 R164 L165 L184 P187 GLN ALA LYS LYS ASP PHE PHE SER SER HIS PRO LEU ARG GLU PRO VAL ASN ALA THR GLU ASP PRO

SER SER GLY TYR TYR SER THR THR ILE ARG TYR GLN ALA THR GLY PHE GLY ASN THR HIS HIS GLN ASP THR GLY GLU GLU SER ALA SER SER GLY LYS LEU GLY LEU ILE THR ASN THR ILE ALA GLY VAL ALA GLY LEU ILE THR GLY ARG ARG THR ARG ARG

• Molecule 3: Envelope glycoprotein

Chain K:

S32 L35 G36 V37 I38 H39 T42 S46 K50 L51 L63 Y99 R130 E156 Y162 D163 R164 F176 I185 L186 P187 GLN ALA LYS LYS ASP PHE PHE SER SER HIS PRO LEU ARG GLU PRO VAL ASN ALA THR GLU ASP PRO SER SER GLY TYR TYR SER

THR THR ILE ARG TYR GLN ALA THR GLY PHE GLY ASN THR HIS HIS GLN ASP THR GLY GLU GLU SER ALA SER SER GLY LYS LEU GLY LEU ILE THR ASN THR ILE ALA GLY VAL ALA GLY LEU ILE THR GLY ARG ARG THR ARG ARG

• Molecule 4: Envelope glycoprotein

Chain H:

GLU ALA I504 N512 T520 Y543 R559 T565 F572 T581 L593 L594 Q595 R596 W597 D607 E611

• Molecule 4: Envelope glycoprotein

Chain J:

86%　　　　13%

E502 A503 I504 V505 N506 N512 T520 Y543 H549 C556 G557 L558 R559 F572 T581 L593 L594 Q595 I610 GLU

• Molecule 4: Envelope glycoprotein

Chain L:

85%　　　　11%　　5%

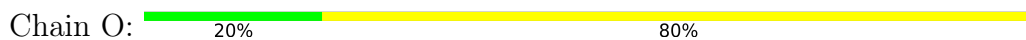GLU ALA I504 K510 T520 E523 GLY ALA A526 Y534 L558 L561 F572 T581 L593 L594 Q595 R596 W597 D607 I610 GLU

• 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 M:

40%　　　60%

NAG1 NAG2 BMA3 MAN4 MAN5

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

Chain O:

20%　　　80%

NAG1 NAG2 BMA3 MAN4 MAN5

• Molecule 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

Chain N:

50%　　　50%

NAG1 NAG2 BMA3 MAN4

4　Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	182.27Å　182.27Å　262.01Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	48.54　–　4.10 48.54　–　4.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.54-4.10) 99.6 (48.54-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 4.14Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.262　,　0.281 0.268　,　0.283	Depositor DCC
R_{free} test set	1796 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	157.7	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 78.3	EDS
L-test for twinning [2]	$< \|L\| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	16530	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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: 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	0/1748	0.47	0/2380
1	C	0.25	0/1805	0.47	0/2457
1	E	0.25	0/1815	0.49	0/2470
2	B	0.25	0/1706	0.45	0/2315
2	D	0.24	0/1706	0.44	0/2315
2	F	0.26	0/1713	0.47	0/2323
3	G	0.26	0/1228	0.49	0/1668
3	I	0.25	0/1219	0.47	0/1656
3	K	0.26	0/1219	0.48	0/1656
4	H	0.25	0/866	0.40	0/1179
4	J	0.24	0/871	0.41	0/1186
4	L	0.24	0/847	0.39	0/1152
All	All	0.25	0/16743	0.46	0/22757

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 ⓘ

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	1706	0	1669	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1763	0	1723	31	0
1	E	1774	0	1719	39	0
2	B	1668	0	1622	20	0
2	D	1668	0	1622	32	0
2	F	1675	0	1626	32	0
3	G	1199	0	1177	17	0
3	I	1190	0	1169	16	0
3	K	1190	0	1169	13	0
4	H	846	0	825	13	0
4	J	851	0	830	14	0
4	L	828	0	810	10	0
5	M	61	0	52	0	0
5	O	61	0	52	1	0
6	N	50	0	43	0	0
All	All	16530	0	16108	234	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 7.

The worst 5 of 234 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:I:38:ILE:HA	3:I:42:THR:O	1.76	0.84
1:E:99:THR:HG21	1:E:118:PHE:HB3	1.60	0.81
1:E:138:SER:O	1:E:160:VAL:HA	1.82	0.78
1:E:65:PRO:O	1:E:69:ARG:NH1	2.21	0.74
4:J:506:ASN:HD22	4:J:556:CYS:HB3	1.52	0.74

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	222/242 (92%)	220 (99%)	2 (1%)	0	100	100
1	C	229/242 (95%)	228 (100%)	1 (0%)	0	100	100
1	E	229/242 (95%)	225 (98%)	4 (2%)	0	100	100
2	B	213/216 (99%)	210 (99%)	3 (1%)	0	100	100
2	D	213/216 (99%)	211 (99%)	2 (1%)	0	100	100
2	F	214/216 (99%)	211 (99%)	3 (1%)	0	100	100
3	G	155/234 (66%)	151 (97%)	4 (3%)	0	100	100
3	I	154/234 (66%)	150 (97%)	4 (3%)	0	100	100
3	K	154/234 (66%)	149 (97%)	5 (3%)	0	100	100
4	H	106/110 (96%)	103 (97%)	3 (3%)	0	100	100
4	J	107/110 (97%)	104 (97%)	3 (3%)	0	100	100
4	L	101/110 (92%)	98 (97%)	3 (3%)	0	100	100
All	All	2097/2406 (87%)	2060 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	189/205 (92%)	189 (100%)	0	100	100
1	C	197/205 (96%)	197 (100%)	0	100	100
1	E	198/205 (97%)	198 (100%)	0	100	100
2	B	189/190 (100%)	189 (100%)	0	100	100
2	D	189/190 (100%)	189 (100%)	0	100	100
2	F	190/190 (100%)	190 (100%)	0	100	100
3	G	129/190 (68%)	129 (100%)	0	100	100
3	I	128/190 (67%)	128 (100%)	0	100	100
3	K	128/190 (67%)	128 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	88/89 (99%)	88 (100%)	0	100	100
4	J	88/89 (99%)	88 (100%)	0	100	100
4	L	87/89 (98%)	87 (100%)	0	100	100
All	All	1800/2022 (89%)	1800 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

14 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
5	NAG	M	1	4,5	14,14,15	0.25	0	17,19,21	0.43	0
5	NAG	M	2	5	14,14,15	0.22	0	17,19,21	0.42	0
5	BMA	M	3	5	11,11,12	1.10	1 (9%)	15,15,17	1.49	3 (20%)
5	MAN	M	4	5	11,11,12	0.88	1 (9%)	15,15,17	1.44	2 (13%)
5	MAN	M	5	5	11,11,12	0.72	1 (9%)	15,15,17	1.16	2 (13%)
6	NAG	N	1	6,4	14,14,15	0.36	0	17,19,21	0.47	0
6	NAG	N	2	6	14,14,15	0.21	0	17,19,21	0.44	0
6	BMA	N	3	6	11,11,12	1.12	1 (9%)	15,15,17	1.26	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths				Bond angles			
					Counts	RMSZ	#|Z| > 2		Counts	RMSZ	#|Z| > 2	
6	MAN	N	4	6	11,11,12	0.87	1 (9%)		15,15,17	0.90	1 (6%)	
5	NAG	O	1	4,5	14,14,15	0.25	0		17,19,21	0.46	0	
5	NAG	O	2	5	14,14,15	0.18	0		17,19,21	0.52	0	
5	BMA	O	3	5	11,11,12	0.96	0		15,15,17	1.24	3 (20%)	
5	MAN	O	4	5	11,11,12	0.83	0		15,15,17	0.89	1 (6%)	
5	MAN	O	5	5	11,11,12	0.98	1 (9%)		15,15,17	1.52	2 (13%)	

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
5	NAG	M	1	4,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
5	MAN	M	4	5	-	0/2/19/22	0/1/1/1
5	MAN	M	5	5	-	0/2/19/22	0/1/1/1
6	NAG	N	1	6,4	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	4/6/23/26	0/1/1/1
6	BMA	N	3	6	-	0/2/19/22	0/1/1/1
6	MAN	N	4	6	-	0/2/19/22	0/1/1/1
5	NAG	O	1	4,5	-	1/6/23/26	0/1/1/1
5	NAG	O	2	5	-	3/6/23/26	0/1/1/1
5	BMA	O	3	5	-	1/2/19/22	0/1/1/1
5	MAN	O	4	5	-	2/2/19/22	0/1/1/1
5	MAN	O	5	5	-	0/2/19/22	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	3	BMA	C2-C3	2.68	1.56	1.52
5	O	5	MAN	C1-C2	2.53	1.58	1.52
5	M	4	MAN	C1-C2	2.45	1.57	1.52
5	M	3	BMA	O3-C3	2.24	1.48	1.43
6	N	4	MAN	O5-C1	-2.14	1.40	1.43

The worst 5 of 16 bond angle outliers are listed below:

| Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	O	5	MAN	C1-O5-C5	4.76	118.65	112.19
5	M	4	MAN	C1-O5-C5	4.19	117.87	112.19
5	M	3	BMA	O3-C3-C2	3.99	117.64	109.99
5	M	3	BMA	C1-O5-C5	3.19	116.52	112.19
5	M	5	MAN	C1-O5-C5	2.91	116.13	112.19

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

| Mol	Chain	Res	Type	Atoms
5	M	2	NAG	O5-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
5	O	2	NAG	C8-C7-N2-C2
5	O	2	NAG	O7-C7-N2-C2
6	N	2	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	2	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 M

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain O

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain N

Bond lengths

Bond angles

Torsions

Rings
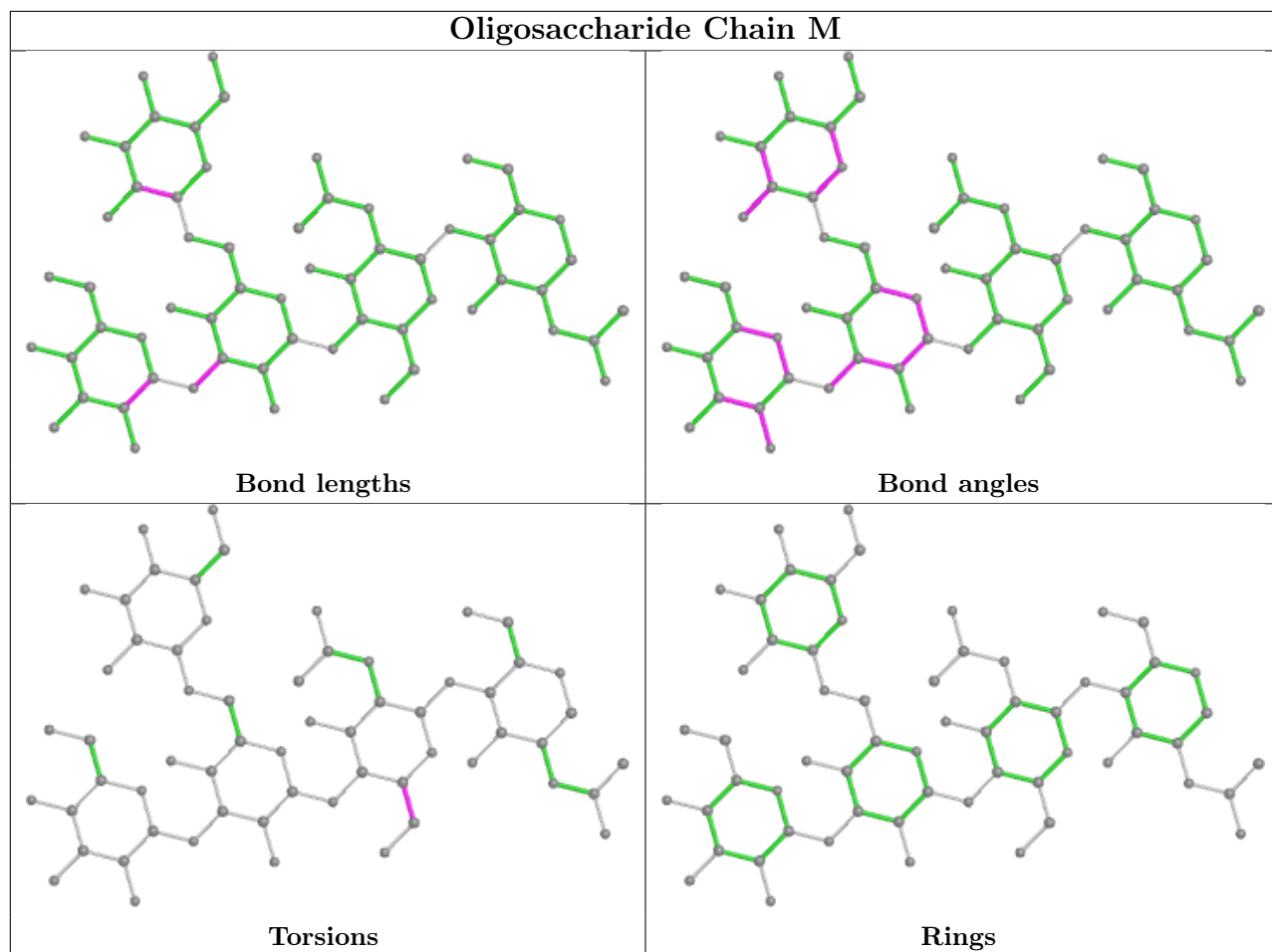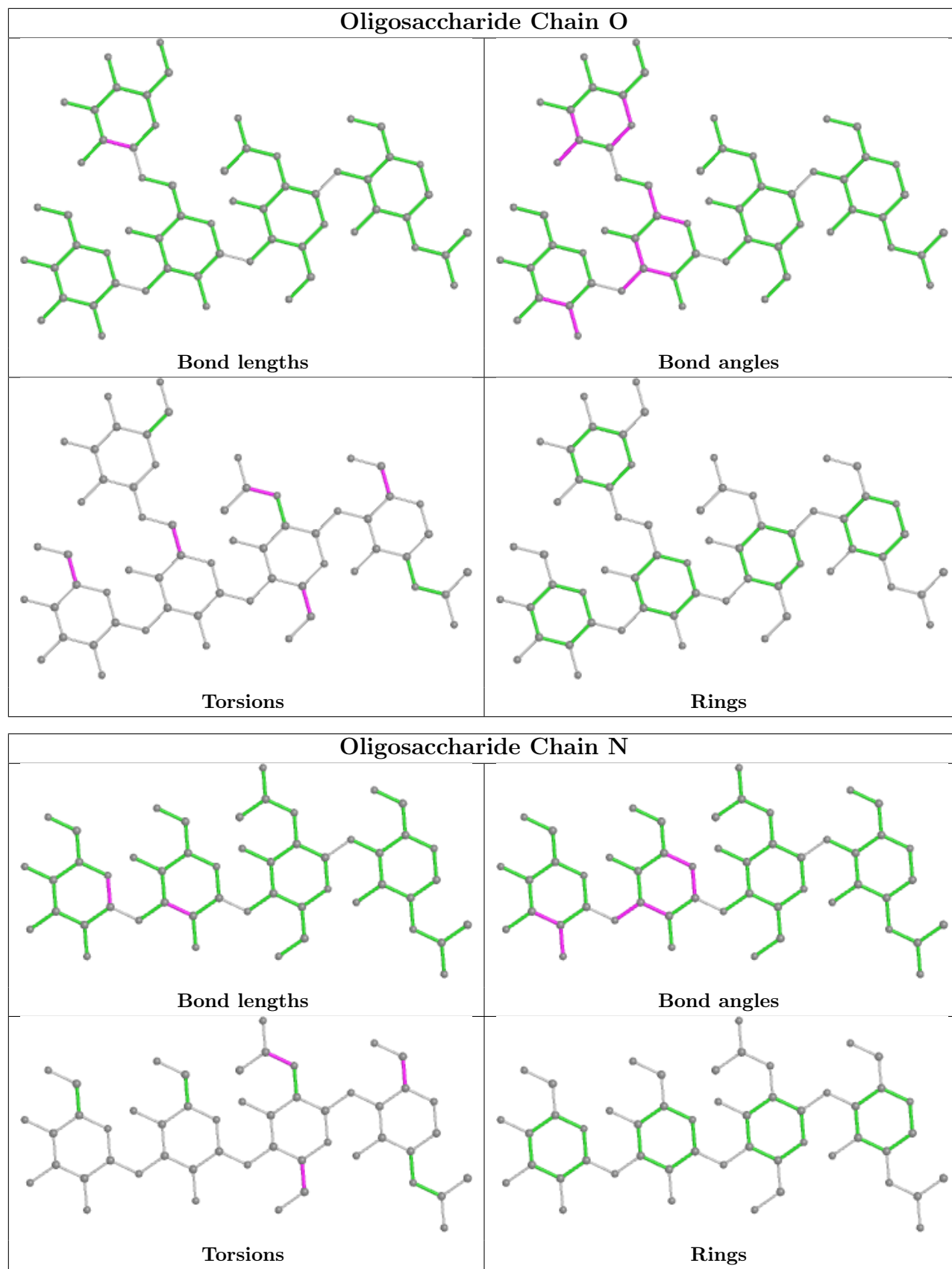
5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

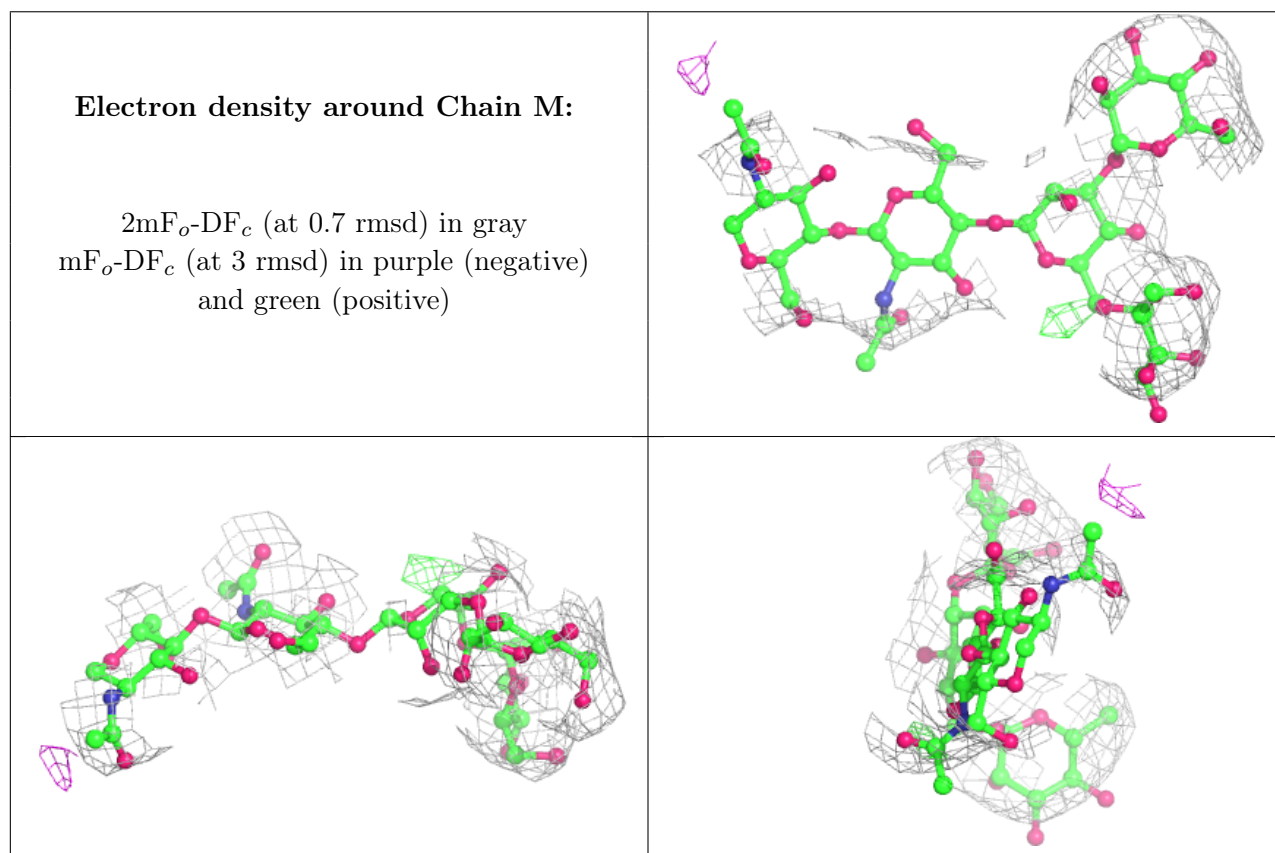Unable to reproduce the depositors R factor - this section is therefore empty.

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 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 O:

$2mF_o\text{-}DF_c$ (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:

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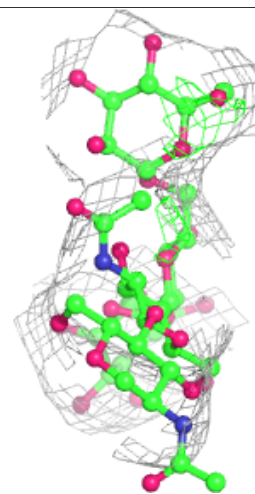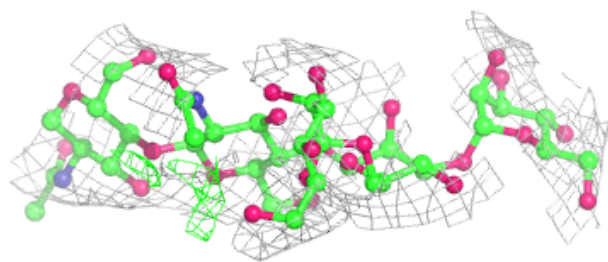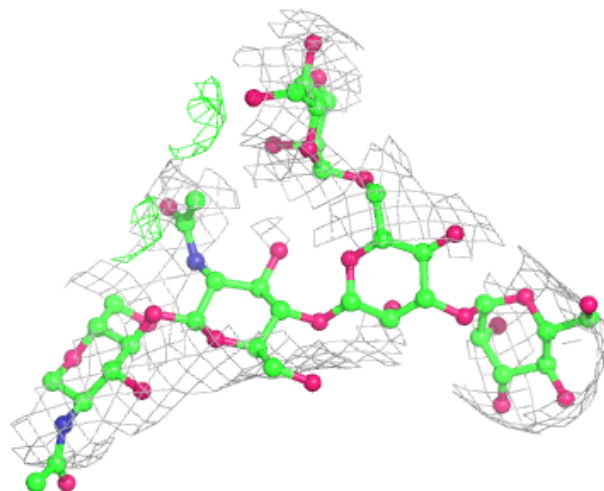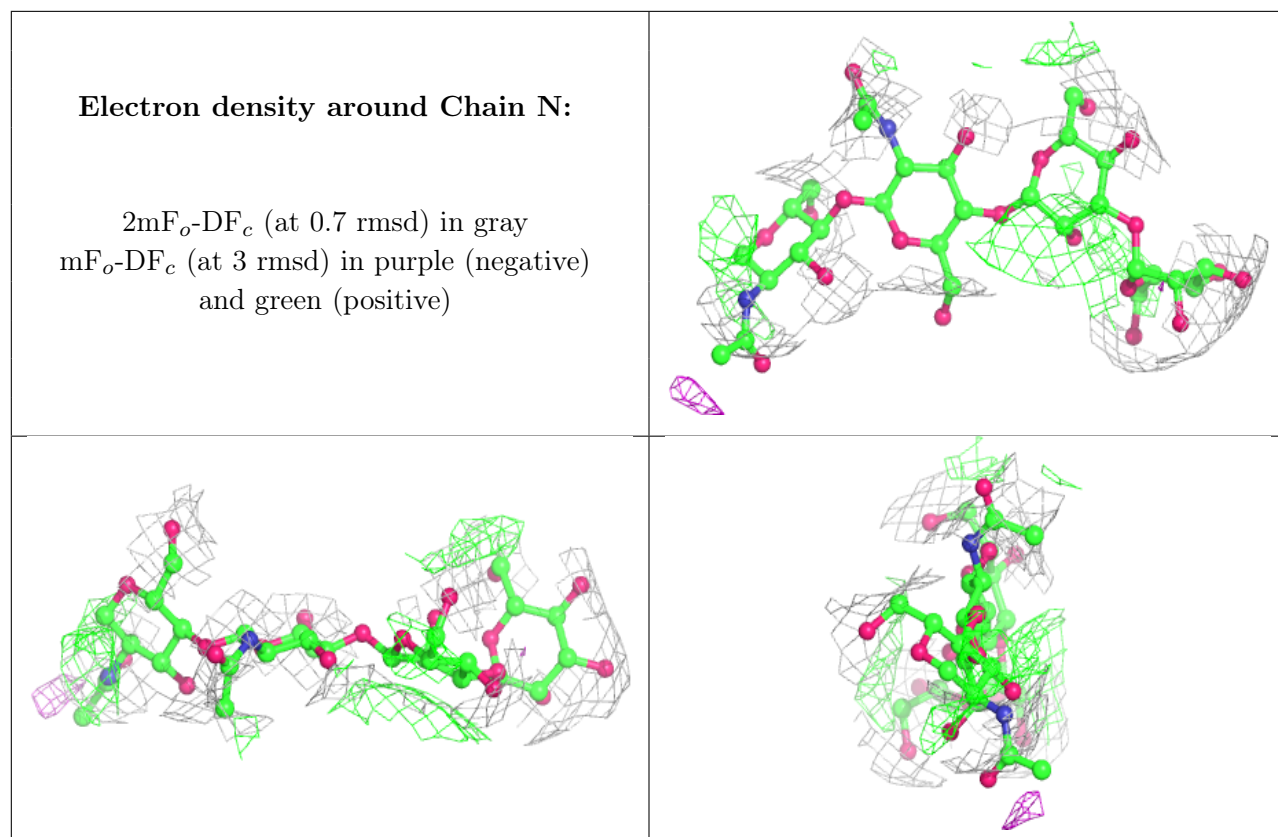
6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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