WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2023 – 12:54 PM EDT

PDB ID	:	1C4Q
Title	:	MUTATED SHIGA-LIKE TOXIN B SUBUNIT (F30A/W34A) COMPLEXED WITH RECEPTOR GB3 ANALOGUE
Authors	:	Ling, H.; Brunton, J.L.; Read, R.J.
Deposited on	:	1999-08-31
Resolution	:	1.52 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

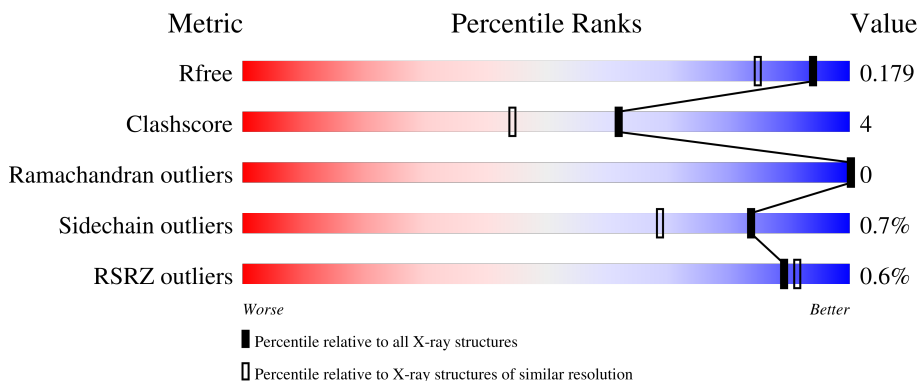|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 1.52 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.
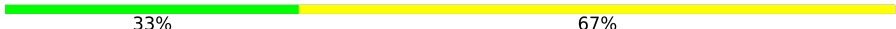
Metric	Percentile Ranks	Value
Rfree		0.179
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		0.7%
RSRZ outliers		0.6%

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	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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	69	90% 10%
1	B	69	94% 6%
1	C	69	% 88% 12%
1	D	69	90% 9% •
1	E	69	% 86% 14%

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Mol	Chain	Length	Quality of chain
2	F	3	100%
2	G	3	33% 67%
2	H	3	67% 33%
2	I	3	33% 67%
2	J	3	67% 33%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 3232 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.
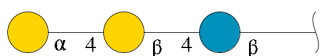
- Molecule 1 is a protein called PROTEIN (SHIGA-LIKE TOXIN I SUBUNIT B).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	69	Total	C	N	O	S	0	2	0
			533	331	89	110	3			
1	B	69	Total	C	N	O	S	0	1	0
			528	328	89	108	3			
1	C	69	Total	C	N	O	S	0	2	0
			533	331	89	110	3			
1	D	69	Total	C	N	O	S	0	4	0
			540	336	90	111	3			
1	E	69	Total	C	N	O	S	0	4	0
			539	337	89	110	3			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	130	ALA	PHE	engineered mutation	UNP P08027
A	134	ALA	TRP	engineered mutation	UNP P08027
B	230	ALA	PHE	engineered mutation	UNP P08027
B	234	ALA	TRP	engineered mutation	UNP P08027
C	330	ALA	PHE	engineered mutation	UNP P08027
C	334	ALA	TRP	engineered mutation	UNP P08027
D	430	ALA	PHE	engineered mutation	UNP P08027
D	434	ALA	TRP	engineered mutation	UNP P08027
E	530	ALA	PHE	engineered mutation	UNP P08027
E	534	ALA	TRP	engineered mutation	UNP P08027

- Molecule 2 is an oligosaccharide called alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	F	3	Total 34	C 18	O 16	0	0	0
2	G	3	Total 34	C 18	O 16	0	0	0
2	H	3	Total 34	C 18	O 16	0	0	0
2	I	3	Total 34	C 18	O 16	0	0	0
2	J	3	Total 34	C 18	O 16	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	77	Total 77	O 77	0	0
3	B	83	Total 83	O 83	0	0
3	C	73	Total 73	O 73	0	0
3	D	81	Total 81	O 81	0	0
3	E	75	Total 75	O 75	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.
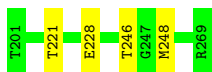
• Molecule 1: PROTEIN (SHIGA-LIKE TOXIN I SUBUNIT B)

Chain A:

90%   10%

T101 V109 T112 V122 E128 H158 N159 V166 R169

• Molecule 1: PROTEIN (SHIGA-LIKE TOXIN I SUBUNIT B)

Chain B:

94%   6%

T201 T221 E228 T246 G247 M248 R269

• Molecule 1: PROTEIN (SHIGA-LIKE TOXIN I SUBUNIT B)

Chain C:

%

88%   12%

T301 T312 V322 K327 E328 I352 H358 N359 R369

• Molecule 1: PROTEIN (SHIGA-LIKE TOXIN I SUBUNIT B)

Chain D:

90%   9%

T401 T412 V422 L440 N459 G460 V466 R469

• Molecule 1: PROTEIN (SHIGA-LIKE TOXIN I SUBUNIT B)

Chain E:

%

86%   14%

T501 V505 K508 Y514 V522 K523 V524 A530 H558 G562 R569
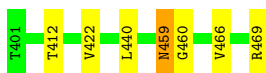
• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain F:

100%

BGC1 GAL2 GLA3

• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain G:

33%   67%

BGC1 GAL2 GLA3

• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain H:

67%   33%

BGC1 GAL2 GLA3

• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain I:

33%   67%

BGC1 GAL2 GLA3

• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain J:

67%   33%

BGC1 GAL2 GLA3

4   Data and refinement statistics   (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	44.27Å 44.16Å 54.01Å 106.24° 106.69° 98.87°	Depositor
Resolution (Å)	38.70 – 1.52 38.67 – 1.50	Depositor EDS
% Data completeness (in resolution range)	96.7 (38.70-1.52) 96.1 (38.67-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 1.50Å)	Xtriage
Refinement program	CNS 0.3D	Depositor
R, R_{free}	0.170 , 0.194 0.164 , 0.179	Depositor DCC
R_{free} test set	1300 reflections (2.32%)	wwPDB-VP
Wilson B-factor (Å^2)	16.3	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.2	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3232	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.08% 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: GAL, BGC, GLA

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	0.93	0/547	1.01	1/739 (0.1%)
1	B	0.88	0/538	0.95	0/727
1	C	1.06	0/547	1.03	0/739
1	D	0.95	0/562	0.99	0/760
1	E	0.88	0/561	0.95	0/759
All	All	0.94	0/2755	0.99	1/3724 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	166	VAL	CB-CA-C	-5.27	101.39	111.40

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	533	0	522	4	0
1	B	528	0	520	2	0
1	C	533	0	522	6	0
1	D	540	0	529	6	0
1	E	539	0	532	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	34	0	30	0	0
2	G	34	0	30	0	0
2	H	34	0	30	0	0
2	I	34	0	30	0	0
2	J	34	0	30	0	0
3	A	77	0	0	1	0
3	B	83	0	0	0	0
3	C	73	0	0	1	0
3	D	81	0	0	2	0
3	E	75	0	0	4	0
All	All	3232	0	2775	25	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 4.

All (25) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:569:ARG:NH2	3:E:896:HOH:O	2.28	0.66
1:D:459[A]:ASN:HD22	1:D:460:GLY:N	1.94	0.66
1:D:412:THR:HG22	1:D:422:VAL:HG12	1.83	0.61
1:C:358:HIS:HE1	3:C:880:HOH:O	1.83	0.60
1:C:312:THR:HG22	1:C:322[A]:VAL:HG12	1.83	0.60
1:E:522[A]:VAL:HG12	1:E:524:VAL:HG23	1.84	0.58
1:A:128:GLU:H	1:A:159:ASN:ND2	2.04	0.54
1:A:109:VAL:HG13	1:A:122[B]:VAL:HG23	1.93	0.50
1:C:328:GLU:H	1:C:359:ASN:HD22	1.60	0.49
1:A:112:THR:HG22	1:A:122[A]:VAL:HG12	1.95	0.47
1:D:469:ARG:NH1	3:D:666:HOH:O	2.46	0.47
1:A:158:HIS:HE1	3:A:858:HOH:O	1.98	0.47
1:B:221:THR:CG2	1:B:228:GLU:HG2	2.46	0.45
1:E:505[A]:VAL:HG21	1:E:524:VAL:O	2.16	0.45
1:D:459[B]:ASN:ND2	3:D:937:HOH:O	2.51	0.44
1:D:466[A]:VAL:HG12	1:E:514:TYR:HB3	2.00	0.44
1:C:327:LYS:HA	1:C:359:ASN:ND2	2.33	0.43
1:C:327:LYS:HA	1:C:359:ASN:HD21	1.83	0.42
1:E:508:LYS:NZ	3:E:981:HOH:O	2.53	0.42
1:E:501:THR:N	3:E:837:HOH:O	2.52	0.42
1:E:558:HIS:HE1	3:E:899:HOH:O	2.02	0.41
1:B:246:THR:OG1	1:B:248:MET:HG3	2.21	0.41
1:C:322[B]:VAL:HG11	1:C:352:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:530:ALA:O	1:E:562:GLY:HA2	2.21	0.41
1:D:422:VAL:HG11	1:D:440:LEU:HD13	2.02	0.40

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	69/69 (100%)	68 (99%)	1 (1%)	0	100	100
1	B	68/69 (99%)	66 (97%)	2 (3%)	0	100	100
1	C	69/69 (100%)	67 (97%)	2 (3%)	0	100	100
1	D	71/69 (103%)	69 (97%)	2 (3%)	0	100	100
1	E	71/69 (103%)	69 (97%)	2 (3%)	0	100	100
All	All	348/345 (101%)	339 (97%)	9 (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	61/59 (103%)	61 (100%)	0	100	100
1	B	60/59 (102%)	60 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	61/59 (103%)	60 (98%)	1 (2%)	62	35
1	D	63/59 (107%)	61 (97%)	2 (3%)	39	10
1	E	63/59 (107%)	63 (100%)	0	100	100
All	All	308/295 (104%)	305 (99%)	3 (1%)	84	56

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	369	ARG
1	D	459[A]	ASN
1	D	459[B]	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	158	HIS
1	A	159	ASN
1	B	244	GLN
1	C	344	GLN
1	C	358	HIS
1	C	359	ASN
1	D	444	GLN
1	E	544	GLN
1	E	558	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 ⓘ

15 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	BGC	F	1	2	12,12,12	0.33	0	17,17,17	0.73	0
2	GAL	F	2	2	11,11,12	0.40	0	15,15,17	0.65	0
2	GLA	F	3	2	11,11,12	0.81	0	15,15,17	0.96	0
2	BGC	G	1	2	12,12,12	0.56	0	17,17,17	1.22	2 (11%)
2	GAL	G	2	2	11,11,12	0.60	0	15,15,17	0.85	0
2	GLA	G	3	2	11,11,12	1.28	3 (27%)	15,15,17	1.24	1 (6%)
2	BGC	H	1	2	12,12,12	0.27	0	17,17,17	0.62	0
2	GAL	H	2	2	11,11,12	0.57	0	15,15,17	0.64	0
2	GLA	H	3	2	11,11,12	1.04	1 (9%)	15,15,17	0.86	0
2	BGC	I	1	2	12,12,12	0.31	0	17,17,17	0.52	0
2	GAL	I	2	2	11,11,12	1.10	1 (9%)	15,15,17	0.71	0
2	GLA	I	3	2	11,11,12	0.77	0	15,15,17	1.22	1 (6%)
2	BGC	J	1	2	12,12,12	0.54	0	17,17,17	0.77	0
2	GAL	J	2	2	11,11,12	0.63	0	15,15,17	0.88	0
2	GLA	J	3	2	11,11,12	0.78	1 (9%)	15,15,17	1.21	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	F	1	2	-	0/2/22/22	0/1/1/1
2	GAL	F	2	2	-	0/2/19/22	0/1/1/1
2	GLA	F	3	2	-	0/2/19/22	0/1/1/1
2	BGC	G	1	2	-	2/2/22/22	0/1/1/1
2	GAL	G	2	2	-	0/2/19/22	0/1/1/1
2	GLA	G	3	2	-	0/2/19/22	0/1/1/1
2	BGC	H	1	2	-	0/2/22/22	0/1/1/1
2	GAL	H	2	2	-	0/2/19/22	0/1/1/1
2	GLA	H	3	2	-	0/2/19/22	0/1/1/1
2	BGC	I	1	2	-	0/2/22/22	0/1/1/1
2	GAL	I	2	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLA	I	3	2	-	0/2/19/22	0/1/1/1
2	BGC	J	1	2	-	0/2/22/22	0/1/1/1
2	GAL	J	2	2	-	0/2/19/22	0/1/1/1
2	GLA	J	3	2	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	3	GLA	C2-C3	2.42	1.56	1.52
2	H	3	GLA	C2-C3	2.23	1.55	1.52
2	J	3	GLA	C2-C3	2.20	1.55	1.52
2	I	2	GAL	O5-C5	2.16	1.47	1.43
2	G	3	GLA	O5-C1	-2.13	1.40	1.43
2	G	3	GLA	O5-C5	2.11	1.47	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	BGC	C6-C5-C4	-3.93	103.80	113.00
2	J	3	GLA	C1-O5-C5	3.48	116.90	112.19
2	I	3	GLA	C1-O5-C5	3.13	116.44	112.19
2	G	3	GLA	C1-O5-C5	2.61	115.73	112.19
2	G	1	BGC	C3-C4-C5	2.02	113.83	110.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	BGC	O5-C5-C6-O6
2	G	1	BGC	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings
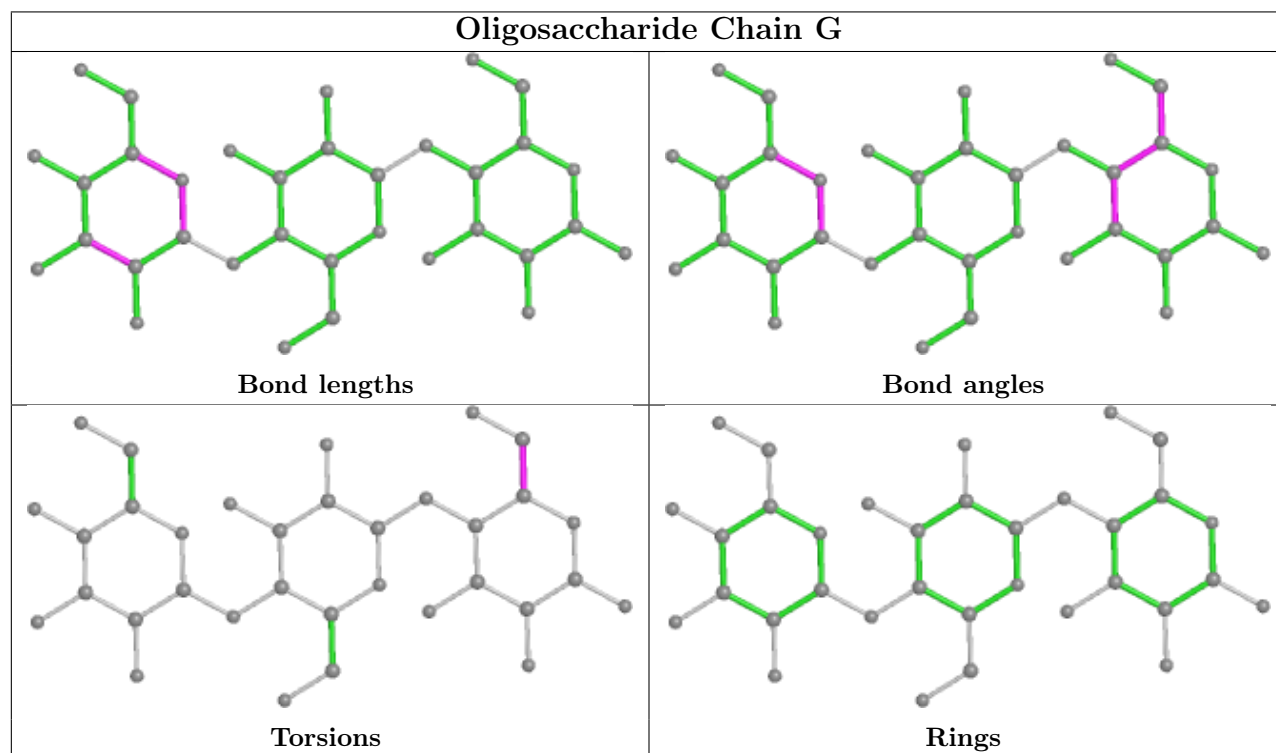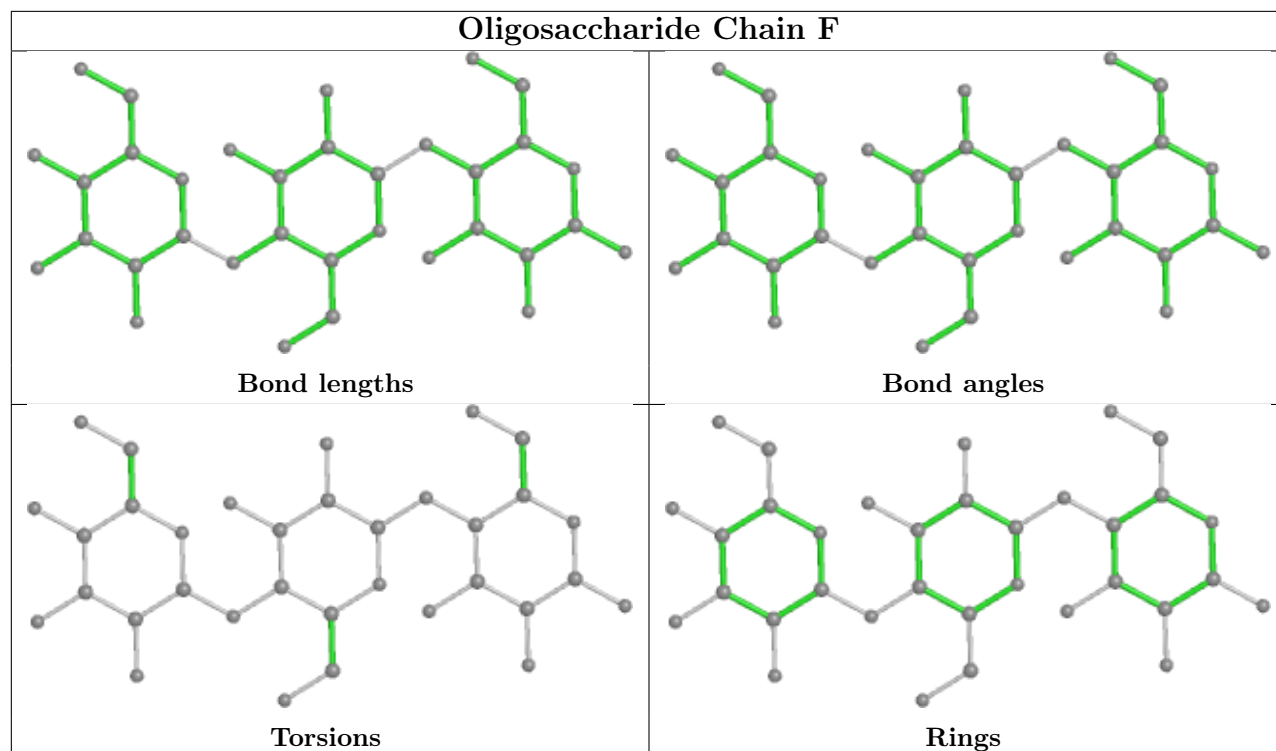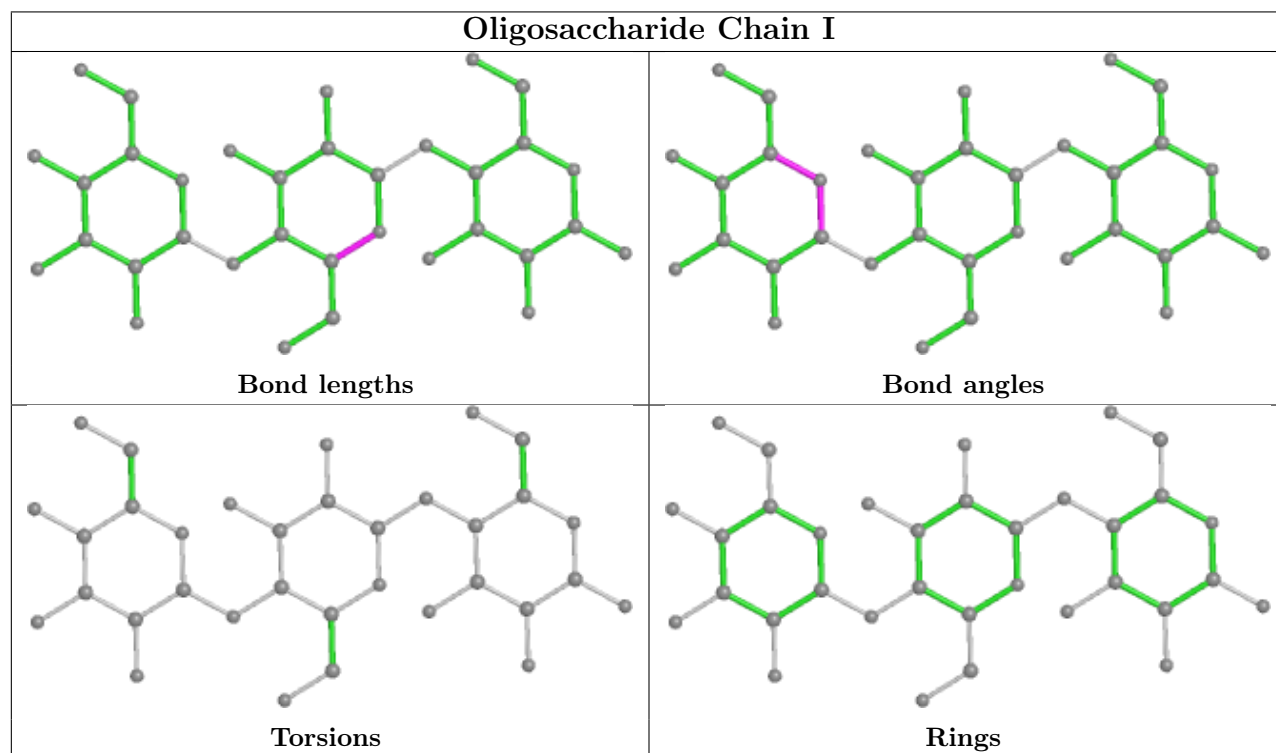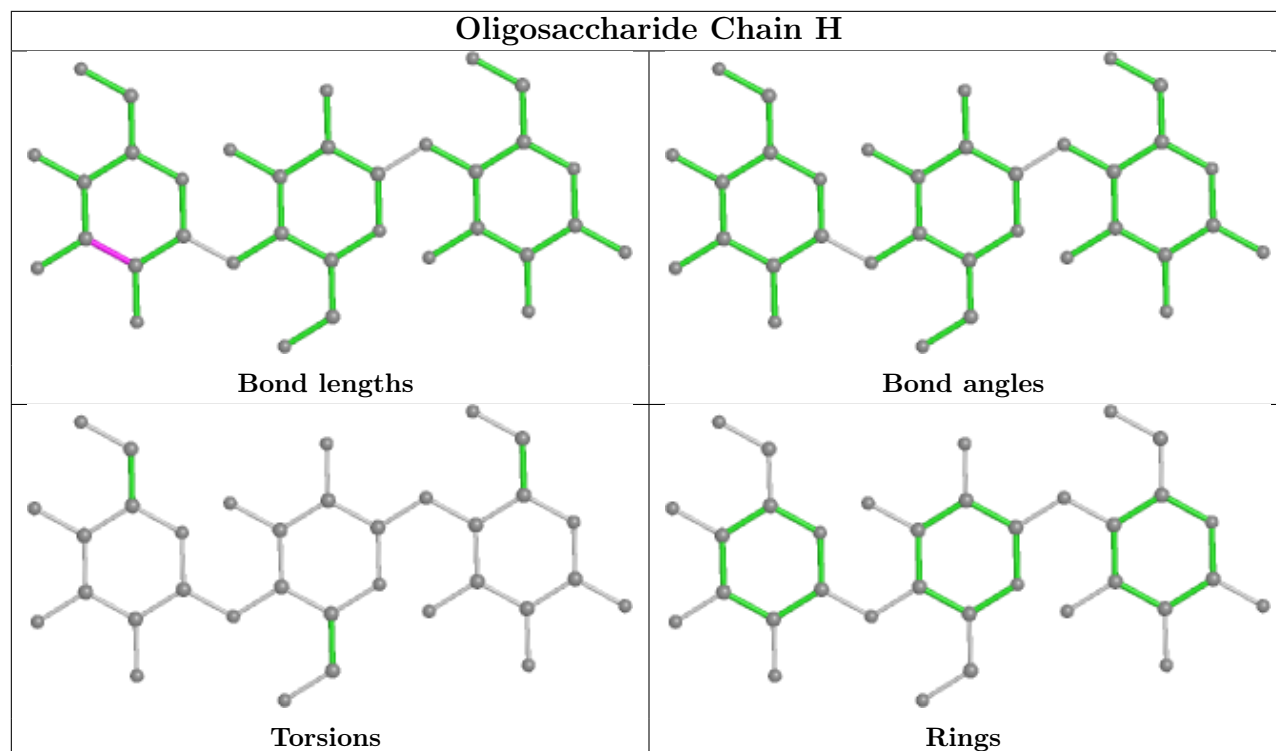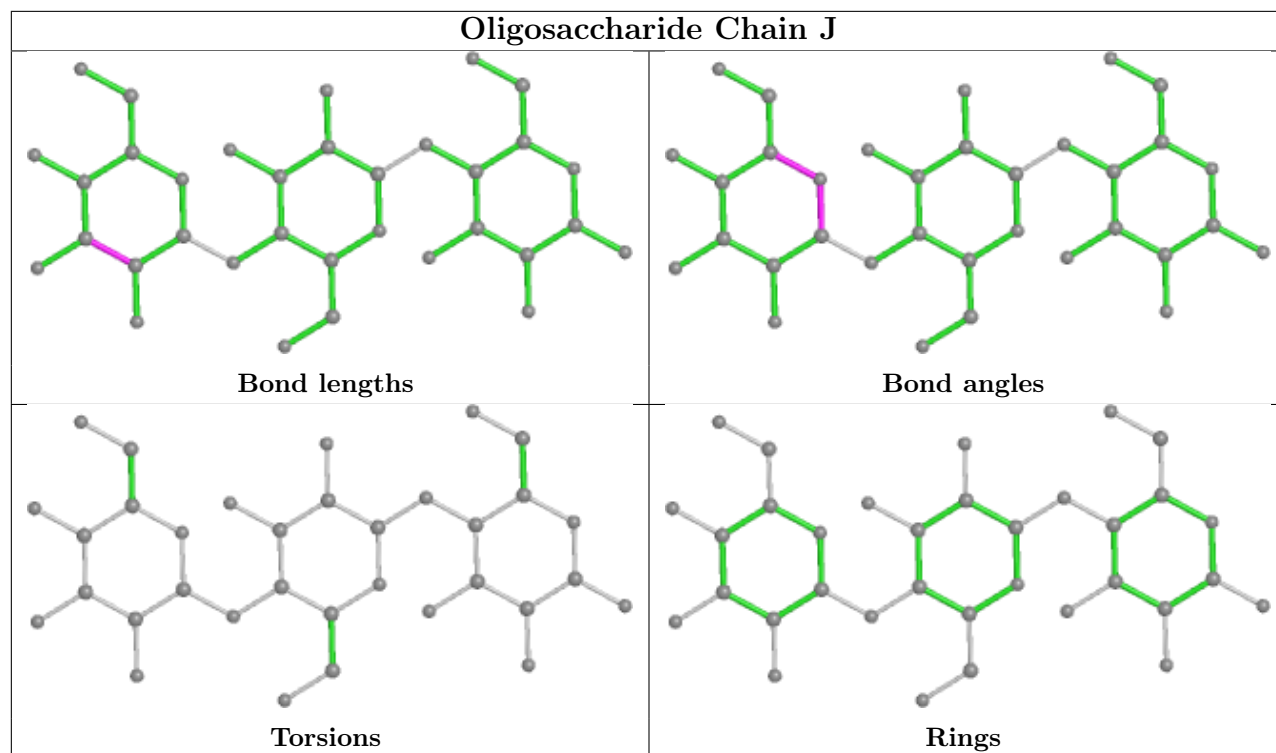
5.6 Ligand geometry ⓘ

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 ⓘ

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	69/69 (100%)	-0.25	0	100	100	11, 15, 20, 26	0
1	B	69/69 (100%)	-0.21	0	100	100	11, 16, 25, 27	0
1	C	69/69 (100%)	-0.27	1 (1%)	75	79	10, 14, 20, 26	0
1	D	69/69 (100%)	-0.26	0	100	100	10, 14, 21, 26	0
1	E	69/69 (100%)	-0.13	1 (1%)	75	79	11, 15, 23, 28	0
All	All	345/345 (100%)	-0.22	2 (0%)	89	91	10, 15, 23, 28	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	369	ARG	2.6
1	E	569	ARG	2.6

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BGC	J	1	12/12	0.83	0.13	23,28,30,30	0
2	BGC	H	1	12/12	0.90	0.15	21,27,29,29	0
2	BGC	G	1	12/12	0.91	0.12	15,21,23,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BGC	F	1	12/12	0.92	0.16	23,29,31,31	0
2	BGC	I	1	12/12	0.94	0.09	14,21,23,24	0
2	GAL	J	2	11/12	0.94	0.11	16,17,21,21	0
2	GAL	H	2	11/12	0.97	0.07	15,16,19,20	0
2	GAL	G	2	11/12	0.97	0.06	12,13,14,15	0
2	GAL	I	2	11/12	0.97	0.06	11,12,13,13	0
2	GLA	G	3	11/12	0.97	0.06	13,13,14,15	0
2	GAL	F	2	11/12	0.97	0.10	15,18,21,21	0
2	GLA	J	3	11/12	0.97	0.07	14,15,15,16	0
2	GLA	F	3	11/12	0.98	0.07	14,15,15,16	0
2	GLA	H	3	11/12	0.98	0.06	13,14,15,16	0
2	GLA	I	3	11/12	0.98	0.05	12,13,14,14	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 F:

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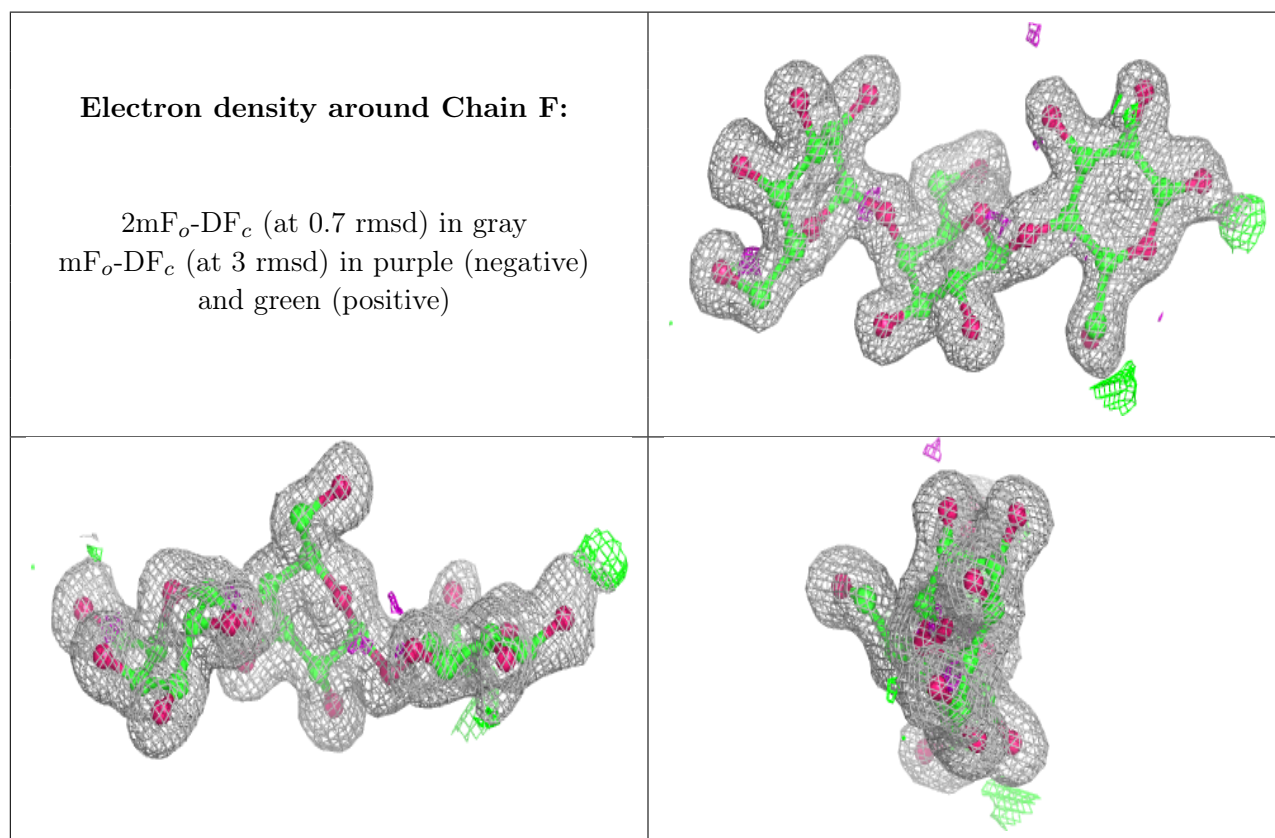
Electron density around Chain G:

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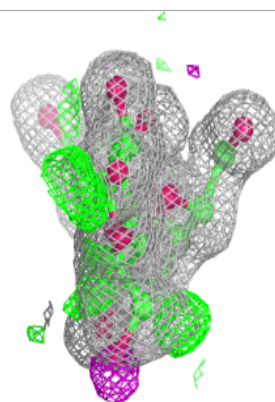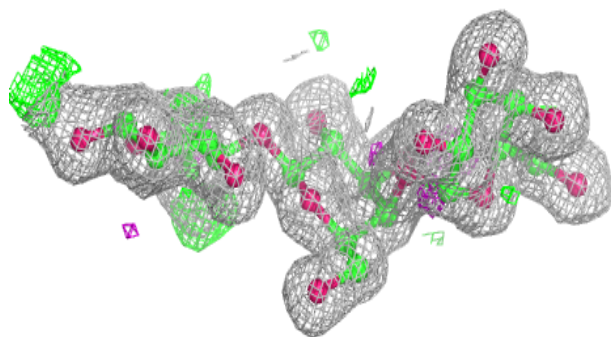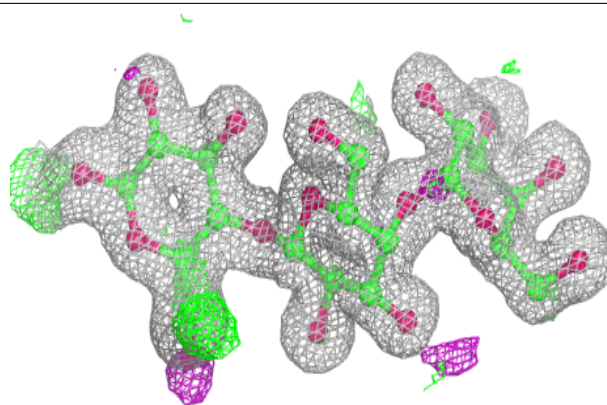
Electron density around Chain H:

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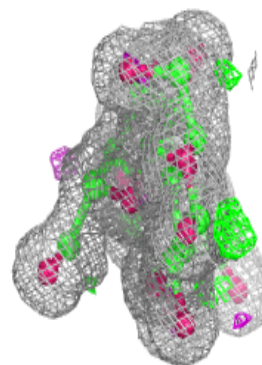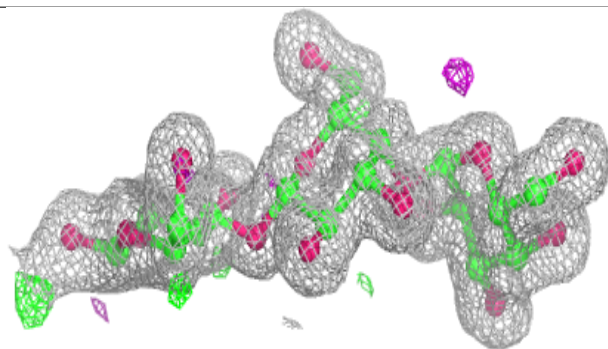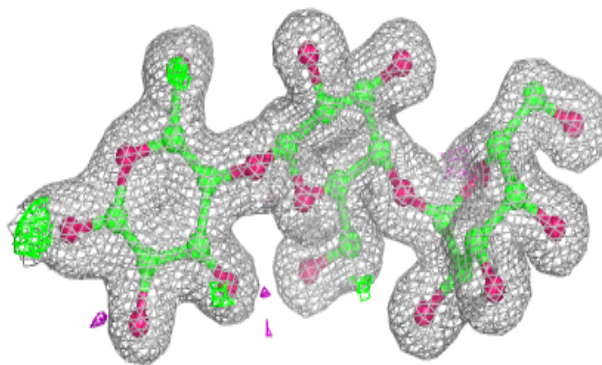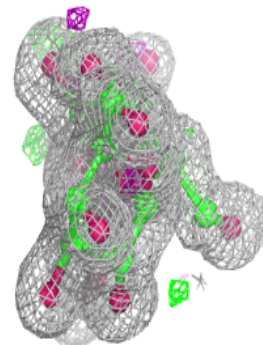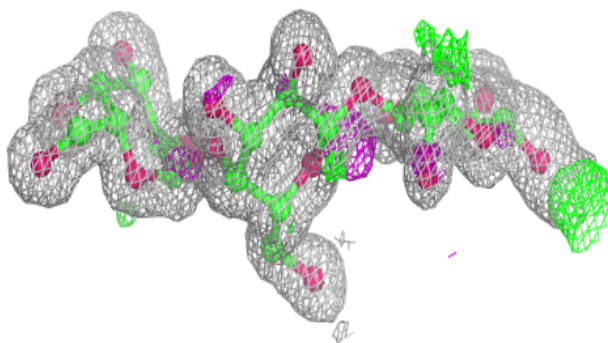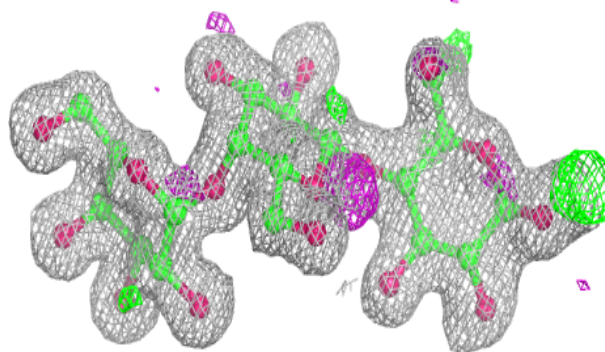mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
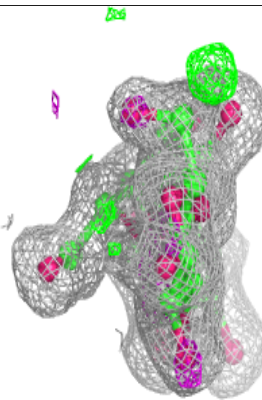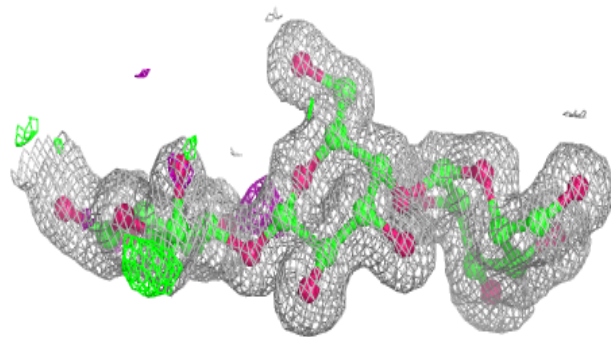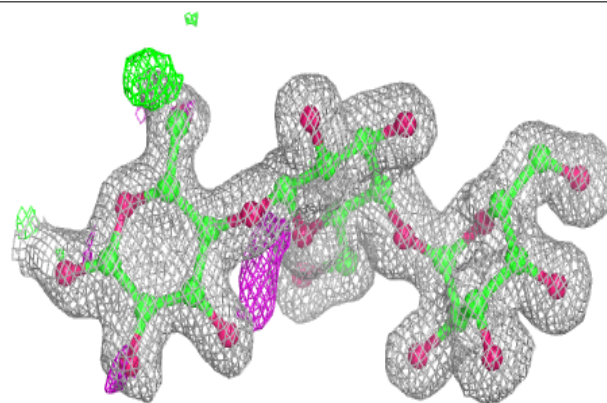
Electron density around Chain I:

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

Electron density around Chain J:

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

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.