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

wwPDB X-ray Structure Validation Summary Report (i)

Aug 19, 2024 – 10:20 am BST

PDB ID	:	8Q6R
Title	:	Structure of complement FP in complex with the TPP-3077 VHH
Authors	:	Andersen, G.R.; Pedersen, D.V.
Deposited on	:	2023-08-14
Resolution	:	1.90 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:

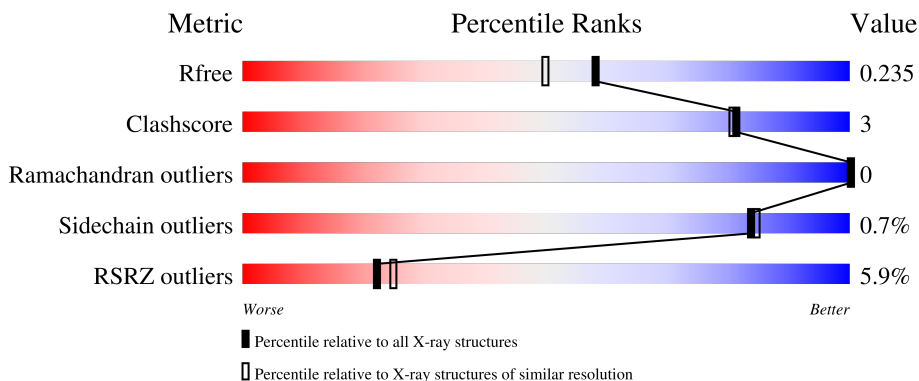|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.90 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		0.235
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		0.7%
RSRZ outliers		5.9%

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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	125	% 91% ··· 5%
1	B	125	2% 91% ····
2	C	108	9% 92% 7% ·
2	E	108	14% 93% 6% ··
3	D	221	6% 92% · 5%

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Mol	Chain	Length	Quality of chain
3	F	221	5% ... 90% ... 5% 5%
4	G	2	100%
4	H	2	100%
4	J	2	100%
4	K	2	100%
5	I	2	50% 50%

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
4	BGC	G	2	-	-	-	X
4	FUC	J	1	-	-	-	X
4	BGC	J	2	-	-	-	X
7	MAN	C	202	-	-	-	X
7	MAN	E	202	-	-	-	X

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 13865 atoms, of which 6373 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 The properdin specific VHH TPP-3077.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	119	Total	C	H	N	O	S	0	0	0
			1806	567	896	161	178	4			
1	B	120	Total	C	H	N	O	S	0	0	0
			1823	573	903	164	179	4			

- Molecule 2 is a protein called Properdin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	107	Total	C	H	N	O	S	0	0	0
			1564	500	752	145	155	12			
2	E	107	Total	C	H	N	O	S	0	0	0
			1564	500	752	145	155	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	132	ALA	CYS	conflict	UNP P27918
E	132	ALA	CYS	conflict	UNP P27918

- Molecule 3 is a protein called Properdin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	211	Total	C	H	N	O	S	0	0	0
			3166	1009	1535	309	291	22			
3	F	211	Total	C	H	N	O	S	0	0	0
			3166	1009	1535	309	291	22			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	255	GLY	-	expression tag	UNP P27918
D	470	HIS	-	expression tag	UNP P27918

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Chain	Residue	Modelled	Actual	Comment	Reference
D	471	HIS	-	expression tag	UNP P27918
D	472	HIS	-	expression tag	UNP P27918
D	473	HIS	-	expression tag	UNP P27918
D	474	HIS	-	expression tag	UNP P27918
D	475	HIS	-	expression tag	UNP P27918
F	255	GLY	-	expression tag	UNP P27918
F	470	HIS	-	expression tag	UNP P27918
F	471	HIS	-	expression tag	UNP P27918
F	472	HIS	-	expression tag	UNP P27918
F	473	HIS	-	expression tag	UNP P27918
F	474	HIS	-	expression tag	UNP P27918
F	475	HIS	-	expression tag	UNP P27918

- Molecule 4 is an oligosaccharide called beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose.
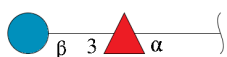
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	G	2	Total 21	C 12	O 9	0	0	0
4	H	2	Total 21	C 12	O 9	0	0	0
4	J	2	Total 21	C 12	O 9	0	0	0
4	K	2	Total 21	C 12	O 9	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 6 is GLYCOCHOLIC ACID (three-letter code: GCH) (formula: $C_{26}H_{43}NO_6$) (labeled as "Ligand of Interest" by depositor).

GCH
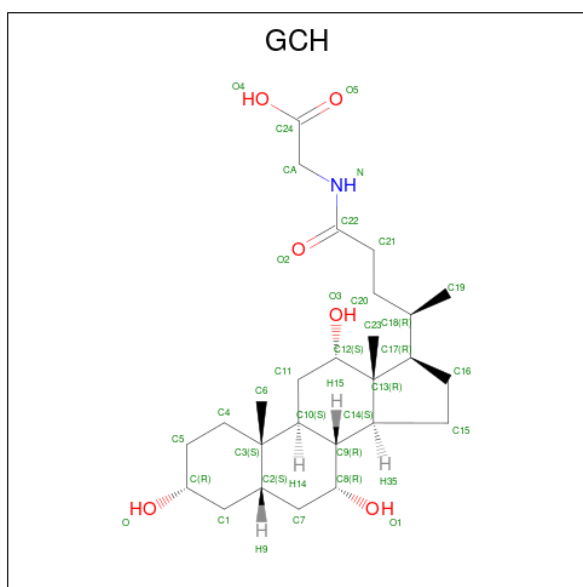
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			33	26	1	6		
6	A	1	Total	C	N	O	0	0
			33	26	1	6		

- Molecule 7 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).

MAN
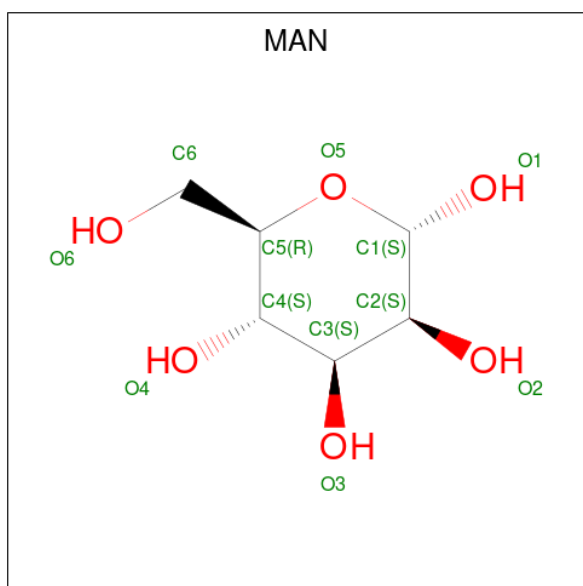
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total 11	C 6	O 5	0	0
7	D	1	Total 11	C 6	O 5	0	0
7	D	1	Total 11	C 6	O 5	0	0
7	D	1	Total 11	C 6	O 5	0	0
7	D	1	Total 11	C 6	O 5	0	0
7	D	1	Total 11	C 6	O 5	0	0
7	D	1	Total 11	C 6	O 5	0	0
7	D	1	Total 11	C 6	O 5	0	0
7	D	1	Total 11	C 6	O 5	0	0
7	E	1	Total 11	C 6	O 5	0	0
7	E	1	Total 11	C 6	O 5	0	0
7	F	1	Total 11	C 6	O 5	0	0
7	F	1	Total 11	C 6	O 5	0	0
7	F	1	Total 11	C 6	O 5	0	0
7	F	1	Total 11	C 6	O 5	0	0
7	F	1	Total 11	C 6	O 5	0	0
7	F	1	Total 11	C 6	O 5	0	0
7	F	1	Total 11	C 6	O 5	0	0
7	F	1	Total 11	C 6	O 5	0	0

- Molecule 8 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).

NAG

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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	82	Total 82	O 82	0	0
9	B	79	Total 79	O 79	0	0
9	C	20	Total 20	O 20	0	0
9	D	74	Total 74	O 74	0	0
9	E	22	Total 22	O 22	0	0
9	F	87	Total 87	O 87	0	0

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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: The properdin specific VHH TPP-3077

• Molecule 1: The properdin specific VHH TPP-3077
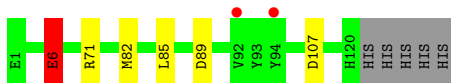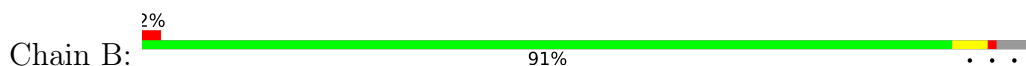
• Molecule 2: Properdin
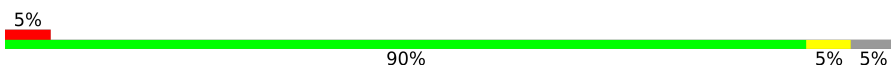
• Molecule 2: Properdin
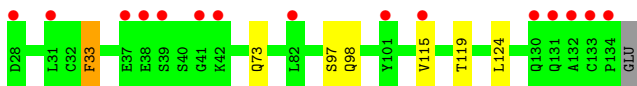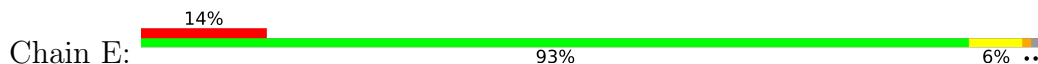
• Molecule 3: Properdin

• Molecule 3: Properdin

Chain F:

5%

90%   5%   5%

G255 V256 A257 L275 E280 Q290 H291 R302 N307 E323 R330 Q344 D356 V418 S419 M420 V421 E422 G423 Q424 G425 E426 K427 C455 K462 E465 GLU GLU GLU LEU HIS HIS HIS HIS HIS HIS
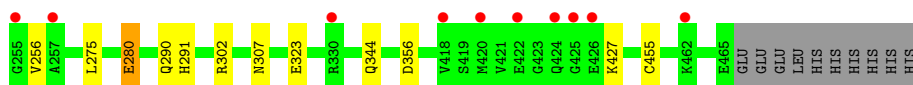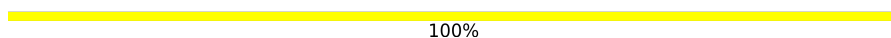
• Molecule 4: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose

Chain G:

100%

FUC1 BGC2

• Molecule 4: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose

Chain H:

100%
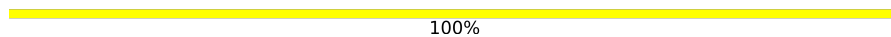
FUC1 BGC2

• Molecule 4: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose

Chain J:

100%

FUC1 BGC2

• Molecule 4: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose

Chain K:

100%

FUC1 BGC2

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

Chain I:

50%   50%

NAG1 NAG2

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.21Å 63.70Å 119.25Å 90.00° 103.75° 90.00°	Depositor
Resolution (Å)	47.86 – 1.90 47.86 – 1.84	Depositor EDS
% Data completeness (in resolution range)	98.1 (47.86-1.90) 93.4 (47.86-1.84)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 1.84Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.202 , 0.238 0.199 , 0.235	Depositor DCC
R_{free} test set	2000 reflections (2.12%)	wwPDB-VP
Wilson B-factor (Å^2)	32.5	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.6	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13865	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.2355e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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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: FUC, MAN, BGC, GCH, 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	0.95	1/926 (0.1%)	1.11	1/1251 (0.1%)
1	B	0.93	1/937 (0.1%)	1.08	2/1266 (0.2%)
2	C	0.59	1/832 (0.1%)	0.82	0/1128
2	E	0.58	1/832 (0.1%)	0.84	3/1128 (0.3%)
3	D	0.76	1/1685 (0.1%)	0.91	1/2295 (0.0%)
3	F	0.72	1/1685 (0.1%)	0.91	3/2295 (0.1%)
All	All	0.77	6/6897 (0.1%)	0.95	10/9363 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	344	GLN	CB-CG	-9.53	1.26	1.52
3	F	344	GLN	CB-CG	-7.87	1.31	1.52
2	C	30	VAL	CB-CG1	-5.52	1.41	1.52
1	A	6	GLU	CB-CG	-5.47	1.41	1.52
1	B	6	GLU	CD-OE1	-5.44	1.19	1.25

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	455	CYS	CA-CB-SG	-6.86	101.64	114.00
3	F	356	ASP	CB-CG-OD1	6.58	124.22	118.30
1	B	89	ASP	CB-CG-OD1	6.16	123.84	118.30
3	D	356	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	71	ARG	CB-CA-C	-5.78	98.83	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	71	ARG	Sidechain
1	B	6	GLU	Sidechain
1	B	71	ARG	Sidechain

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	910	896	896	4	0
1	B	920	903	903	1	0
2	C	812	752	754	4	0
2	E	812	752	754	3	0
3	D	1631	1535	1544	4	0
3	F	1631	1535	1544	5	0
4	G	21	0	19	2	0
4	H	21	0	19	0	0
4	J	21	0	19	1	0
4	K	21	0	19	0	0
5	I	28	0	25	1	0
6	A	66	0	74	9	0
7	C	22	0	20	0	0
7	D	88	0	80	5	0
7	E	22	0	20	0	0
7	F	88	0	80	2	0
8	F	14	0	13	0	0
9	A	82	0	0	3	0
9	B	79	0	0	0	0
9	C	20	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	74	0	0	1	0
9	E	22	0	0	1	0
9	F	87	0	0	1	0
All	All	7492	6373	6783	36	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 3.

The worst 5 of 36 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)
6:A:1102:GCH:C7	6:A:1102:GCH:C8	1.76	1.58
6:A:1102:GCH:C17	6:A:1102:GCH:C16	1.75	1.54
6:A:1102:GCH:C16	6:A:1102:GCH:C18	2.49	0.89
2:C:84:SER:O	9:C:301:HOH:O	1.93	0.86
3:D:374:GLN:OE1	9:D:601:HOH:O	1.97	0.81

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	117/125 (94%)	116 (99%)	1 (1%)	0	100	100
1	B	118/125 (94%)	116 (98%)	2 (2%)	0	100	100
2	C	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	E	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
3	D	209/221 (95%)	204 (98%)	5 (2%)	0	100	100
3	F	209/221 (95%)	205 (98%)	4 (2%)	0	100	100
All	All	863/908 (95%)	836 (97%)	27 (3%)	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	98/104 (94%)	97 (99%)	1 (1%)	76	76
1	B	99/104 (95%)	98 (99%)	1 (1%)	76	76
2	C	89/90 (99%)	88 (99%)	1 (1%)	73	73
2	E	89/90 (99%)	88 (99%)	1 (1%)	73	73
3	D	180/190 (95%)	180 (100%)	0	100	100
3	F	180/190 (95%)	179 (99%)	1 (1%)	86	87
All	All	735/768 (96%)	730 (99%)	5 (1%)	84	84

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	B	6	GLU
2	C	33	PHE
2	E	33	PHE
3	F	427	LYS

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 ⓘ

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	#$|Z| > 2$
4	FUC	G	1	2,4	10,10,11	1.52	2 (20%)	14,14,16	1.35	0
4	BGC	G	2	4	11,11,12	1.78	2 (18%)	15,15,17	2.61	2 (13%)
4	FUC	H	1	4,3	10,10,11	1.37	2 (20%)	14,14,16	1.12	1 (7%)
4	BGC	H	2	4	11,11,12	1.93	2 (18%)	15,15,17	1.59	2 (13%)
5	NAG	I	1	5,3	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	I	2	5	14,14,15	0.64	1 (7%)	17,19,21	0.89	1 (5%)
4	FUC	J	1	2,4	10,10,11	1.23	1 (10%)	14,14,16	1.21	1 (7%)
4	BGC	J	2	4	11,11,12	1.76	2 (18%)	15,15,17	2.77	4 (26%)
4	FUC	K	1	4,3	10,10,11	2.00	3 (30%)	14,14,16	1.38	1 (7%)
4	BGC	K	2	4	11,11,12	1.22	2 (18%)	15,15,17	1.44	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUC	G	1	2,4	-	-	0/1/1/1
4	BGC	G	2	4	-	2/2/19/22	0/1/1/1
4	FUC	H	1	4,3	-	-	0/1/1/1
4	BGC	H	2	4	-	0/2/19/22	0/1/1/1
5	NAG	I	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	1/6/23/26	0/1/1/1
4	FUC	J	1	2,4	-	-	0/1/1/1
4	BGC	J	2	4	-	2/2/19/22	0/1/1/1
4	FUC	K	1	4,3	-	-	0/1/1/1
4	BGC	K	2	4	-	0/2/19/22	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	1	FUC	O5-C1	-4.89	1.35	1.43
4	G	2	BGC	O5-C1	4.83	1.51	1.43
4	J	2	BGC	O5-C1	4.71	1.51	1.43
4	H	2	BGC	O5-C1	4.33	1.50	1.43
4	H	2	BGC	C2-C3	-3.90	1.46	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	2	BGC	C1-C2-C3	8.82	120.51	109.67
4	J	2	BGC	C1-C2-C3	8.18	119.72	109.67
4	J	2	BGC	O5-C1-C2	4.96	118.42	110.77
4	H	2	BGC	C2-C3-C4	-4.20	103.63	110.89
4	K	2	BGC	O4-C4-C5	-2.92	102.05	109.30

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	2	BGC	O5-C5-C6-O6
5	I	2	NAG	C1-C2-N2-C7
4	G	2	BGC	C4-C5-C6-O6
4	J	2	BGC	C4-C5-C6-O6
4	J	2	BGC	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 4 short contacts:

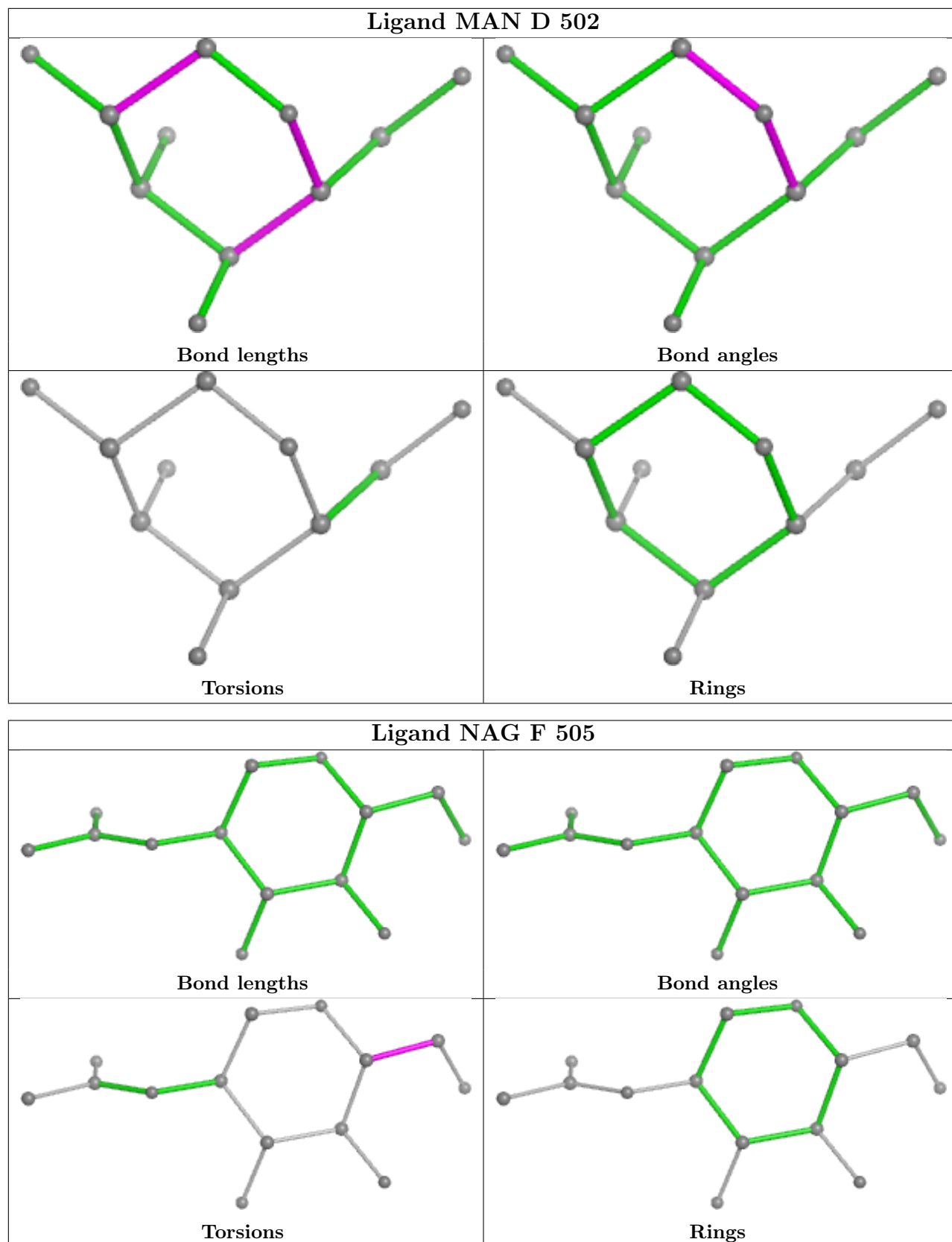| Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2	BGC	1	0
4	J	2	BGC	1	0
4	J	1	FUC	1	0
4	G	1	FUC	2	0
5	I	2	NAG	1	0
5	I	1	NAG	1	0

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 G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

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 I

Bond lengths

Bond angles

Torsions

Rings
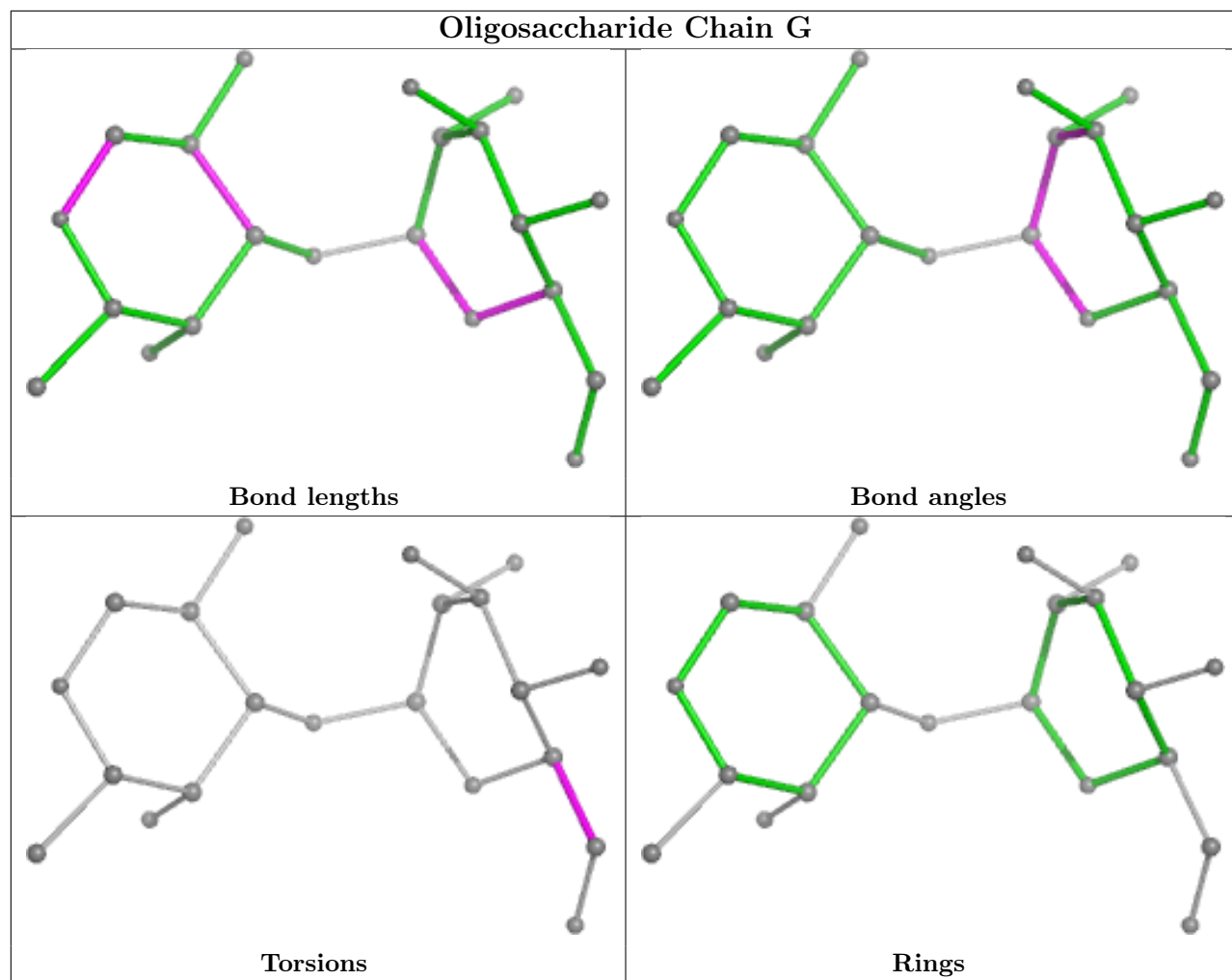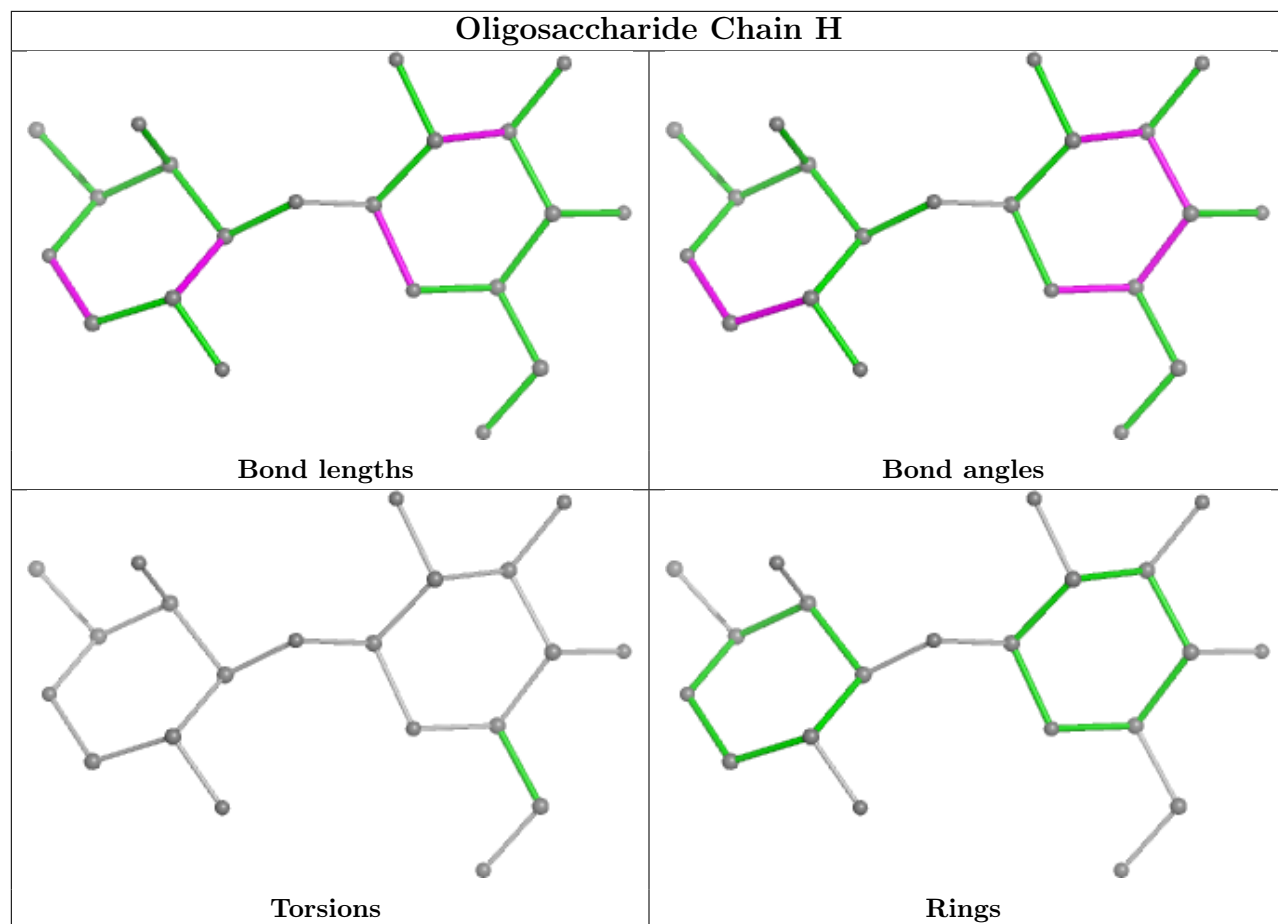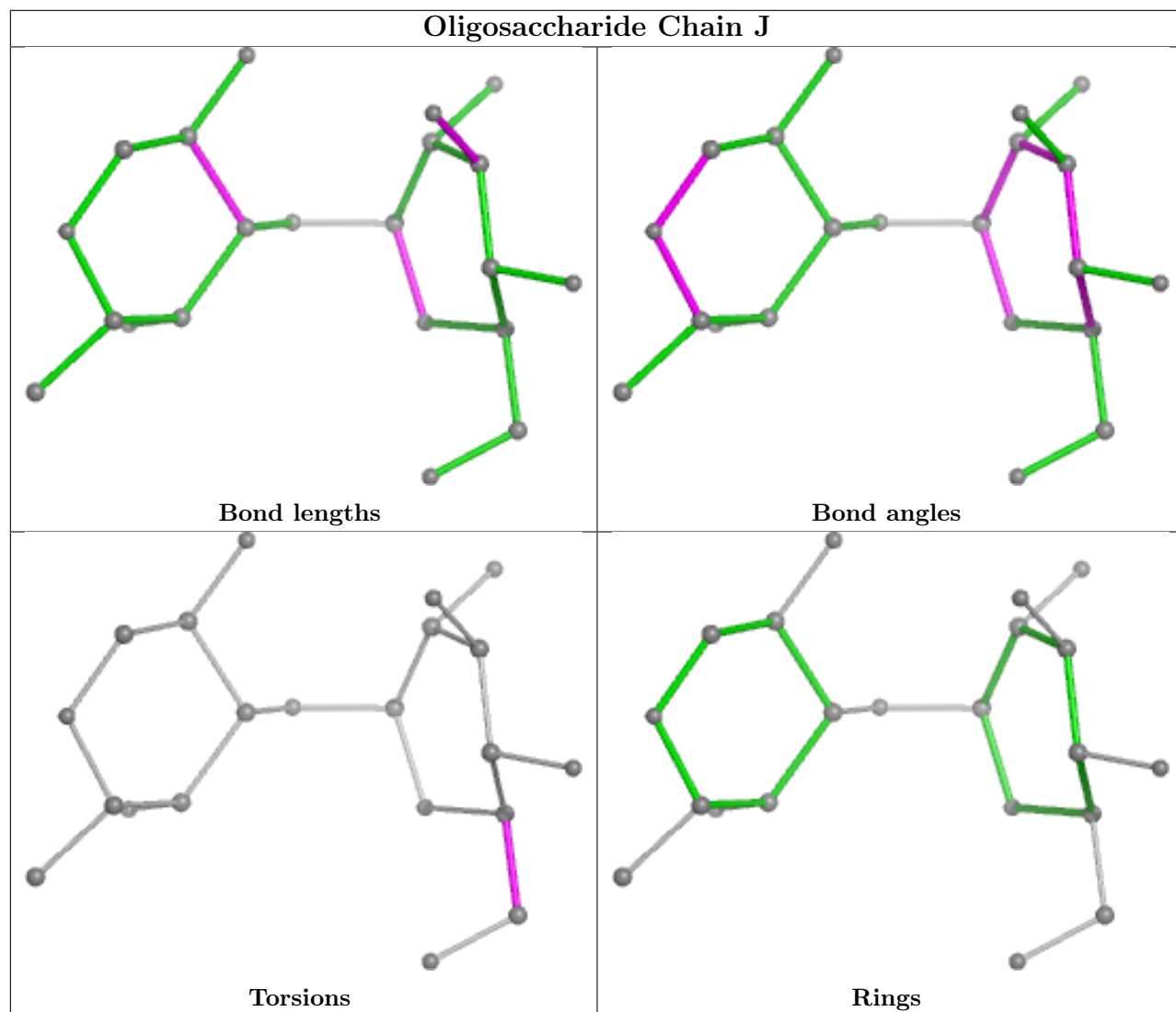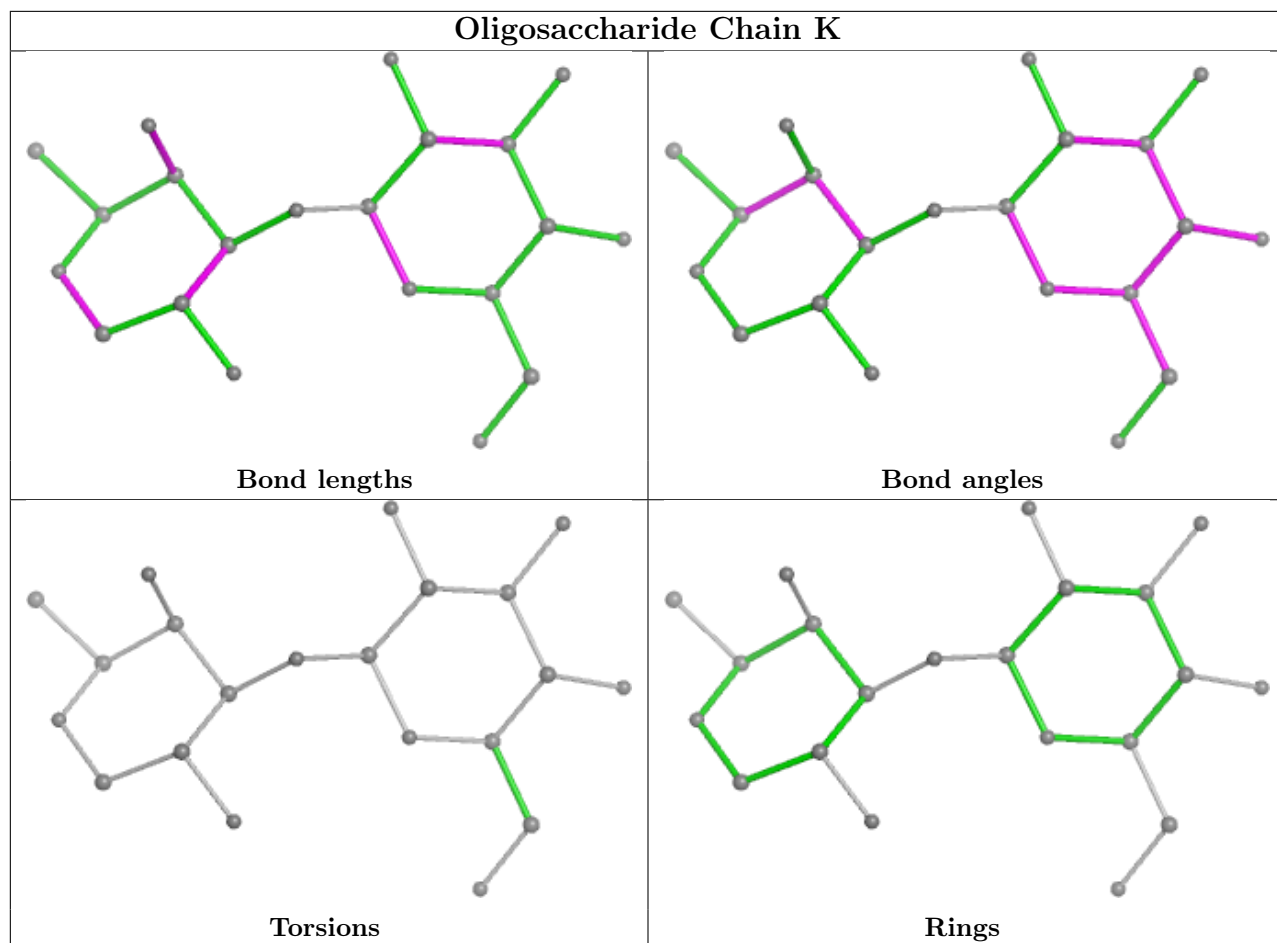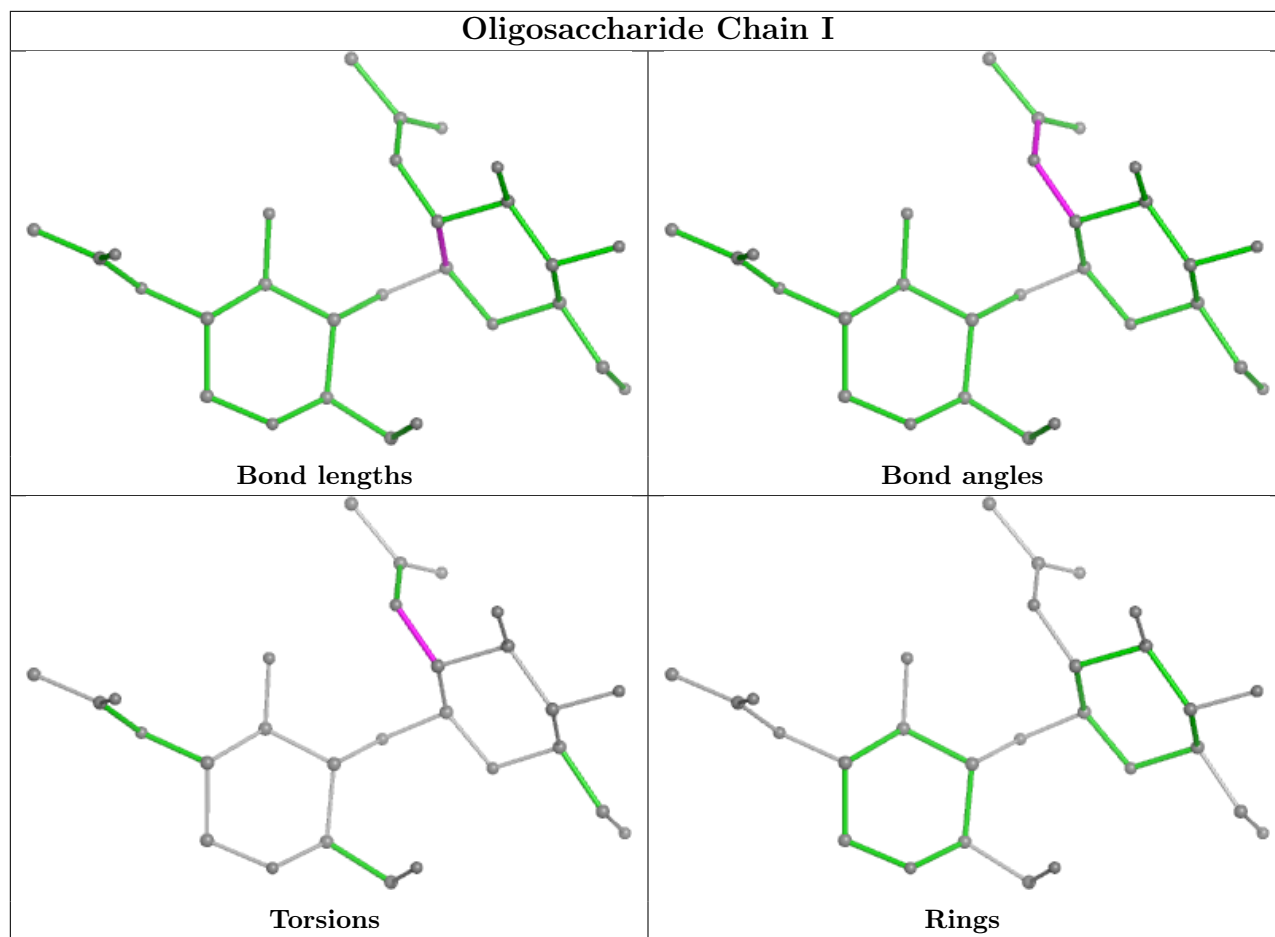
5.6 Ligand geometry ⓘ

23 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	MAN	F	509	3	11,11,12	1.34	1 (9%)	15,15,17	1.78	2 (13%)
7	MAN	D	506	3	11,11,12	1.06	0	15,15,17	1.41	2 (13%)
7	MAN	F	507	3	11,11,12	1.17	2 (18%)	15,15,17	1.23	2 (13%)
7	MAN	F	506	3	11,11,12	1.23	1 (9%)	15,15,17	1.42	2 (13%)
7	MAN	D	502	3	11,11,12	1.53	3 (27%)	15,15,17	1.35	1 (6%)
8	NAG	F	505	3	14,14,15	0.46	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|>2$	Counts	RMSZ	#$\|Z\|>2$
7	MAN	E	202	2	11,11,12	1.34	0	15,15,17	1.62	3 (20%)
7	MAN	F	504	3	11,11,12	2.62	3 (27%)	15,15,17	2.25	6 (40%)
6	GCH	A	1102	-	36,36,36	8.19	27 (75%)	56,56,56	2.58	26 (46%)
7	MAN	C	202	2	11,11,12	1.06	1 (9%)	15,15,17	1.59	4 (26%)
7	MAN	F	503	3	11,11,12	1.74	3 (27%)	15,15,17	1.44	3 (20%)
7	MAN	D	503	3	11,11,12	1.52	2 (18%)	15,15,17	1.68	5 (33%)
7	MAN	D	501	3	11,11,12	2.31	5 (45%)	15,15,17	1.73	5 (33%)
7	MAN	D	504	3	11,11,12	2.25	3 (27%)	15,15,17	2.16	3 (20%)
7	MAN	C	201	2	11,11,12	1.09	0	15,15,17	1.24	1 (6%)
7	MAN	D	505	3	11,11,12	1.16	1 (9%)	15,15,17	1.27	2 (13%)
7	MAN	F	501	3	11,11,12	1.80	2 (18%)	15,15,17	2.24	6 (40%)
7	MAN	D	507	3	11,11,12	1.65	2 (18%)	15,15,17	1.80	2 (13%)
6	GCH	A	1101	-	36,36,36	8.06	26 (72%)	56,56,56	3.07	28 (50%)
7	MAN	E	201	2	11,11,12	0.86	0	15,15,17	0.76	0
7	MAN	D	508	3	11,11,12	1.44	2 (18%)	15,15,17	1.27	1 (6%)
7	MAN	F	502	3	11,11,12	1.17	0	15,15,17	1.79	1 (6%)
7	MAN	F	508	3	11,11,12	1.87	3 (27%)	15,15,17	1.48	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
7	MAN	F	509	3	-	0/2/19/22	0/1/1/1
7	MAN	D	506	3	-	1/2/19/22	0/1/1/1
7	MAN	F	507	3	-	1/2/19/22	0/1/1/1
7	MAN	F	506	3	-	2/2/19/22	0/1/1/1
7	MAN	D	502	3	-	0/2/19/22	0/1/1/1
8	NAG	F	505	3	-	2/6/23/26	0/1/1/1
7	MAN	E	202	2	-	0/2/19/22	0/1/1/1
7	MAN	F	504	3	-	0/2/19/22	0/1/1/1
6	GCH	A	1102	-	-	1/14/79/79	0/4/4/4
7	MAN	C	202	2	-	0/2/19/22	0/1/1/1
7	MAN	F	503	3	-	0/2/19/22	0/1/1/1
7	MAN	D	503	3	-	0/2/19/22	0/1/1/1
7	MAN	D	501	3	-	0/2/19/22	0/1/1/1
7	MAN	D	504	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	C	201	2	-	0/2/19/22	0/1/1/1
7	MAN	D	505	3	-	1/2/19/22	0/1/1/1
7	MAN	F	501	3	-	0/2/19/22	0/1/1/1
7	MAN	D	507	3	-	1/2/19/22	0/1/1/1
6	GCH	A	1101	-	-	2/14/79/79	0/4/4/4
7	MAN	E	201	2	-	0/2/19/22	0/1/1/1
7	MAN	D	508	3	-	2/2/19/22	0/1/1/1
7	MAN	F	502	3	-	0/2/19/22	0/1/1/1
7	MAN	F	508	3	-	1/2/19/22	0/1/1/1

The worst 5 of 87 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1102	GCH	C9-C14	-23.62	1.07	1.53
6	A	1101	GCH	C9-C14	-22.68	1.09	1.53
6	A	1102	GCH	C9-C8	-21.05	1.17	1.53
6	A	1101	GCH	C9-C8	-20.62	1.18	1.53
6	A	1101	GCH	C3-C2	-14.03	1.32	1.55

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1101	GCH	C19-C18-C20	-7.13	99.19	110.36
6	A	1101	GCH	O3-C12-C13	-6.23	100.49	111.03
6	A	1102	GCH	O3-C12-C13	-6.23	100.50	111.03
6	A	1101	GCH	C7-C8-C9	6.17	118.06	111.48
6	A	1101	GCH	O1-C8-C7	-6.10	94.80	109.94

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1101	GCH	O4-C24-CA-N
6	A	1101	GCH	O5-C24-CA-N
8	F	505	NAG	C4-C5-C6-O6
8	F	505	NAG	O5-C5-C6-O6
7	F	506	MAN	O5-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	507	MAN	1	0
6	A	1102	GCH	8	0
7	F	503	MAN	1	0
7	D	503	MAN	1	0
7	D	501	MAN	1	0
7	D	504	MAN	1	0
7	D	505	MAN	1	0
6	A	1101	GCH	1	0
7	D	508	MAN	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 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 MAN F 509

Bond lengths

Bond angles

Torsions

Rings

Ligand MAN D 506

Bond lengths

Bond angles

Torsions

Rings

Ligand MAN F 507

Bond lengths

Bond angles

Torsions

Rings

wwPDB X-ray Structure Validation Summary Report

Ligand MAN F 506

Bond lengths

Bond angles

Torsions

Rings

Ligand MAN D 502

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG F 505

Bond lengths

Bond angles

Torsions

Rings

Ligand MAN E 202

Bond lengths

Bond angles

Torsions

Rings

Ligand MAN F 504

Bond lengths

Bond angles

Torsions

Rings

Ligand GCH A 1102

Bond lengths

Bond angles

Torsions

Rings

Ligand MAN C 202

Bond lengths

Bond angles

Torsions

Rings

Ligand MAN F 503

Bond lengths

Bond angles

Torsions

Rings

Ligand MAN D 503

Bond lengths

Bond angles

Torsions

Rings

Ligand MAN D 501

Bond lengths

Bond angles

Torsions

Rings

Ligand MAN D 504

Bond lengths

Bond angles

Torsions

Rings

Ligand MAN C 201

Bond lengths

Bond angles

Torsions

Rings

Ligand MAN D 505

Bond lengths

Bond angles

Torsions

Rings

Ligand MAN F 501

Bond lengths

Bond angles

Torsions

Rings

Ligand MAN D 507

Bond lengths

Bond angles

Torsions

Rings

Ligand GCH A 1101

Bond lengths

Bond angles

Torsions

Rings

wwPDB X-ray Structure Validation Summary Report

Ligand MAN E 201

Bond lengths

Bond angles

Torsions

Rings

Ligand MAN D 508

Bond lengths

Bond angles

Torsions

Rings

Ligand MAN F 502

Bond lengths

Bond angles

Torsions

Rings

Ligand MAN F 508

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 ⓘ

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(Å^2)	Q<0.9
1	A	119/125 (95%)	0.24	1 (0%)	86	87	24, 33, 68, 99	0
1	B	120/125 (96%)	0.28	2 (1%)	70	72	25, 34, 71, 110	0
2	C	107/108 (99%)	0.43	10 (9%)	8	10	43, 66, 113, 140	0
2	E	107/108 (99%)	0.86	15 (14%)	2	2	37, 72, 122, 148	0
3	D	211/221 (95%)	0.29	14 (6%)	18	20	29, 58, 111, 132	0
3	F	211/221 (95%)	0.20	10 (4%)	31	34	28, 57, 108, 127	0
All	All	875/908 (96%)	0.35	52 (5%)	22	25	24, 56, 112, 148	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	421	VAL	12.0
2	E	132	ALA	8.9
3	F	255	GLY	8.4
2	E	133	CYS	7.4
3	F	422	GLU	7.0

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

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

6.3   Carbohydrates ⓘ

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.

WORLDWIDE
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PROTEIN DATA BANK

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BGC	J	2	11/12	0.31	0.42	106,132,141,146	0
4	FUC	J	1	10/11	0.52	0.42	130,137,150,154	0
5	NAG	I	1	14/15	0.65	0.31	120,136,151,165	0
5	NAG	I	2	14/15	0.66	0.40	138,148,165,170	0
4	BGC	G	2	11/12	0.68	0.42	100,135,149,151	0
4	FUC	G	1	10/11	0.75	0.27	113,130,141,142	0
4	BGC	K	2	11/12	0.94	0.10	44,50,57,60	0
4	BGC	H	2	11/12	0.95	0.08	55,58,64,67	0
4	FUC	H	1	10/11	0.96	0.07	54,61,65,70	0
4	FUC	K	1	10/11	0.97	0.09	39,44,49,49	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 G:

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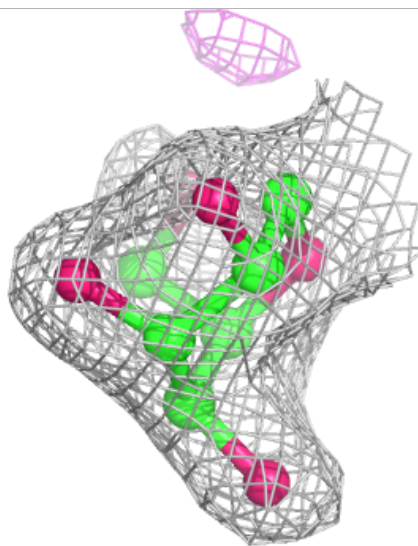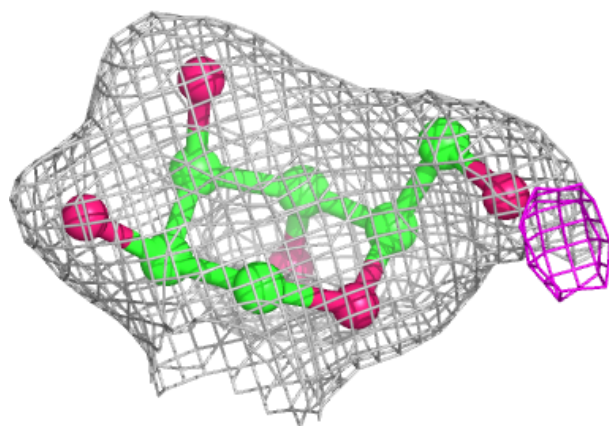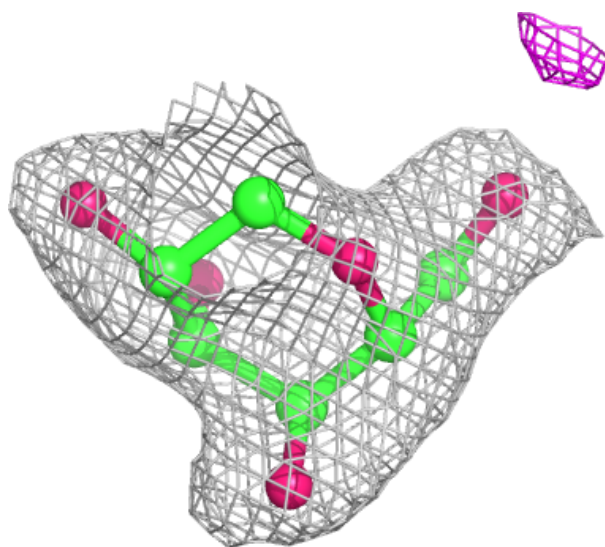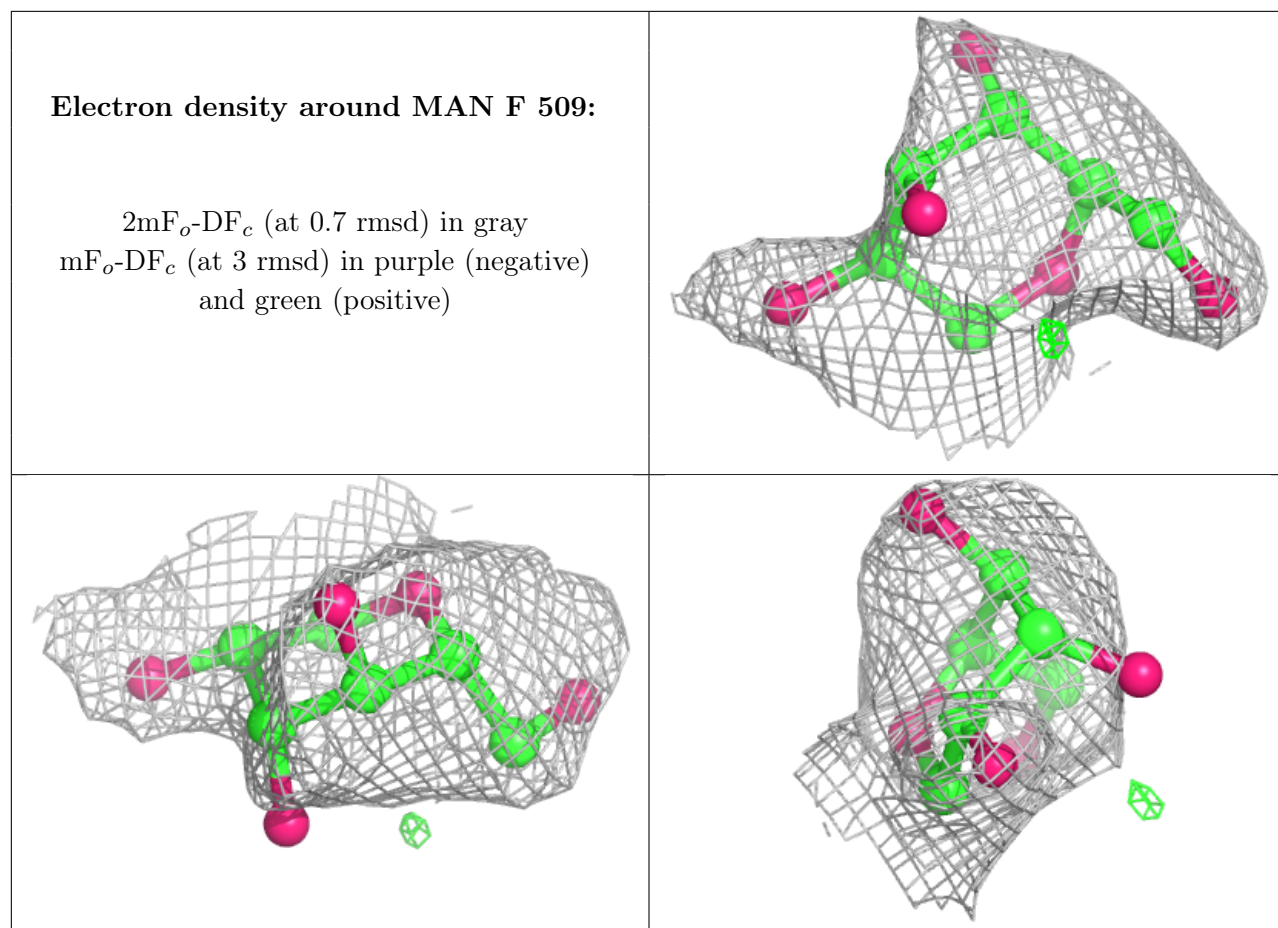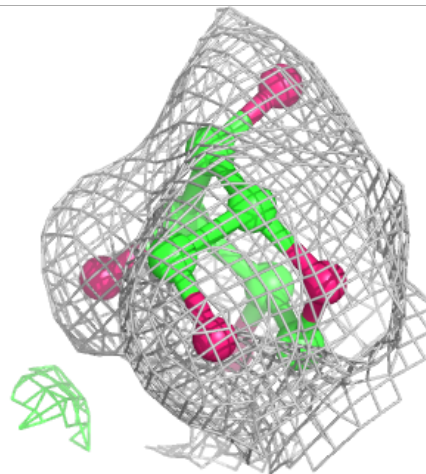mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around Chain H:

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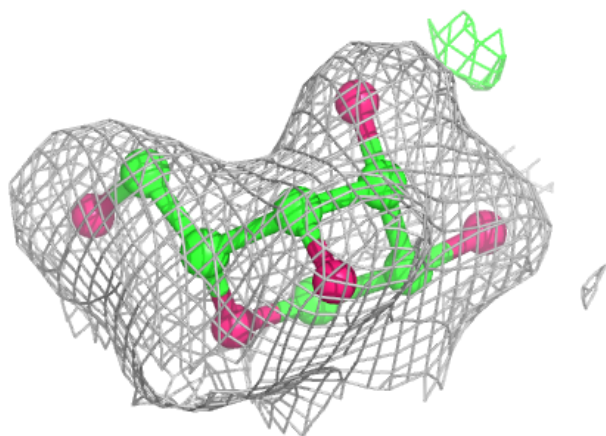and green (positive)
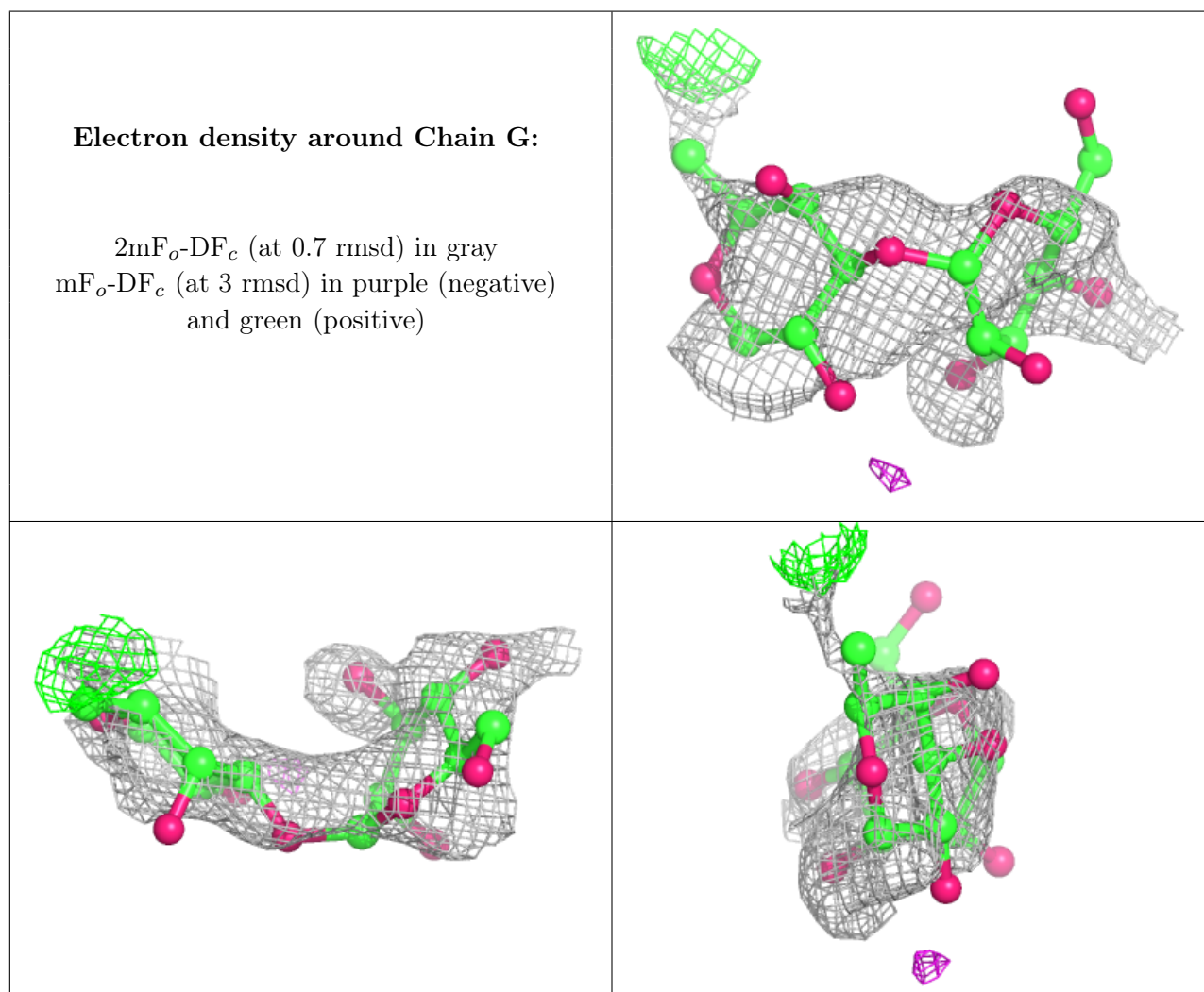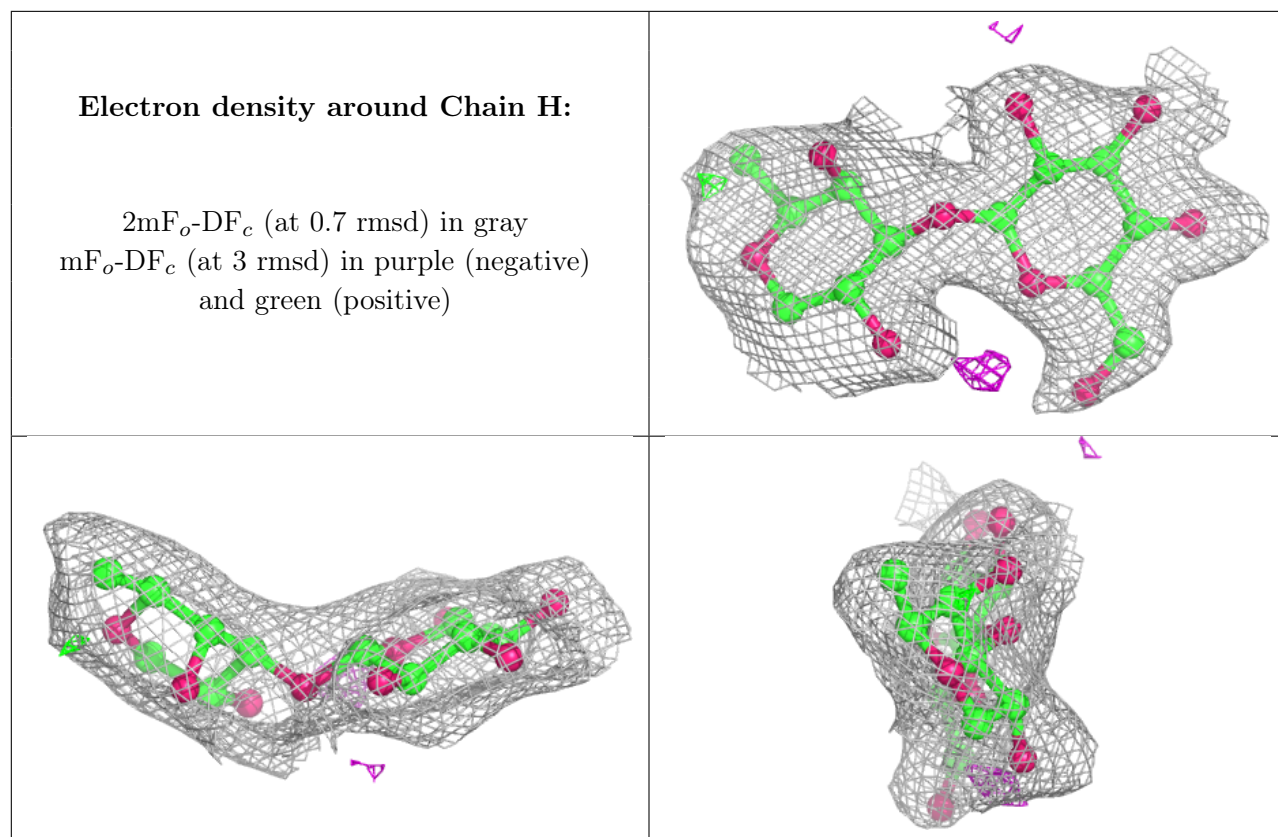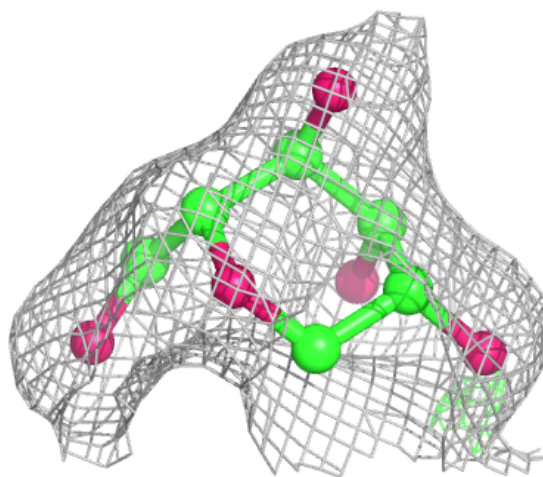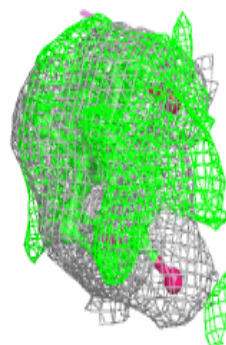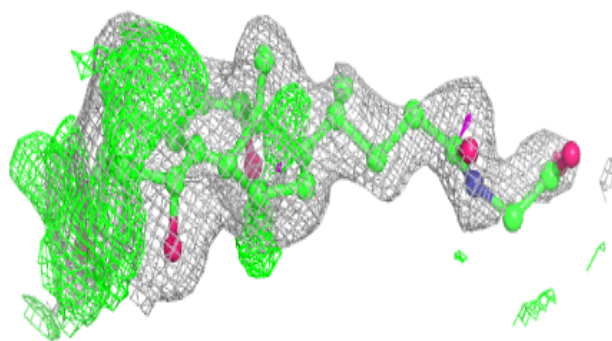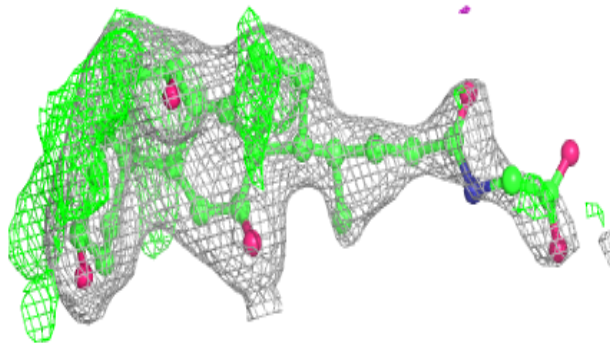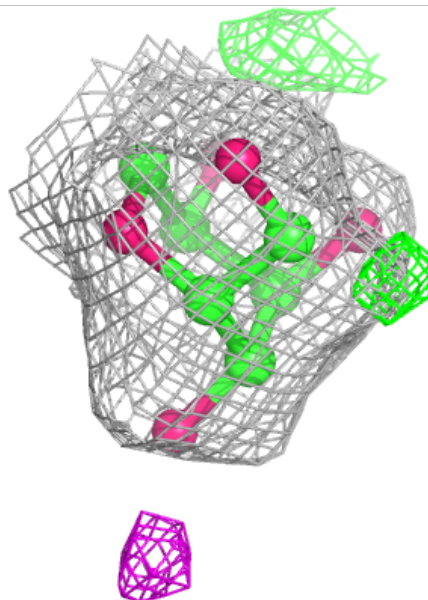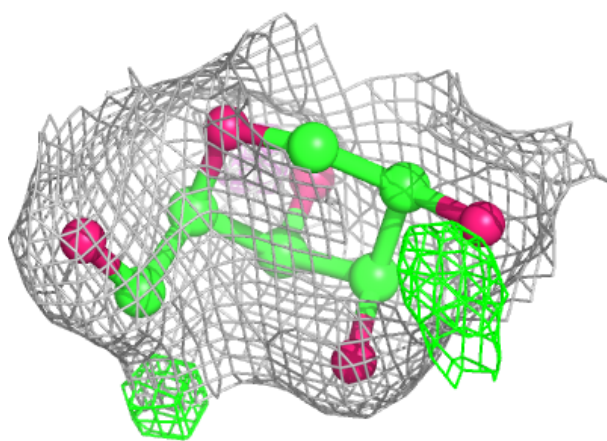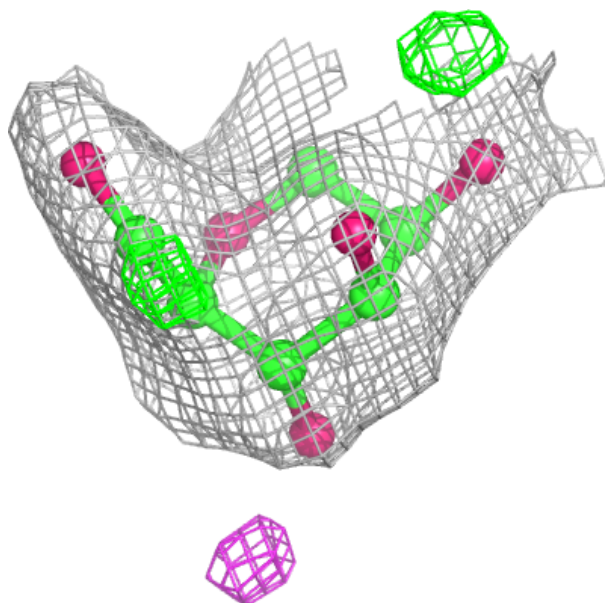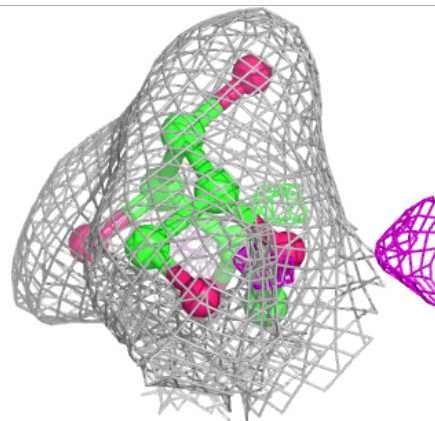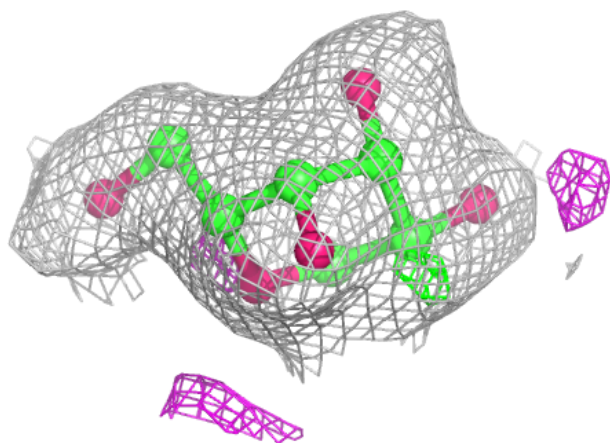
Electron density around Chain J:

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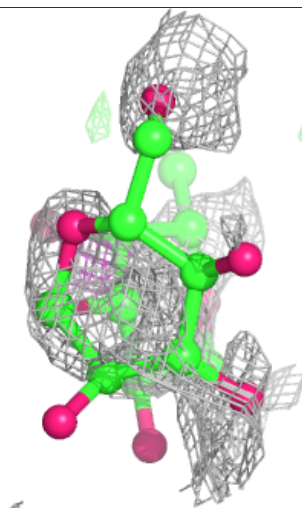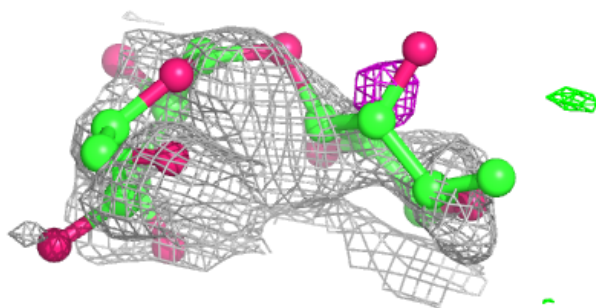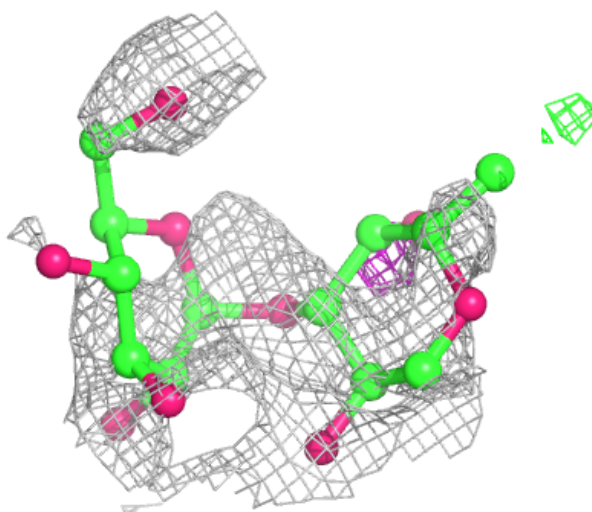
Electron density around Chain K:

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

Electron density around Chain 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)
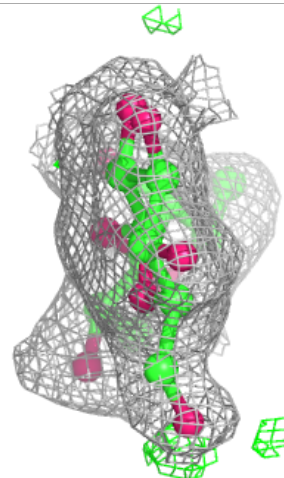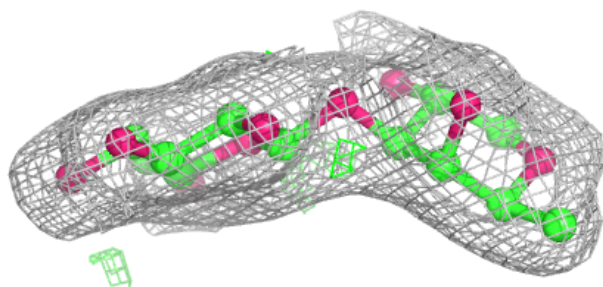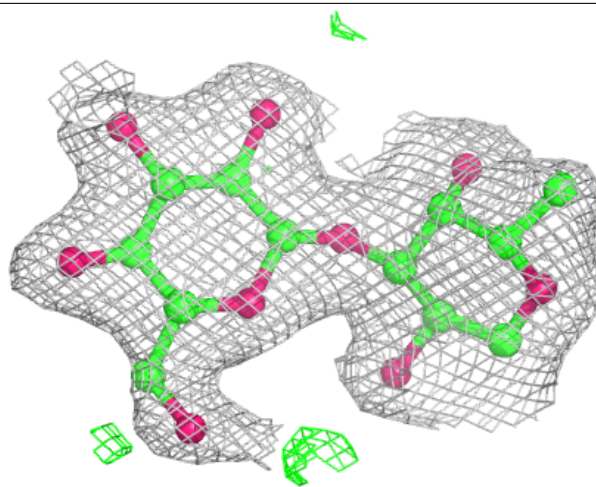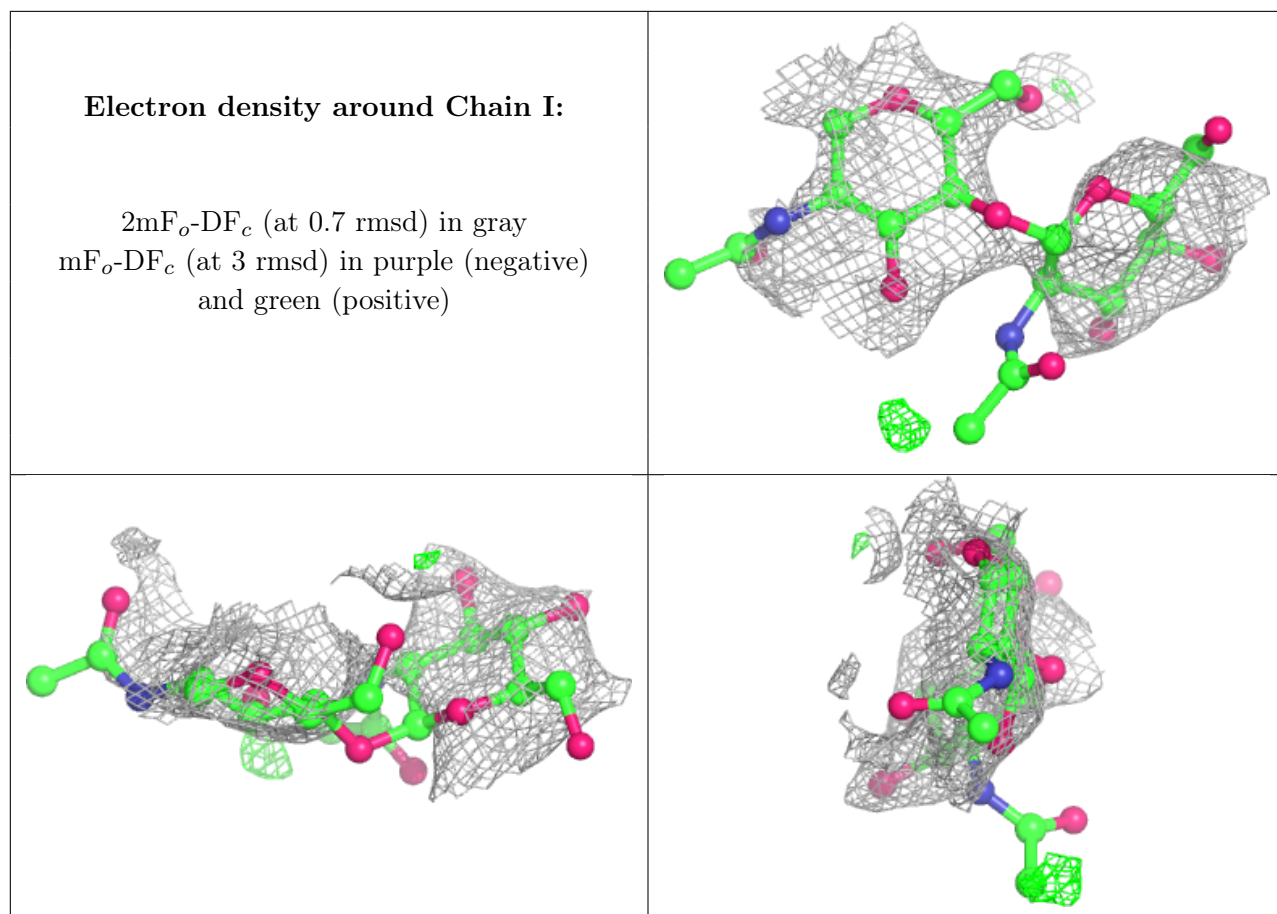
6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	MAN	C	202	11/12	0.55	0.47	77,86,101,105	11
7	MAN	E	202	11/12	0.59	0.63	80,90,98,102	11
7	MAN	D	504	11/12	0.73	0.26	58,79,90,91	0
7	MAN	F	501	11/12	0.73	0.19	40,56,62,67	11
8	NAG	F	505	14/15	0.73	0.26	107,125,135,136	0
7	MAN	F	504	11/12	0.75	0.26	56,75,90,111	0
7	MAN	D	506	11/12	0.82	0.16	70,73,79,80	0
7	MAN	F	508	11/12	0.86	0.09	72,79,83,83	0
7	MAN	D	501	11/12	0.87	0.26	41,49,56,60	11
7	MAN	D	507	11/12	0.88	0.14	64,67,73,79	0
7	MAN	F	509	11/12	0.88	0.17	73,85,98,100	0
7	MAN	F	506	11/12	0.88	0.19	62,67,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GCH	A	1101	33/33	0.90	0.20	30,39,95,106	0
7	MAN	D	505	11/12	0.90	0.10	69,72,81,82	0
7	MAN	F	502	11/12	0.90	0.08	42,51,56,58	0
7	MAN	E	201	11/12	0.90	0.18	67,70,74,75	0
7	MAN	C	201	11/12	0.91	0.13	61,64,69,73	0
7	MAN	D	508	11/12	0.92	0.11	67,70,77,79	0
7	MAN	D	502	11/12	0.93	0.08	43,50,56,57	0
6	GCH	A	1102	33/33	0.93	0.16	31,39,72,84	0
7	MAN	F	507	11/12	0.93	0.09	64,68,71,75	0
7	MAN	D	503	11/12	0.94	0.08	43,47,51,52	0
7	MAN	F	503	11/12	0.94	0.09	46,48,51,51	0

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 MAN C 202:

$2\text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray
$\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)
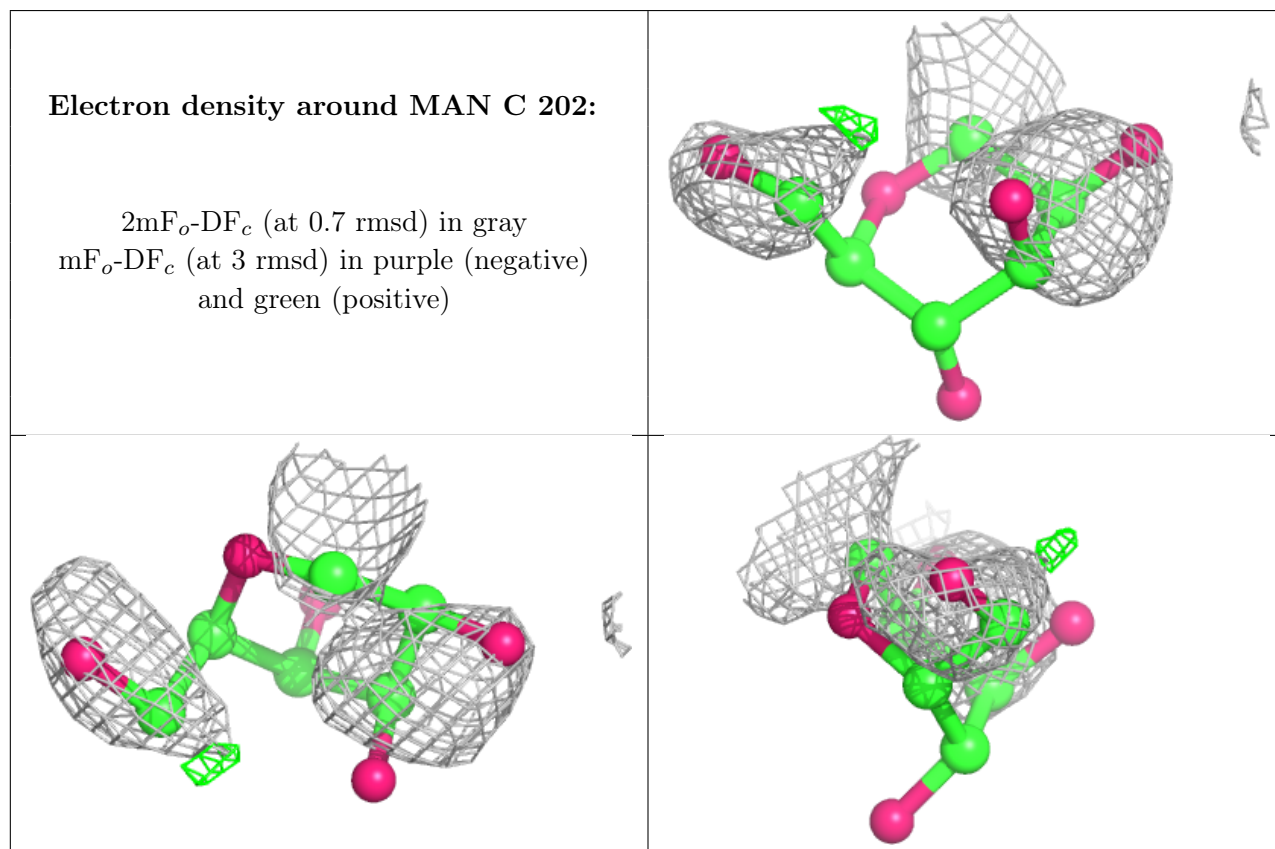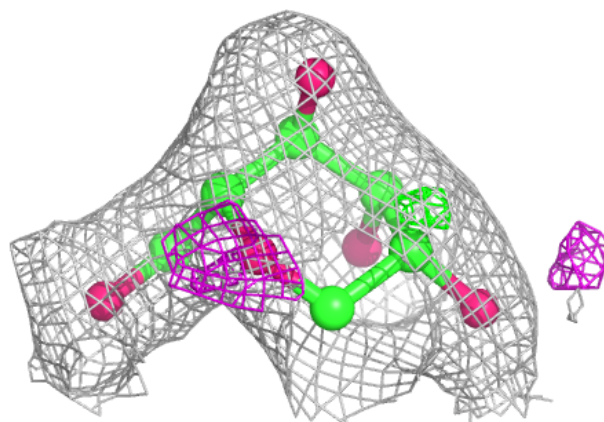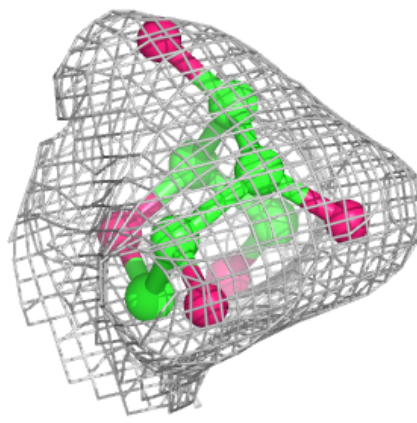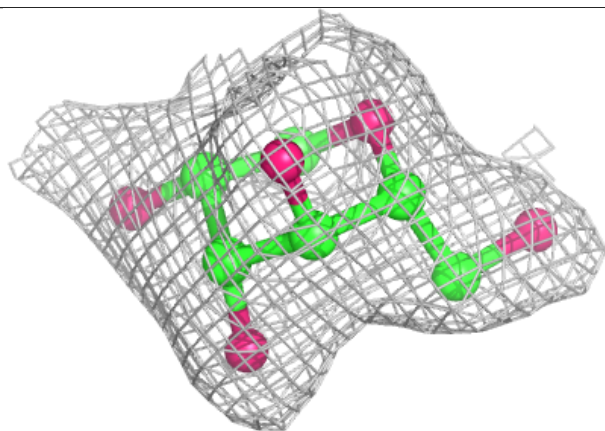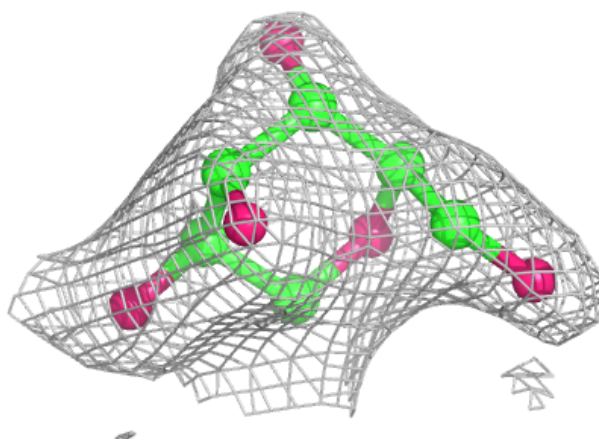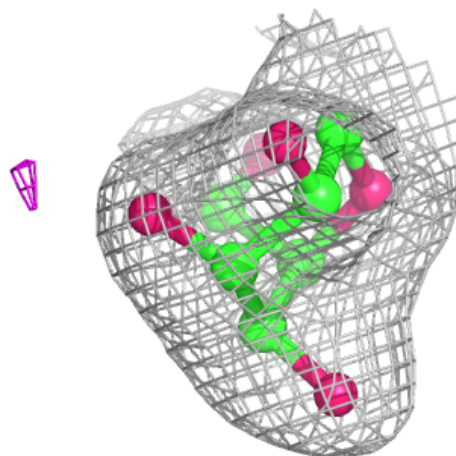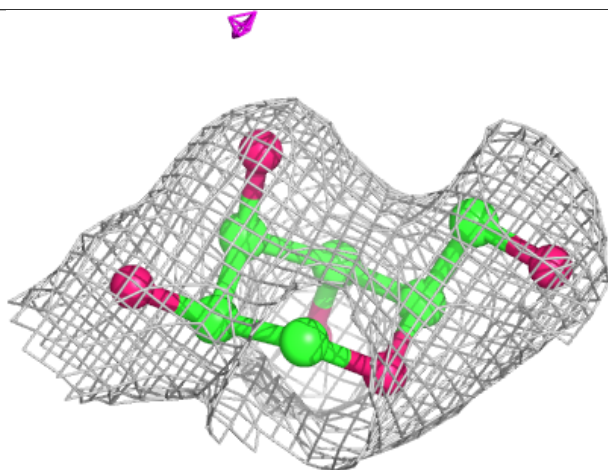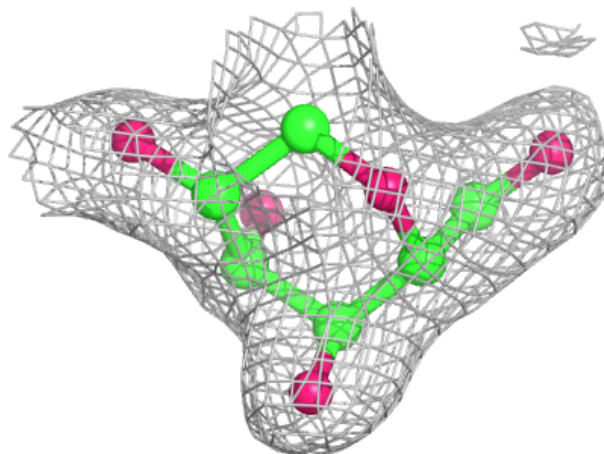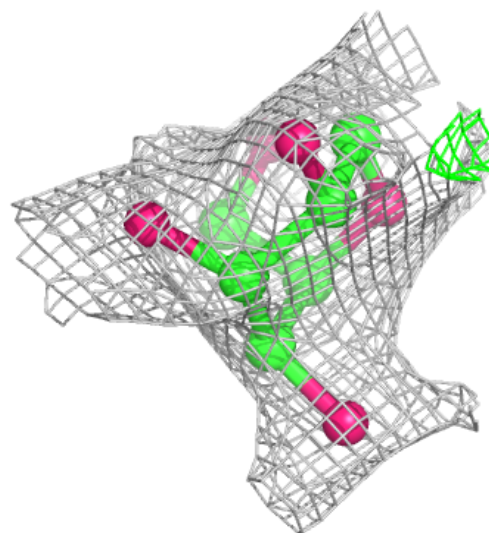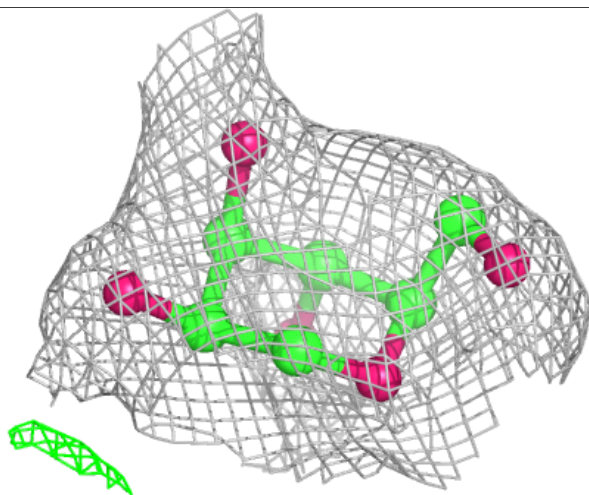
Electron density around MAN E 202:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
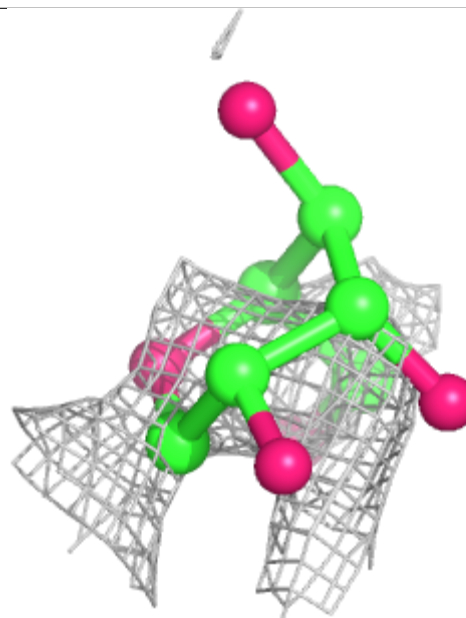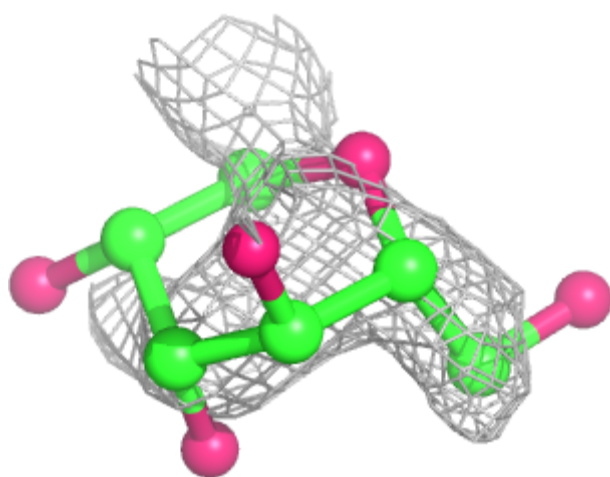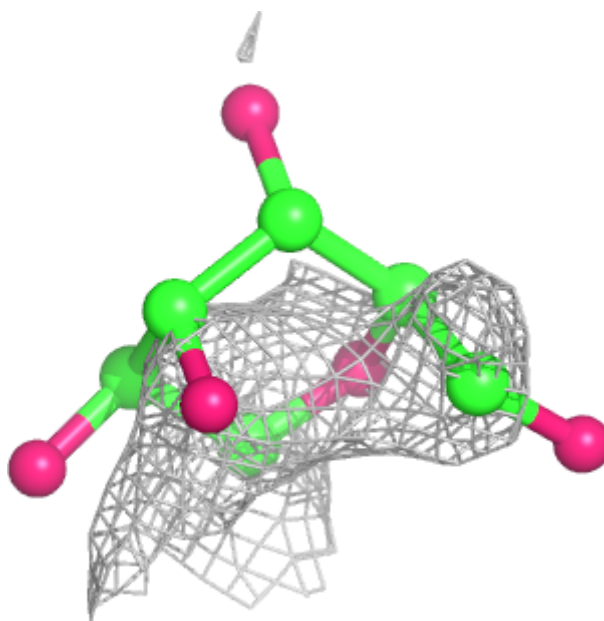
Electron density around MAN D 504:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
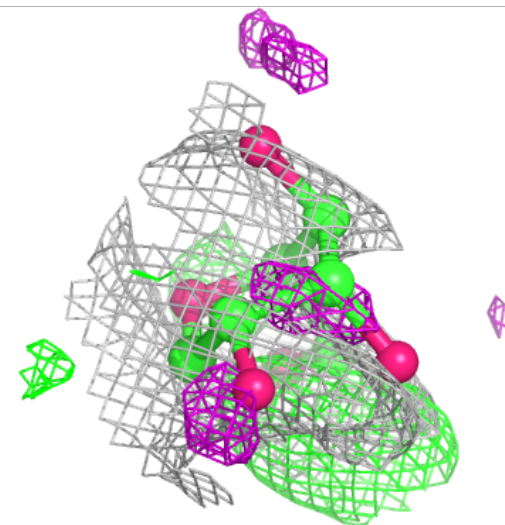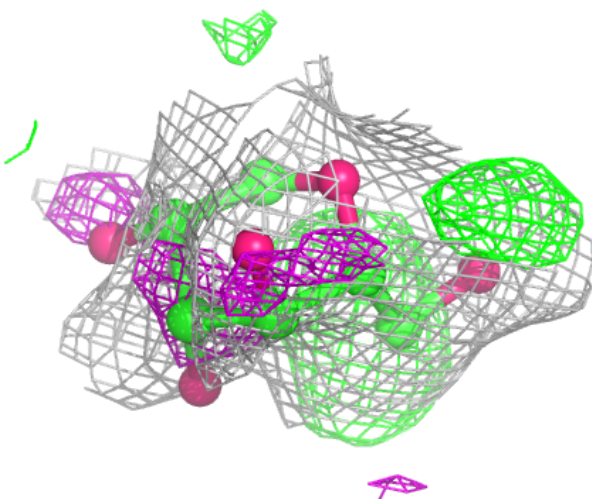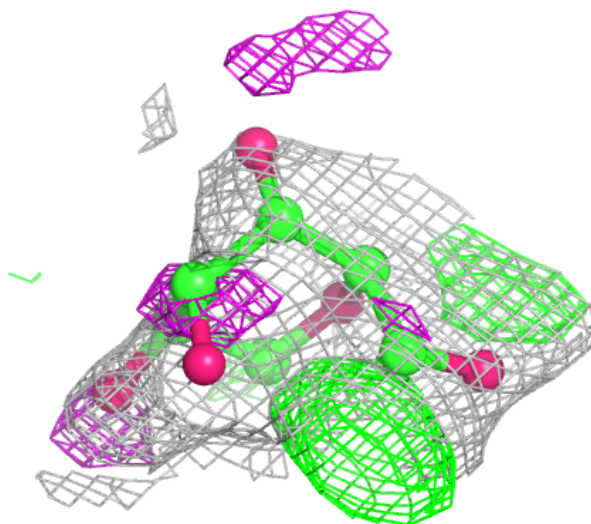
Electron density around MAN F 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
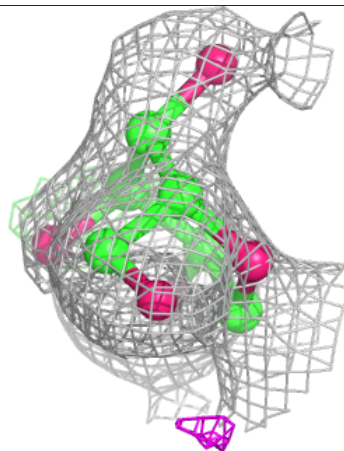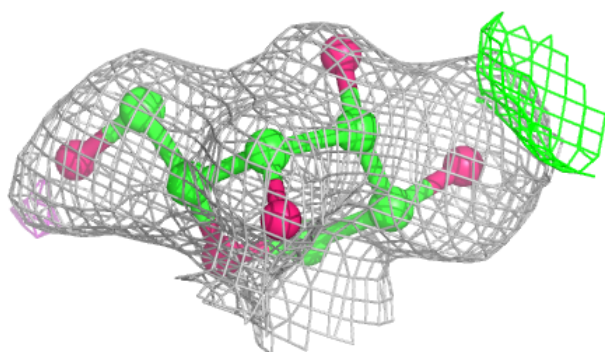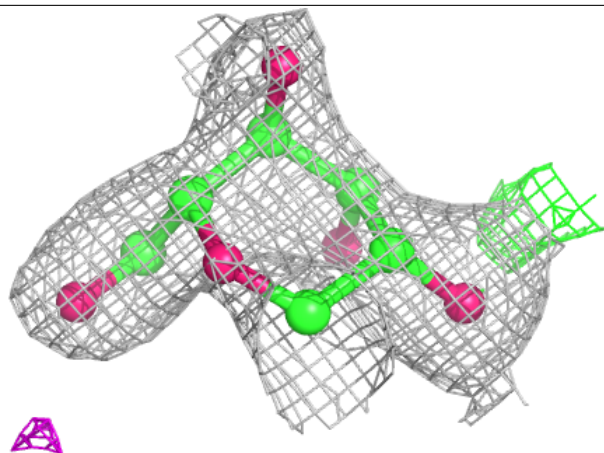
Electron density around NAG F 505:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
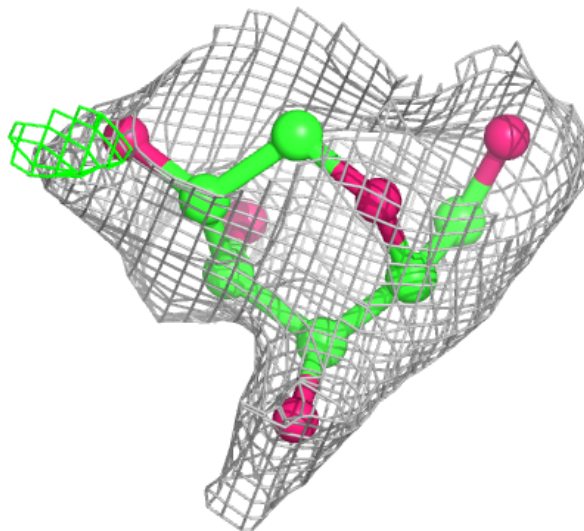$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
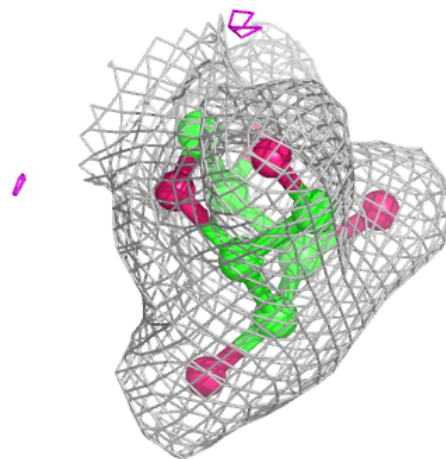and green (positive)
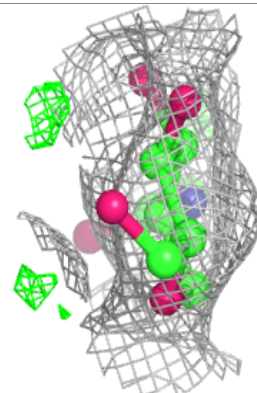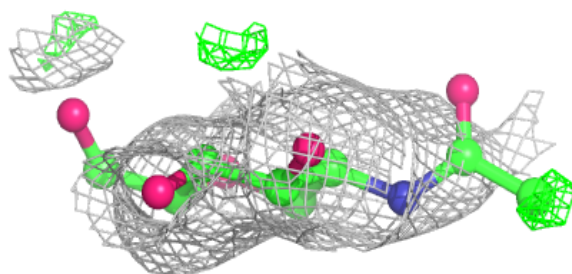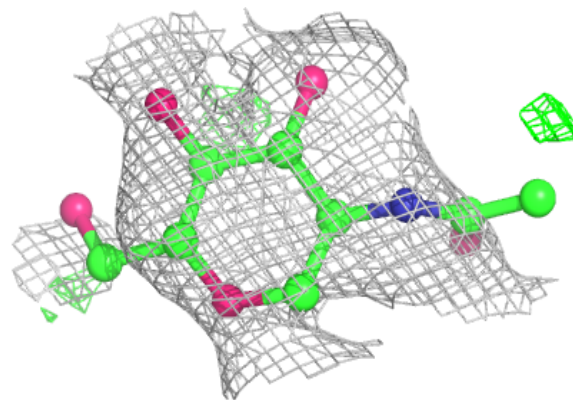
Electron density around MAN F 504:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
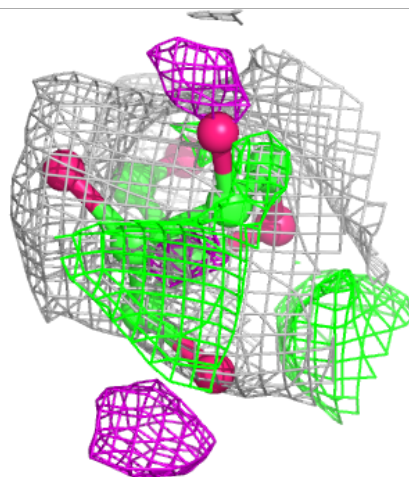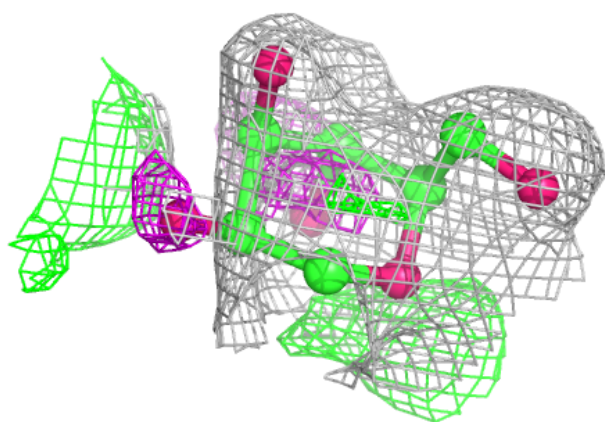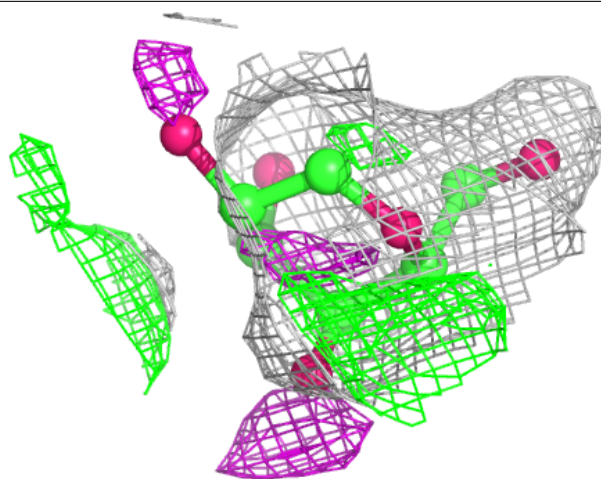
Electron density around MAN D 506:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
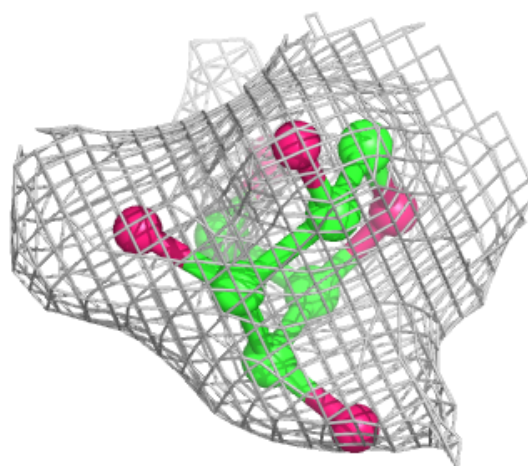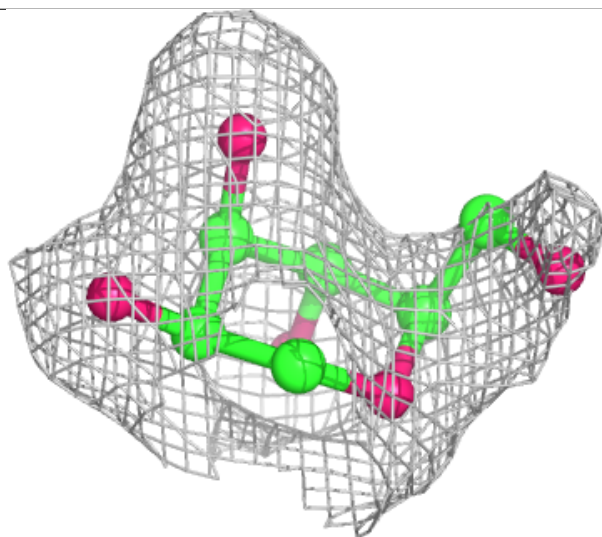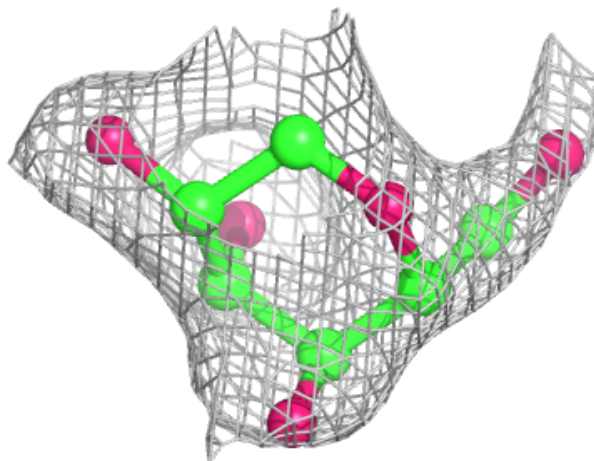
Electron density around MAN F 508:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
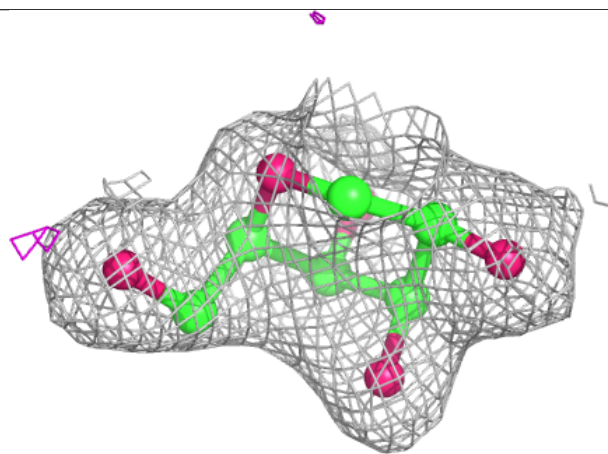$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
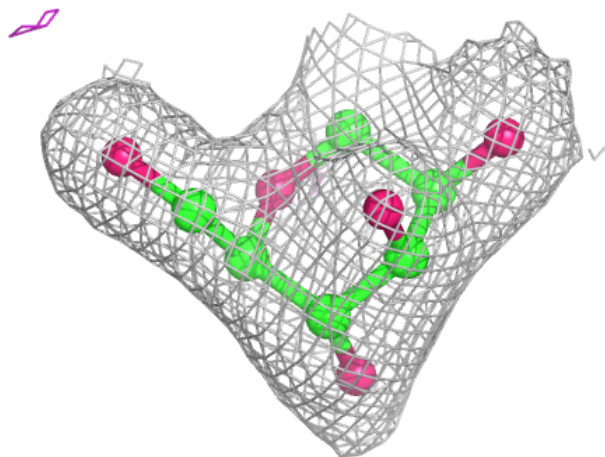and green (positive)
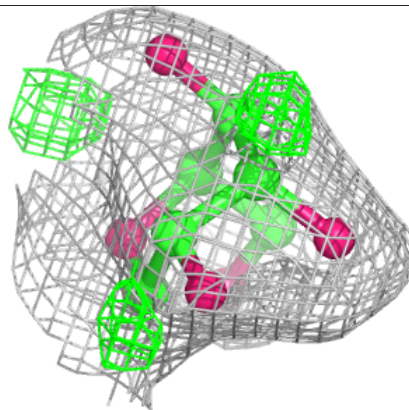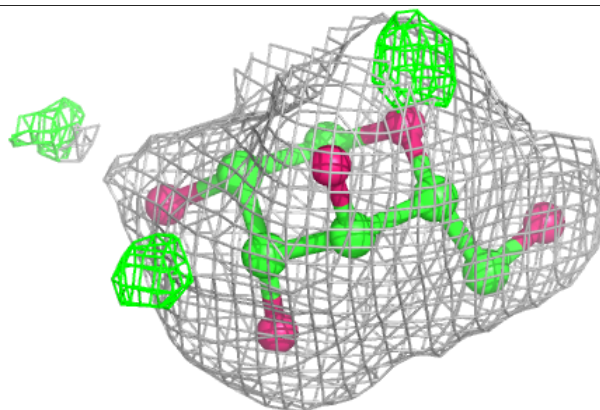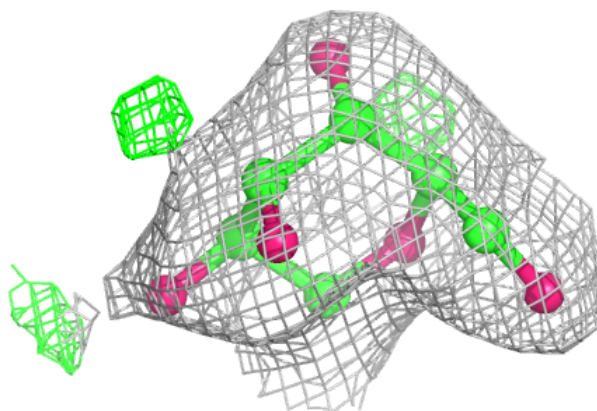
Electron density around MAN D 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
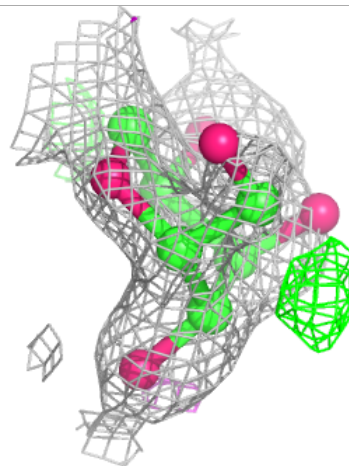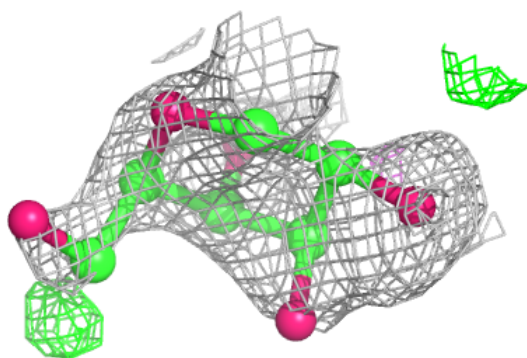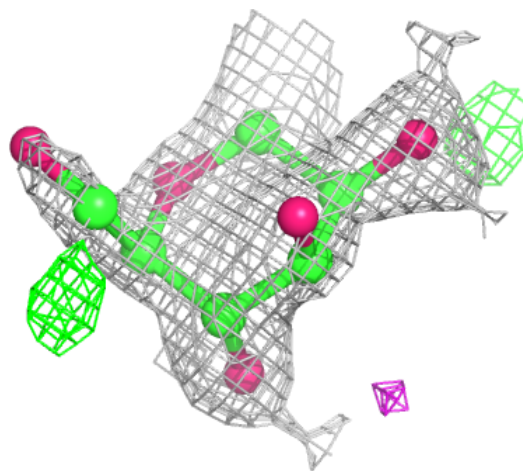
Electron density around MAN D 507:

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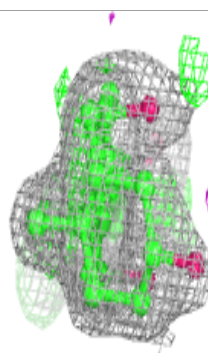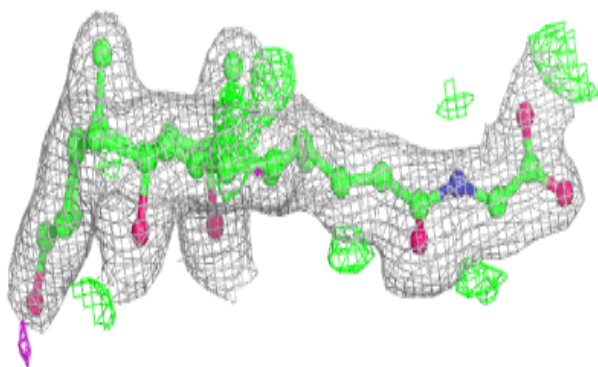and green (positive)

Electron density around MAN F 509:

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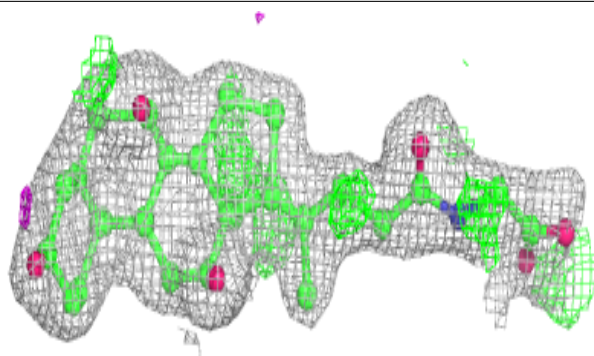and green (positive)

Electron density around MAN F 506:

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

Electron density around GCH A 1101:

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

Electron density around MAN D 505:

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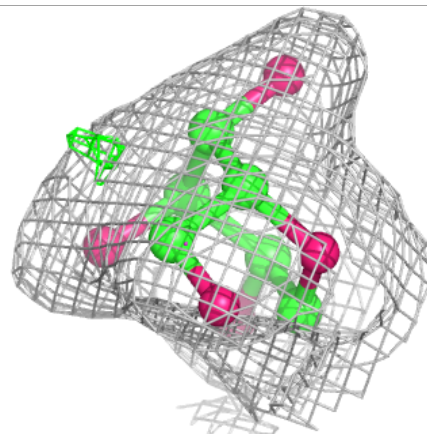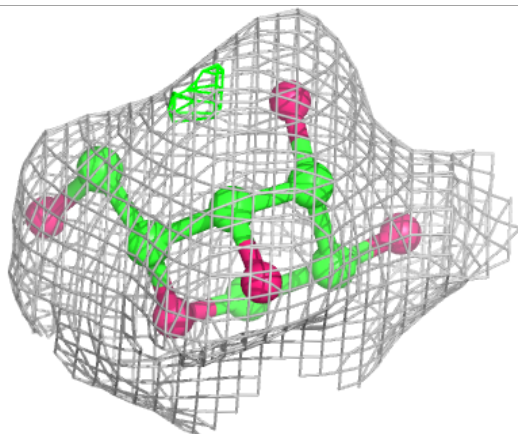and green (positive)

Electron density around MAN F 502:

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

Electron density around MAN E 201:

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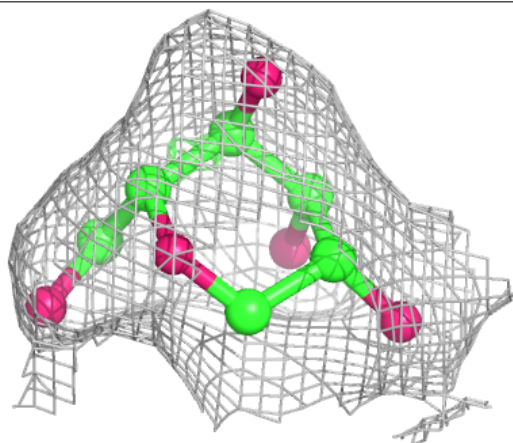and green (positive)

Electron density around MAN C 201:

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

Electron density around MAN D 508:

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

Electron density around MAN D 502:

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

Electron density around GCH A 1102:

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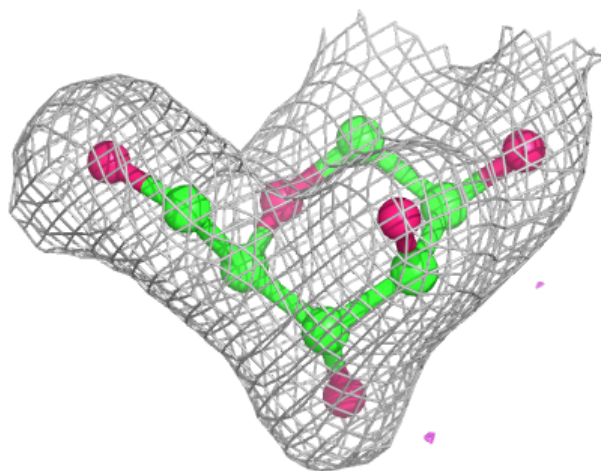and green (positive)

Electron density around MAN F 507:

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 MAN D 503:

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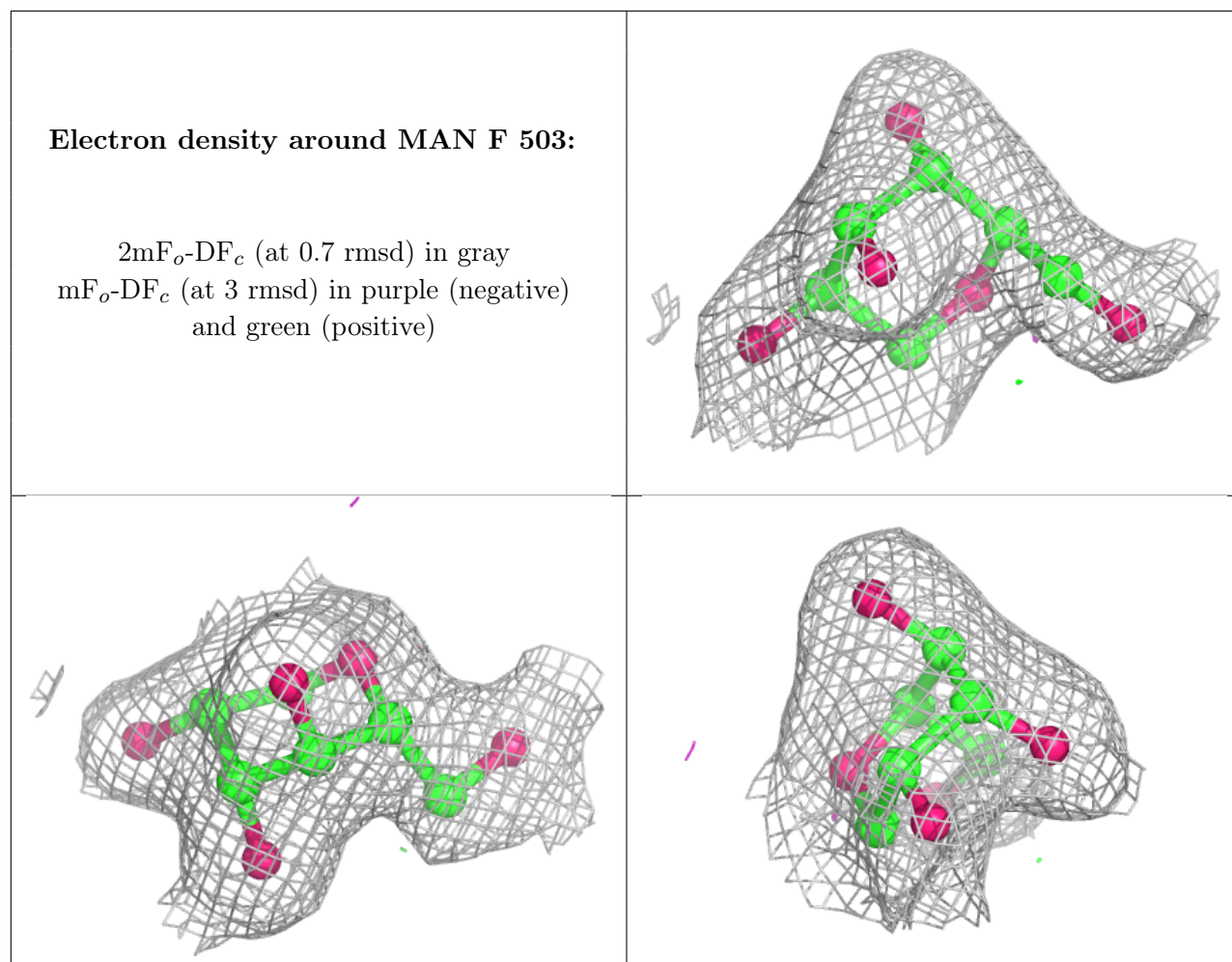and green (positive)

Electron density around MAN F 503:

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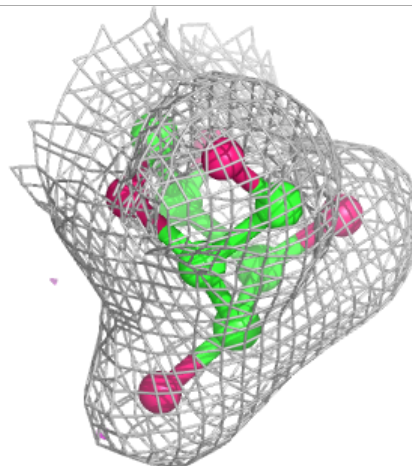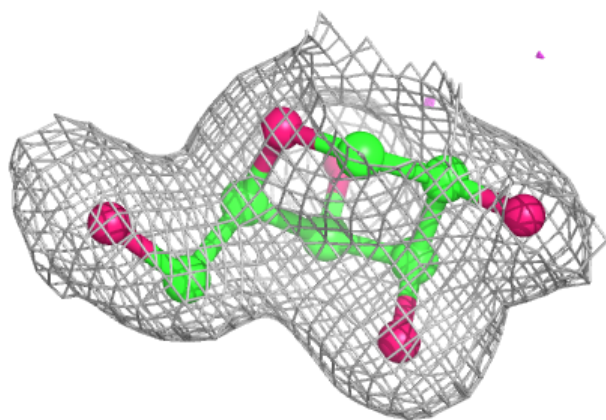
6.5 Other polymers (i)

There are no such residues in this entry.