



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 07:16 AM BST

PDB ID : 4X3R
Title : Avi-GCPII structure in complex with FITC-conjugated GCPII-specific inhibitor
Authors : Tykvart, J.; Konvalinka, J.
Deposited on : 2014-12-01
Resolution : 1.86 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

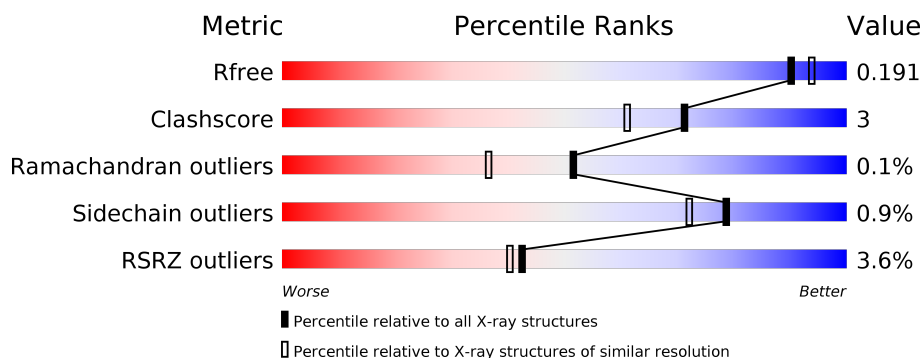
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 on 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 $\leq 5\%$. 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	739	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>7%</div> </div> </div>
2	B	2	<div> <div>100%</div> </div>
2	C	2	<div> <div>100%</div> </div>
2	D	2	<div> <div>100%</div> </div>
3	E	3	<div> <div>100%</div> </div>
4	F	4	<div> <div>100%</div> </div>

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
2	NAG	C	2	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6517 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 Glutamate carboxypeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	690	Total	C	N	O	S	0	8	0
			5540	3564	931	1026	19			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	ARG	-	expression tag	UNP Q04609
A	13	SER	-	expression tag	UNP Q04609
A	14	GLY	-	expression tag	UNP Q04609
A	15	LEU	-	expression tag	UNP Q04609
A	16	ASN	-	expression tag	UNP Q04609
A	17	ASP	-	expression tag	UNP Q04609
A	18	ILE	-	expression tag	UNP Q04609
A	19	PHE	-	expression tag	UNP Q04609
A	20	GLU	-	expression tag	UNP Q04609
A	21	ALA	-	expression tag	UNP Q04609
A	22	GLN	-	expression tag	UNP Q04609
A	23	LYS	-	expression tag	UNP Q04609
A	24	ILE	-	expression tag	UNP Q04609
A	25	GLU	-	expression tag	UNP Q04609
A	26	TRP	-	expression tag	UNP Q04609
A	27	HIS	-	expression tag	UNP Q04609
A	28	GLU	-	expression tag	UNP Q04609
A	29	GLY	-	expression tag	UNP Q04609
A	30	SER	-	expression tag	UNP Q04609
A	31	GLY	-	expression tag	UNP Q04609
A	32	SER	-	expression tag	UNP Q04609
A	33	GLY	-	expression tag	UNP Q04609
A	34	SER	-	expression tag	UNP Q04609
A	35	GLU	-	expression tag	UNP Q04609
A	36	ASN	-	expression tag	UNP Q04609
A	37	LEU	-	expression tag	UNP Q04609
A	38	TYR	-	expression tag	UNP Q04609

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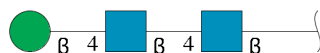
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	PHE	-	expression tag	UNP Q04609
A	40	GLN	-	expression tag	UNP Q04609
A	41	GLY	-	expression tag	UNP Q04609
A	42	ARG	-	expression tag	UNP Q04609
A	43	SER	-	expression tag	UNP Q04609

- Molecule 2 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
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

- Molecule 4 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
4	F	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Zn	0	0
			2	2		

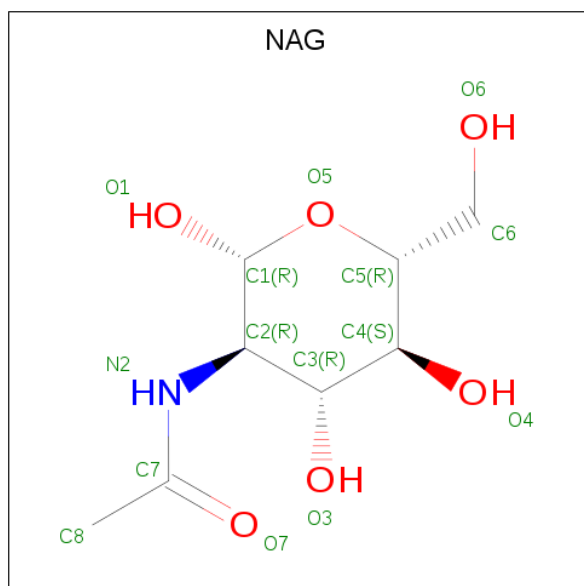
- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



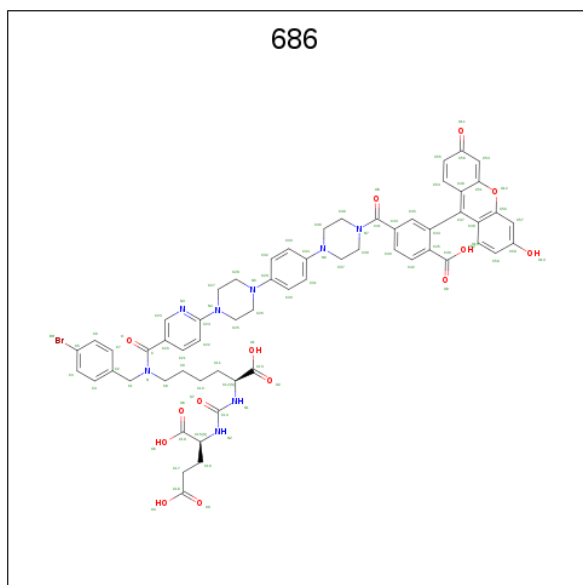
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 9 is N-((1S)-5-[(4-bromobenzyl)((6-[4-(4-{4-[4-carboxy-3-(6-hydroxy-3-oxo-3H-xanthen-9-yl)benzoyl]piperazin-1-yl}phenyl)piperazin-1-yl]pyridin-3-yl}carbonyl)amino]-1-carboxypentyl}carbamoyl)-L-glutamic acid (three-letter code: 686) (formula: C₆₀H₅₉BrN₈O₁₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	Br	C	N	O	0	1
			138	3	95	16	24		

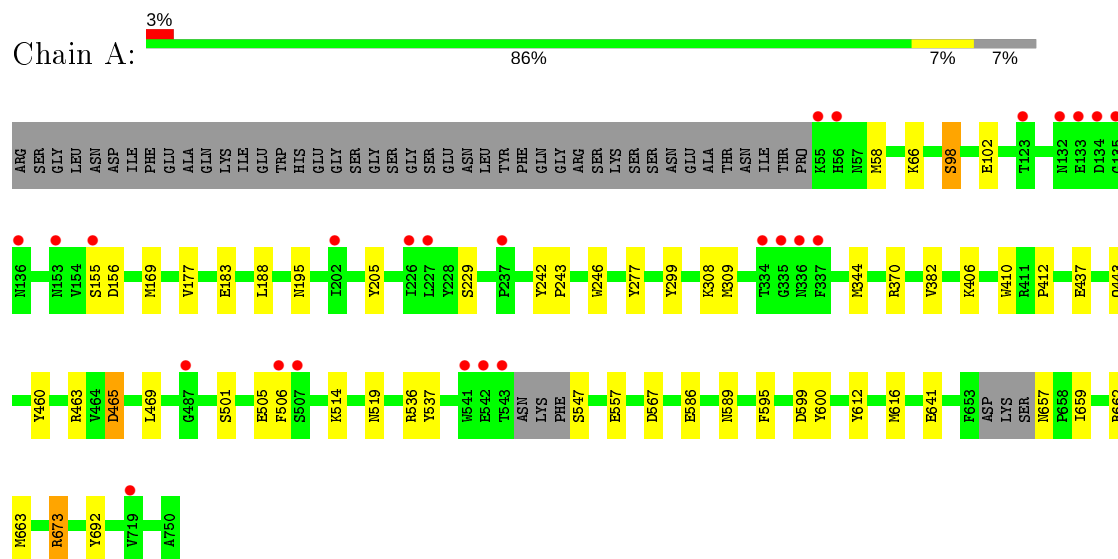
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	632	Total	O	0	5
			634	634		

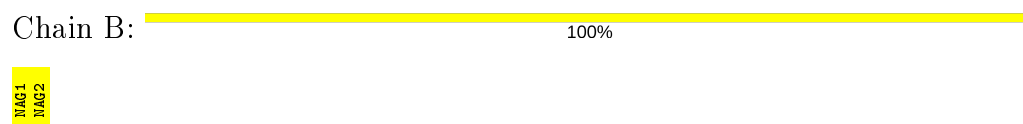
3 Residue-property plots [i](#)

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.

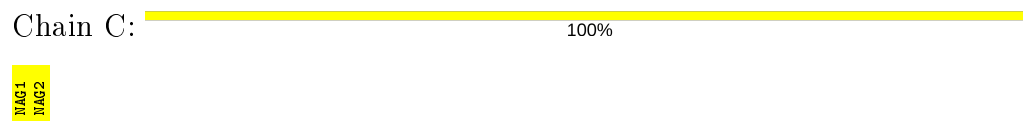
- Molecule 1: Glutamate carboxypeptidase 2



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



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



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



NAG1
NAG2

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

Chain E:

100%

NAG1
NAG2
BMA3

- Molecule 4: 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 F:

100%

NAG1
NAG2
BMA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	101.71Å 130.16Å 159.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.86 29.55 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-1.86) 99.5 (29.55-1.86)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.148 , 0.180 0.160 , 0.191	Depositor DCC
R_{free} test set	4429 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6517	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: ZN, BMA, NAG, CL, CA, 686, MAN

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	1.03	8/5715 (0.1%)	0.96	8/7743 (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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	437	GLU	CD-OE2	-7.60	1.17	1.25
1	A	657	ASN	N-CA	7.50	1.61	1.46
1	A	557	GLU	CB-CG	-6.42	1.40	1.52
1	A	309	MET	CG-SD	-5.45	1.67	1.81
1	A	98	SER	CB-OG	-5.30	1.35	1.42
1	A	460	TYR	CG-CD1	5.21	1.46	1.39
1	A	501	SER	CB-OG	-5.19	1.35	1.42
1	A	277	TYR	CE1-CZ	5.12	1.45	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	465	ASP	CB-CG-OD1	8.92	126.33	118.30
1	A	673	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	599	ASP	CB-CG-OD2	6.63	124.26	118.30
1	A	662	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	A	370	ARG	NE-CZ-NH1	6.21	123.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	567	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	673	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	465	ASP	CB-CG-OD2	-5.40	113.44	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	TYR	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	5540	0	5400	31	0
2	B	28	0	25	0	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
3	E	39	0	34	0	0
4	F	50	0	43	0	0
5	A	2	0	0	0	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	28	0	26	2	0
9	A	138	0	99	17	0
10	A	634	0	0	5	0
All	All	6517	0	5677	40	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.

All (40) 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:A:659:ILE:O	1:A:663[B]:MET:HG3	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1320[B]:686:O	9:A:1320[B]:686:H25	1.86	0.74
1:A:463[B]:ARG:HH22	9:A:1320[B]:686:H16	1.56	0.70
1:A:58:MET:HE1	1:A:586:GLU:HG2	1.79	0.65
1:A:463[B]:ARG:HH22	9:A:1320[B]:686:C23	2.13	0.62
1:A:465:ASP:OD2	9:A:1320[B]:686:H20	2.00	0.61
9:A:1320[B]:686:H19	10:A:1684:HOH:O	2.01	0.60
1:A:505:GLU:HB3	1:A:506:PHE:CD2	2.37	0.60
9:A:1320[B]:686:O	9:A:1320[B]:686:C9	2.50	0.58
1:A:463[B]:ARG:HG2	9:A:1320[B]:686:BR	2.61	0.55
1:A:612:TYR:CZ	1:A:616:MET:HG3	2.43	0.54
1:A:505:GLU:HB3	1:A:506:PHE:CE2	2.43	0.53
1:A:169:MET:HA	1:A:344:MET:O	2.09	0.53
1:A:58:MET:CE	1:A:586:GLU:HG2	2.39	0.52
1:A:195:ASN:HD22	8:A:1311:NAG:H83	1.75	0.52
1:A:183:GLU:HG3	10:A:1956:HOH:O	2.11	0.51
1:A:463[B]:ARG:NH2	9:A:1320[B]:686:H16	2.24	0.50
1:A:66:LYS:HE2	10:A:1727:HOH:O	2.12	0.50
1:A:641:GLU:HG3	10:A:1805:HOH:O	2.13	0.49
1:A:155:SER:O	1:A:156:ASP:HB2	2.14	0.48
1:A:412:PRO:HA	1:A:589[B]:ASN:OD1	2.14	0.48
1:A:536:ARG:HG2	9:A:1320[B]:686:BR	2.70	0.47
9:A:1320[B]:686:C23	9:A:1320[B]:686:H18	2.45	0.46
9:A:1320[C]:686:H14	9:A:1320[C]:686:H8	1.76	0.46
1:A:469:LEU:O	1:A:595:PHE:HA	2.16	0.45
1:A:505:GLU:CB	1:A:506:PHE:CD2	3.00	0.45
9:A:1320[A]:686:H10	9:A:1320[A]:686:H5	1.83	0.45
1:A:246:TRP:CD1	8:A:1312:NAG:H83	2.53	0.44
9:A:1320[A]:686:C7	9:A:1320[A]:686:C20	2.95	0.44
1:A:514[A]:LYS:HD2	1:A:692:TYR:HE1	1.82	0.44
1:A:242:TYR:CG	1:A:243:PRO:HA	2.53	0.43
1:A:547:SER:N	9:A:1320[C]:686:C6	2.82	0.42
9:A:1320[C]:686:H5	9:A:1320[C]:686:H10	1.84	0.42
1:A:406:LYS:HA	1:A:410:TRP:O	2.19	0.42
1:A:465:ASP:OD2	9:A:1320[B]:686:C6	2.67	0.41
9:A:1320[B]:686:O7	9:A:1320[B]:686:C19	2.66	0.41
1:A:308:LYS:HB2	10:A:1537:HOH:O	2.20	0.41
1:A:98:SER:O	1:A:102:GLU:HG3	2.20	0.41
1:A:177:VAL:HG12	1:A:188:LEU:HD11	2.03	0.41
1:A:229:SER:O	1:A:299:TYR:HB3	2.21	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	692/739 (94%)	672 (97%)	19 (3%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	382	VAL

5.3.2 Protein sidechains [i](#)

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	593/629 (94%)	587 (99%)	6 (1%)	76	69

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	443[A]	GLN
1	A	443[B]	GLN
1	A	519	ASN
1	A	537	TYR
1	A	600	TYR
1	A	673	ARG

Some 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 ⓘ

13 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	NAG	B	1	1,2	14,14,15	0.92	1 (7%)	17,19,21	2.11	7 (41%)
2	NAG	B	2	2	14,14,15	0.90	1 (7%)	17,19,21	1.80	6 (35%)
2	NAG	C	1	1,2	14,14,15	1.29	1 (7%)	17,19,21	2.93	11 (64%)
2	NAG	C	2	2	14,14,15	0.85	1 (7%)	17,19,21	1.47	1 (5%)
2	NAG	D	1	1,2	14,14,15	1.16	2 (14%)	17,19,21	1.29	2 (11%)
2	NAG	D	2	2	14,14,15	0.90	1 (7%)	17,19,21	1.94	5 (29%)
3	NAG	E	1	1,3	14,14,15	1.19	1 (7%)	17,19,21	1.78	6 (35%)
3	NAG	E	2	3	14,14,15	0.79	0	17,19,21	1.25	1 (5%)
3	BMA	E	3	3	11,11,12	0.95	0	15,15,17	1.75	5 (33%)
4	NAG	F	1	1,4	14,14,15	1.24	0	17,19,21	1.57	3 (17%)
4	NAG	F	2	4	14,14,15	1.07	1 (7%)	17,19,21	1.89	6 (35%)
4	BMA	F	3	4	11,11,12	1.01	0	15,15,17	1.19	1 (6%)
4	MAN	F	4	4	11,11,12	0.96	1 (9%)	15,15,17	2.17	5 (33%)

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	NAG	B	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	2/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	NAG	C4-C5	2.94	1.59	1.53
4	F	2	NAG	O5-C1	-2.73	1.39	1.43
2	C	1	NAG	C6-C5	2.44	1.60	1.51
2	B	1	NAG	C1-C2	-2.31	1.48	1.52
4	F	4	MAN	O2-C2	-2.25	1.38	1.43
2	C	2	NAG	C4-C5	2.21	1.57	1.53
2	D	2	NAG	O3-C3	-2.20	1.37	1.43
3	E	1	NAG	C7-N2	-2.07	1.27	1.34
2	B	2	NAG	C3-C2	2.06	1.56	1.52
2	D	1	NAG	C1-C2	2.01	1.55	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	O5-C5-C6	5.54	115.88	107.20
2	C	1	NAG	O6-C6-C5	4.90	128.11	111.29
2	C	2	NAG	O4-C4-C5	4.72	121.02	109.30
2	D	2	NAG	O4-C4-C5	4.60	120.72	109.30
4	F	1	NAG	O5-C1-C2	-4.46	104.25	111.29
4	F	4	MAN	O2-C2-C1	-4.42	100.10	109.15
2	B	1	NAG	O5-C5-C6	4.38	114.07	107.20
2	C	1	NAG	O4-C4-C3	-4.00	101.11	110.35
2	B	1	NAG	C1-O5-C5	3.99	117.60	112.19
2	C	1	NAG	C6-C5-C4	3.95	122.25	113.00
2	C	1	NAG	C1-C2-N2	-3.86	103.90	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	4	MAN	O5-C5-C6	3.74	113.06	107.20
2	B	2	NAG	C4-C3-C2	3.73	116.48	111.02
3	E	3	BMA	O5-C5-C6	3.71	113.02	107.20
4	F	2	NAG	C1-C2-N2	-3.69	104.19	110.49
2	D	2	NAG	C3-C4-C5	-3.65	103.74	110.24
4	F	2	NAG	C3-C4-C5	-3.56	103.89	110.24
3	E	1	NAG	O4-C4-C3	-3.45	102.37	110.35
4	F	4	MAN	C1-O5-C5	3.31	116.68	112.19
4	F	2	NAG	O3-C3-C4	3.23	117.81	110.35
2	C	1	NAG	C4-C3-C2	3.20	115.71	111.02
2	B	2	NAG	C2-N2-C7	3.09	127.30	122.90
2	B	1	NAG	O4-C4-C3	-2.88	103.69	110.35
2	B	2	NAG	C3-C4-C5	-2.88	105.11	110.24
4	F	3	BMA	O3-C3-C2	-2.79	104.65	109.99
2	B	1	NAG	O5-C1-C2	-2.77	106.91	111.29
2	D	1	NAG	C3-C4-C5	2.76	115.16	110.24
3	E	1	NAG	O5-C1-C2	-2.67	107.07	111.29
3	E	1	NAG	C3-C4-C5	-2.64	105.52	110.24
2	D	2	NAG	O3-C3-C4	-2.57	104.41	110.35
4	F	4	MAN	O5-C1-C2	-2.50	106.92	110.77
3	E	2	NAG	O5-C5-C6	2.48	111.09	107.20
2	D	1	NAG	O3-C3-C2	-2.47	104.35	109.47
2	B	1	NAG	C2-N2-C7	-2.46	119.40	122.90
2	C	1	NAG	O4-C4-C5	2.44	115.36	109.30
3	E	3	BMA	C1-O5-C5	-2.44	108.89	112.19
3	E	1	NAG	C1-O5-C5	-2.42	108.92	112.19
2	C	1	NAG	C8-C7-N2	2.40	120.16	116.10
2	D	2	NAG	O7-C7-C8	-2.36	117.68	122.06
4	F	2	NAG	C6-C5-C4	2.34	118.49	113.00
2	B	2	NAG	O4-C4-C5	2.31	115.03	109.30
4	F	4	MAN	C2-C3-C4	2.29	114.86	110.89
3	E	3	BMA	O2-C2-C3	2.29	114.72	110.14
2	C	1	NAG	O5-C5-C4	-2.27	105.31	110.83
3	E	3	BMA	C3-C4-C5	2.26	114.28	110.24
3	E	3	BMA	O3-C3-C2	2.26	114.33	109.99
2	C	1	NAG	O7-C7-C8	-2.25	117.88	122.06
3	E	1	NAG	O6-C6-C5	-2.23	103.64	111.29
4	F	1	NAG	C6-C5-C4	-2.21	107.83	113.00
4	F	2	NAG	O5-C5-C4	-2.20	105.47	110.83
2	B	1	NAG	O7-C7-C8	-2.20	117.97	122.06
2	D	2	NAG	O7-C7-N2	2.18	125.97	121.95
2	B	1	NAG	O7-C7-N2	2.17	125.94	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	NAG	C1-O5-C5	2.17	115.13	112.19
4	F	2	NAG	O6-C6-C5	-2.15	103.91	111.29
2	B	2	NAG	O5-C1-C2	-2.11	107.96	111.29
2	B	2	NAG	O4-C4-C3	2.08	115.15	110.35
3	E	1	NAG	O5-C5-C4	-2.02	105.92	110.83
2	C	1	NAG	C2-N2-C7	-2.01	120.03	122.90

There are no chirality outliers.

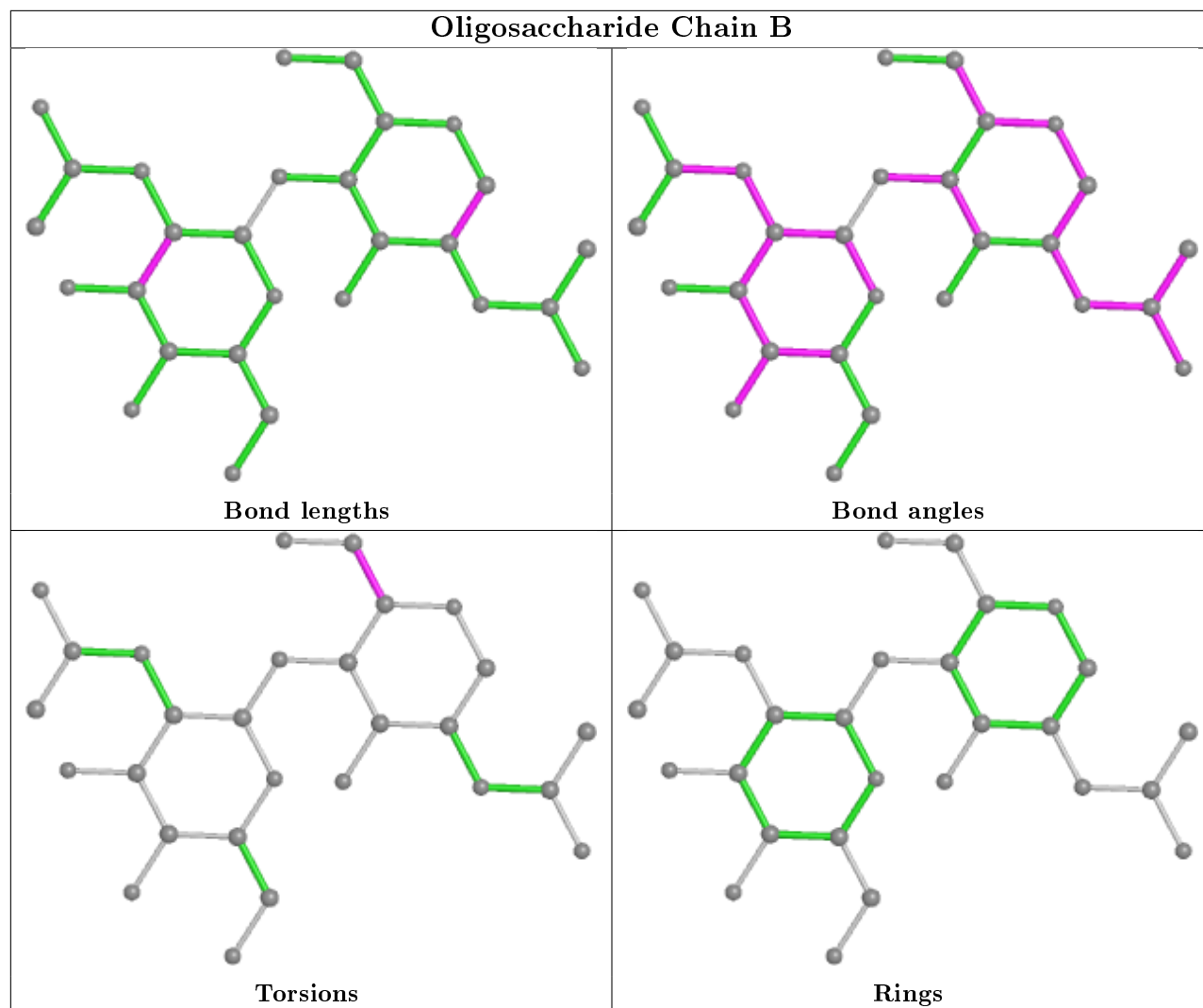
All (9) torsion outliers are listed below:

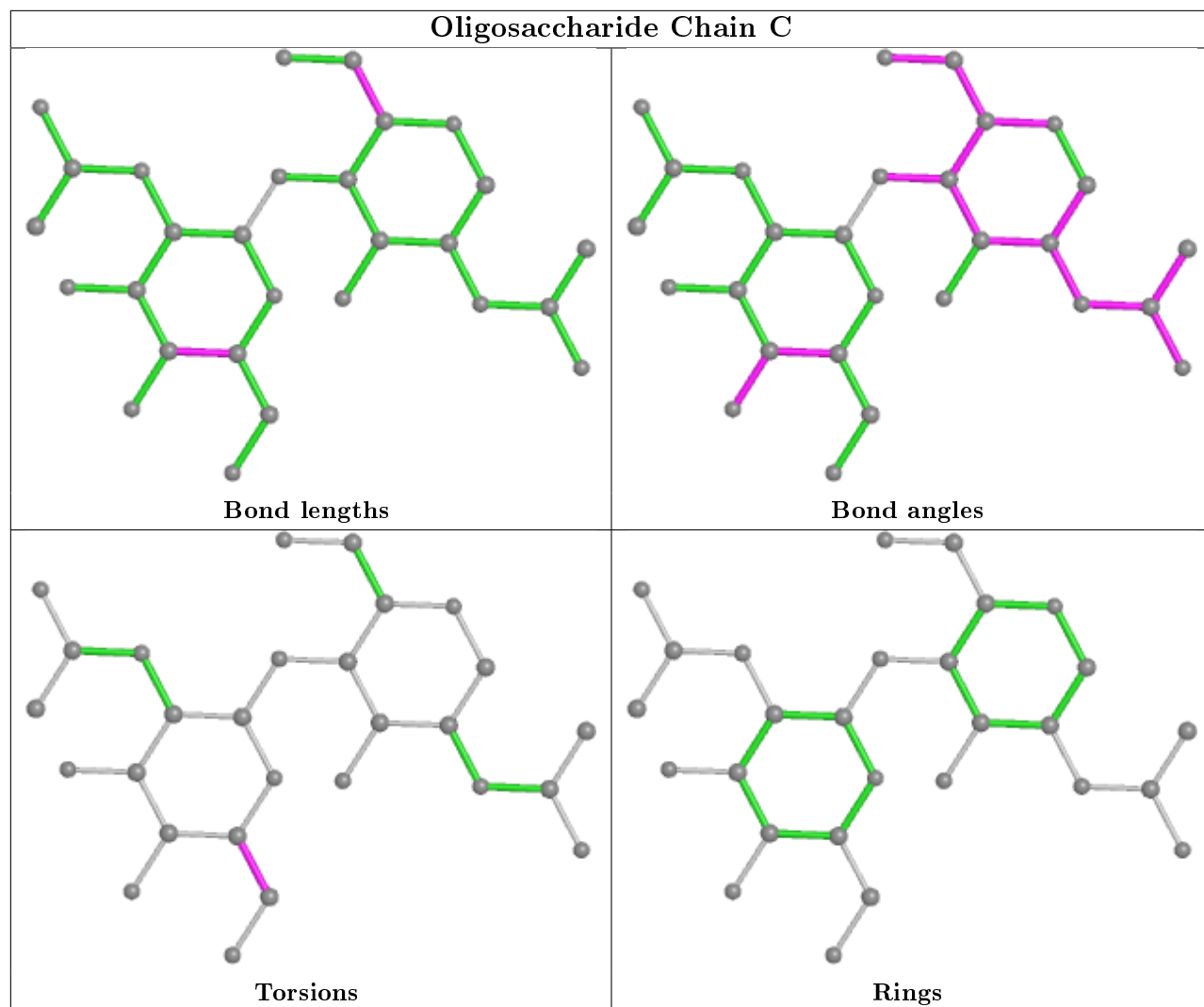
Mol	Chain	Res	Type	Atoms
3	E	3	BMA	O5-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

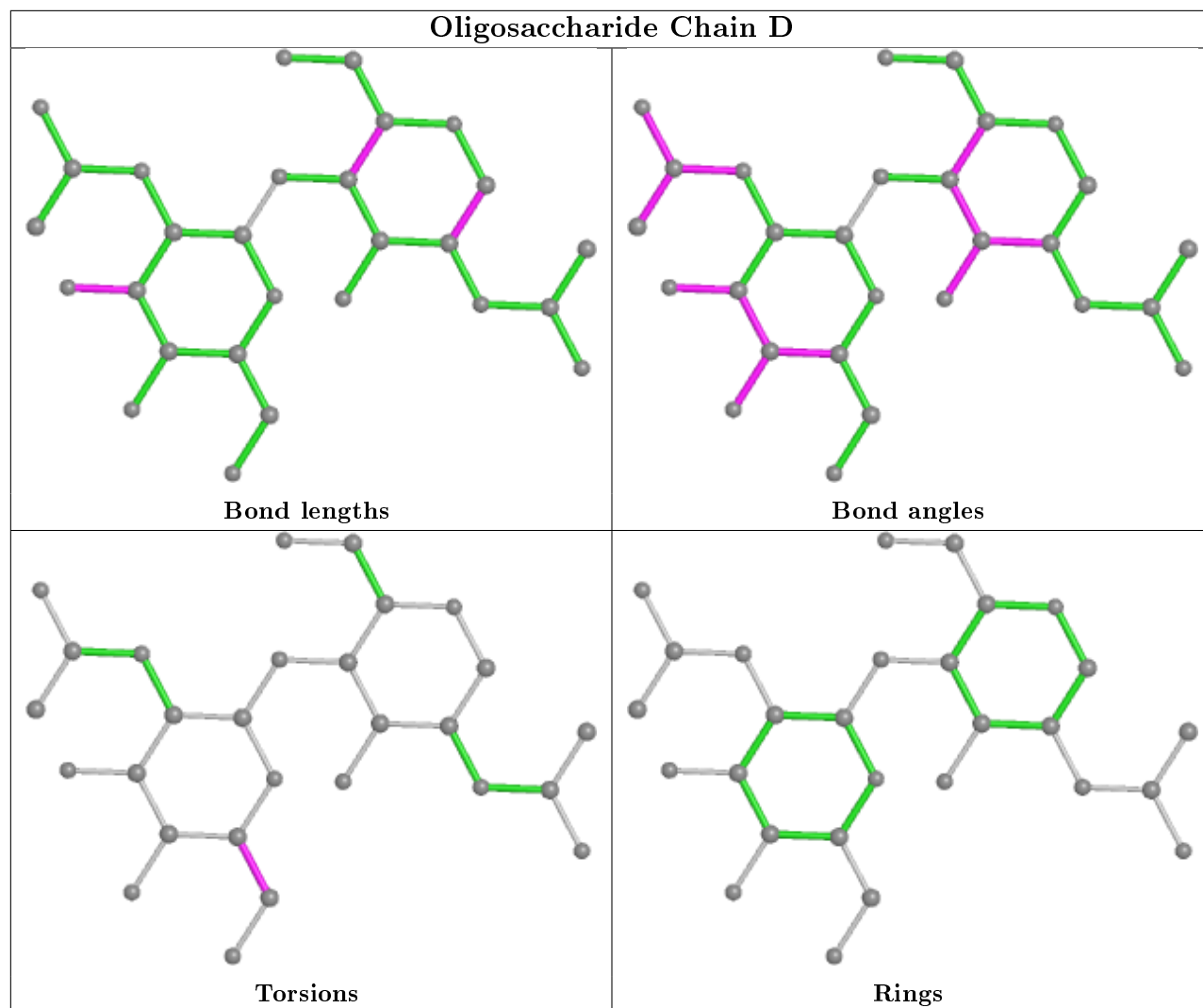
There are no ring outliers.

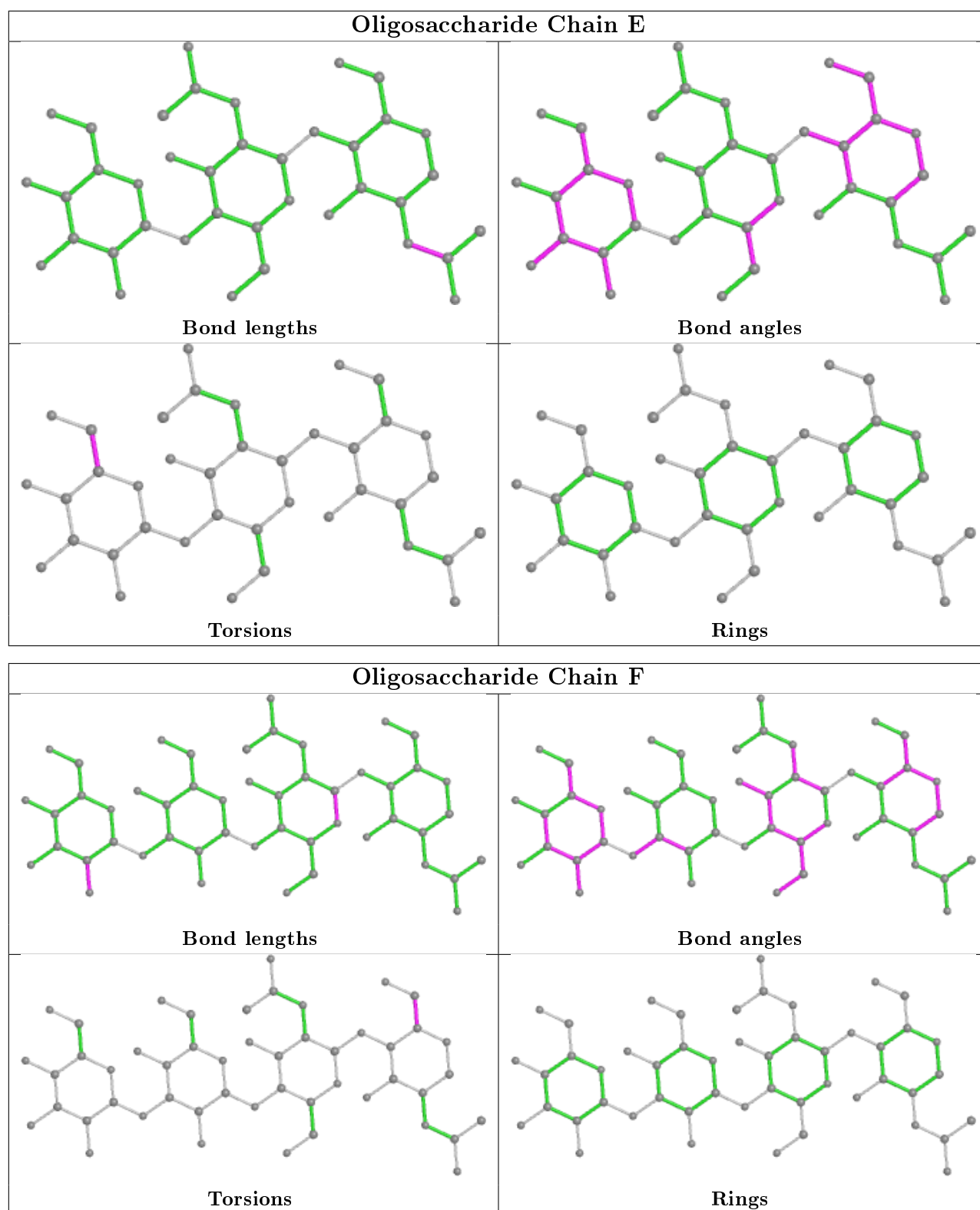
No monomer is involved in short contacts.

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









5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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
8	NAG	A	1311	1	14,14,15	0.94	1 (7%)	17,19,21	3.63	8 (47%)
9	686	A	1320[C]	5	44,53,91	0.93	2 (4%)	56,71,129	1.89	13 (23%)
9	686	A	1320[A]	5	44,53,91	0.97	2 (4%)	56,71,129	1.75	12 (21%)
8	NAG	A	1312	1	14,14,15	0.96	1 (7%)	17,19,21	2.51	8 (47%)

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
8	NAG	A	1311	1	-	4/6/23/26	0/1/1/1
9	686	A	1320[C]	5	-	2/38/58/92	0/4/4/9
9	686	A	1320[A]	5	-	2/38/58/92	0/4/4/9
8	NAG	A	1312	1	-	1/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1312	NAG	C3-C2	2.64	1.58	1.52
9	A	1320[A]	686	C24-N4	2.62	1.42	1.37
9	A	1320[C]	686	C24-N4	2.44	1.42	1.37
9	A	1320[C]	686	C15-N2	-2.21	1.43	1.46
9	A	1320[A]	686	C15-N2	-2.14	1.43	1.46
8	A	1311	NAG	O5-C1	2.12	1.47	1.43

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1311	NAG	C1-O5-C5	6.99	121.66	112.19
8	A	1311	NAG	O5-C5-C6	6.52	117.42	107.20
8	A	1311	NAG	C8-C7-N2	5.86	126.03	116.10
8	A	1311	NAG	O5-C1-C2	-5.73	102.24	111.29
9	A	1320[C]	686	C28-N5-C26	5.54	123.75	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1320[A]	686	C28-N5-C26	5.39	123.41	111.52
9	A	1320[C]	686	N3-C24-N4	4.93	124.17	116.79
8	A	1312	NAG	O3-C3-C4	-4.70	99.48	110.35
8	A	1311	NAG	O3-C3-C2	-4.67	99.81	109.47
9	A	1320[C]	686	C20-C-N	4.67	124.64	118.72
9	A	1320[A]	686	N3-C24-N4	4.63	123.73	116.79
9	A	1320[A]	686	C16-C15-N2	4.60	116.89	110.19
9	A	1320[C]	686	C16-C15-N2	4.55	116.82	110.19
8	A	1312	NAG	O5-C1-C2	-4.30	104.51	111.29
8	A	1311	NAG	C1-C2-N2	4.07	117.44	110.49
8	A	1312	NAG	C1-O5-C5	3.55	117.00	112.19
8	A	1312	NAG	O3-C3-C2	3.42	116.55	109.47
9	A	1320[A]	686	C2-C1-N	-3.33	107.78	113.13
8	A	1312	NAG	O7-C7-C8	-3.27	115.98	122.06
9	A	1320[A]	686	O-C-N	-3.19	117.06	122.34
9	A	1320[C]	686	C28-C27-N4	-3.10	104.67	110.70
8	A	1312	NAG	C8-C7-N2	3.03	121.22	116.10
9	A	1320[A]	686	C22-C24-N3	-2.99	117.92	123.41
8	A	1311	NAG	O7-C7-C8	-2.84	116.77	122.06
9	A	1320[A]	686	C21-C22-C24	2.80	121.39	117.53
9	A	1320[C]	686	C11-C12-N1	-2.68	106.29	110.19
8	A	1312	NAG	C3-C4-C5	-2.67	105.47	110.24
9	A	1320[A]	686	C23-N3-C24	2.67	122.17	117.30
9	A	1320[C]	686	C22-C24-N3	-2.63	118.58	123.41
9	A	1320[C]	686	C20-C23-N3	-2.60	120.04	123.67
8	A	1311	NAG	O7-C7-N2	-2.58	117.20	121.95
9	A	1320[C]	686	C21-C22-C24	2.55	121.04	117.53
8	A	1312	NAG	O4-C4-C5	2.51	115.54	109.30
9	A	1320[C]	686	C23-N3-C24	2.50	121.87	117.30
9	A	1320[C]	686	C22-C24-N4	-2.48	117.24	121.70
9	A	1320[A]	686	C11-C12-N1	-2.48	106.58	110.19
9	A	1320[A]	686	C28-C27-N4	-2.43	105.99	110.70
9	A	1320[A]	686	C20-C-N	2.33	121.67	118.72
9	A	1320[A]	686	C20-C23-N3	-2.20	120.59	123.67
9	A	1320[C]	686	BR-C5-C4	2.14	122.42	119.30
9	A	1320[C]	686	O-C-C20	-2.03	116.28	120.23

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1311	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	A	1311	NAG	C4-C5-C6-O6
8	A	1311	NAG	C8-C7-N2-C2
8	A	1311	NAG	O7-C7-N2-C2
9	A	1320[C]	686	C19-C15-N2-C14
9	A	1320[A]	686	C19-C15-N2-C14
8	A	1312	NAG	O5-C5-C6-O6
9	A	1320[C]	686	C13-C12-N1-C14
9	A	1320[A]	686	C13-C12-N1-C14

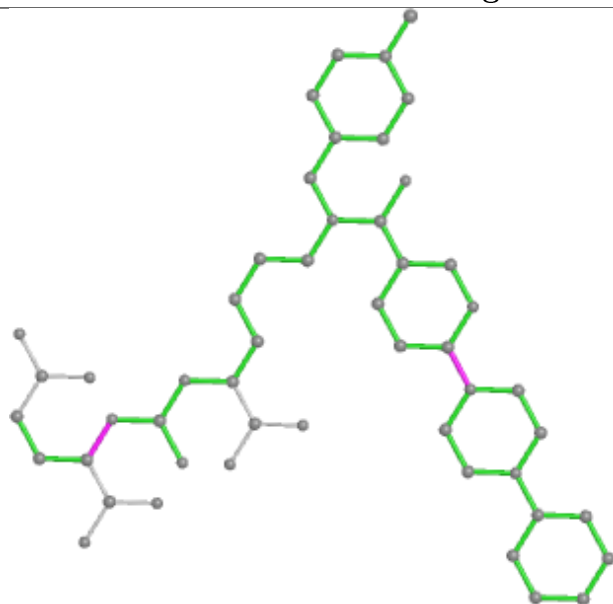
There are no ring outliers.

4 monomers are involved in 7 short contacts:

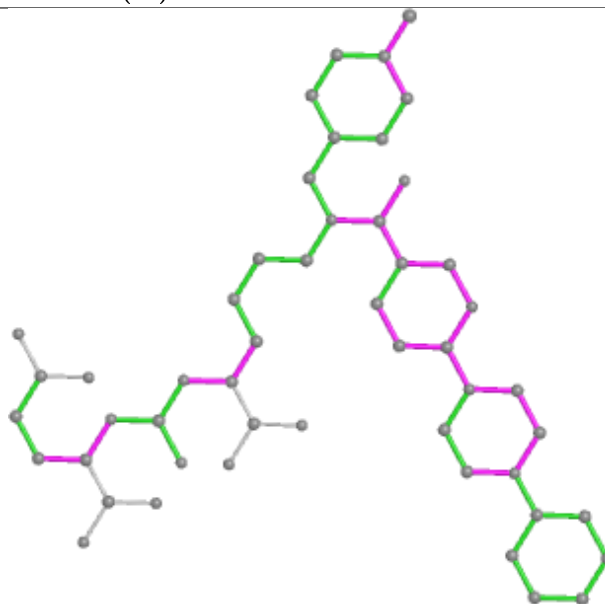
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1311	NAG	1	0
9	A	1320[C]	686	3	0
9	A	1320[A]	686	2	0
8	A	1312	NAG	1	0

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

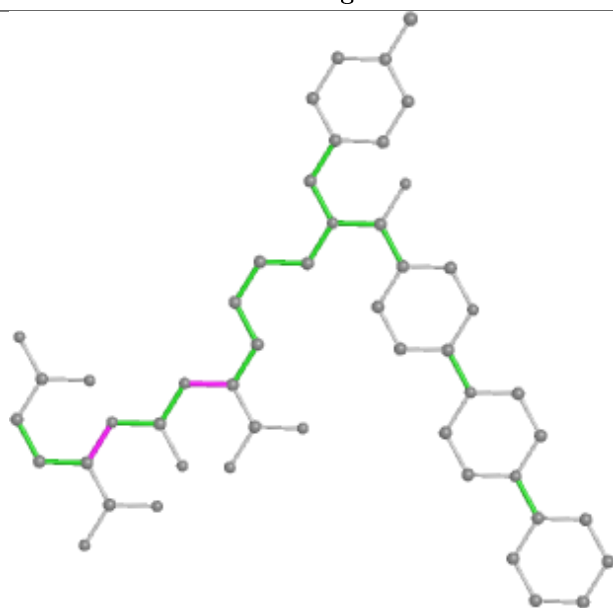
Ligand 686 A 1320 (C)



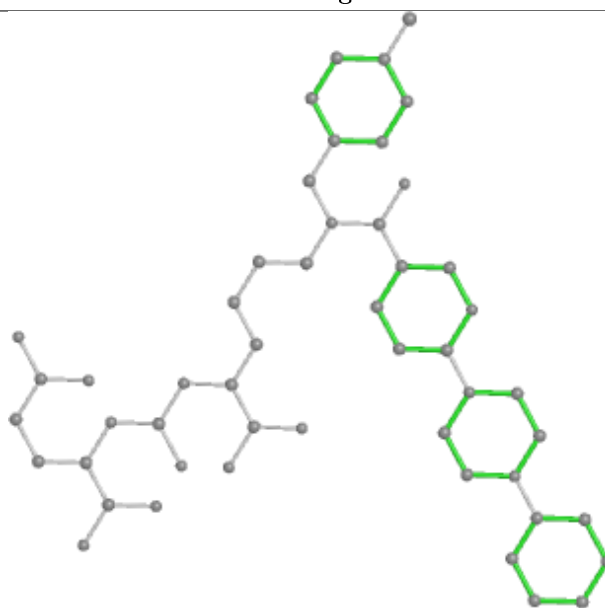
Bond lengths



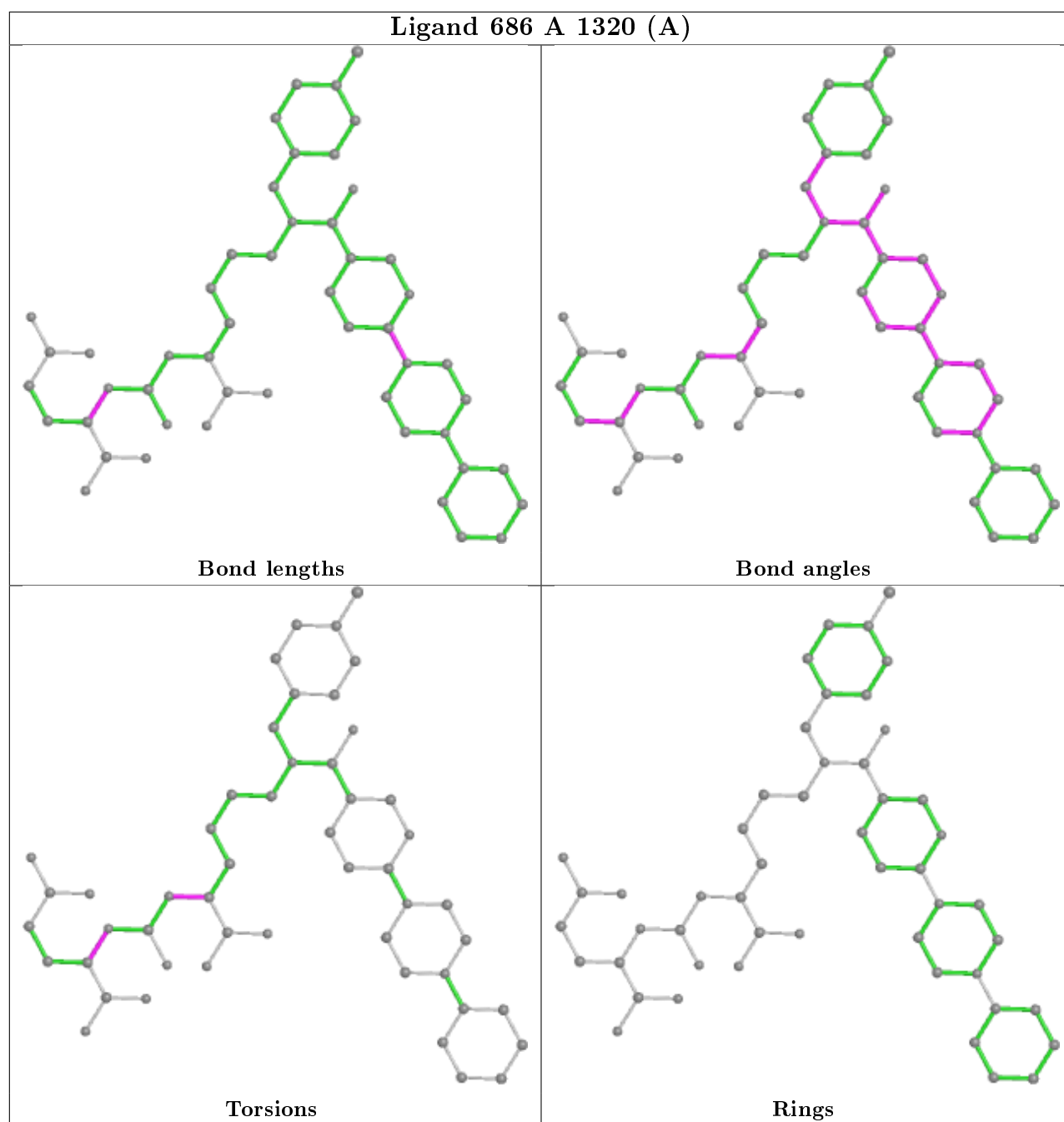
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	690/739 (93%)	-0.11	25 (3%) 42 40	16, 27, 49, 92	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	543	THR	6.3
1	A	541	TRP	3.9
1	A	135	GLY	3.5
1	A	155	SER	3.4
1	A	336	ASN	3.3
1	A	136	ASN	3.2
1	A	134	ASP	3.1
1	A	335	GLY	3.1
1	A	227	LEU	3.0
1	A	153	ASN	2.9
1	A	719	VAL	2.8
1	A	542	GLU	2.8
1	A	506	PHE	2.8
1	A	123	THR	2.7
1	A	55	LYS	2.6
1	A	487	GLY	2.5
1	A	507	SER	2.5
1	A	237	PRO	2.5
1	A	56	HIS	2.5
1	A	334	THR	2.4
1	A	337	PHE	2.4
1	A	133	GLU	2.3
1	A	132	ASN	2.3
1	A	202	ILE	2.2
1	A	226	ILE	2.0

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 ⓘ

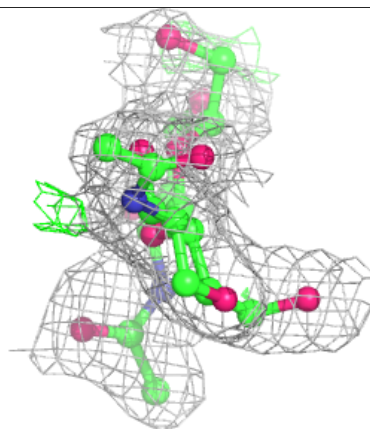
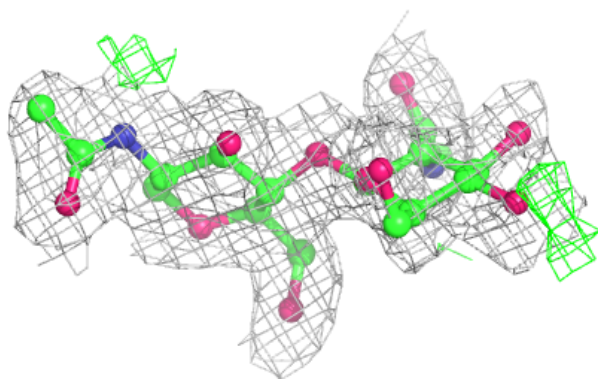
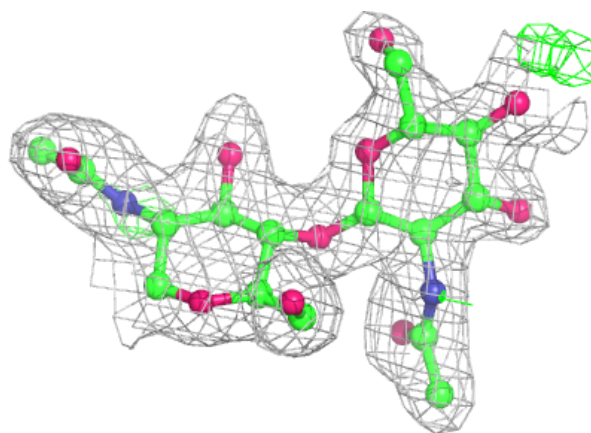
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	B	2	14/15	0.67	0.30	41,58,68,70	0
3	BMA	E	3	11/12	0.73	0.35	60,67,72,80	0
2	NAG	C	2	14/15	0.78	0.43	69,75,82,91	0
2	NAG	D	2	14/15	0.82	0.32	56,63,71,72	0
2	NAG	C	1	14/15	0.83	0.24	46,58,76,85	0
2	NAG	D	1	14/15	0.87	0.18	39,43,49,57	0
4	BMA	F	3	11/12	0.88	0.19	44,47,52,56	0
4	NAG	F	1	14/15	0.89	0.11	22,29,42,53	0
4	NAG	F	2	14/15	0.90	0.27	40,48,57,61	0
3	NAG	E	2	14/15	0.94	0.20	35,44,54,58	0
3	NAG	E	1	14/15	0.94	0.14	28,30,35,44	0
4	MAN	F	4	11/12	0.94	0.20	50,52,60,61	0
2	NAG	B	1	14/15	0.95	0.11	30,39,45,55	0

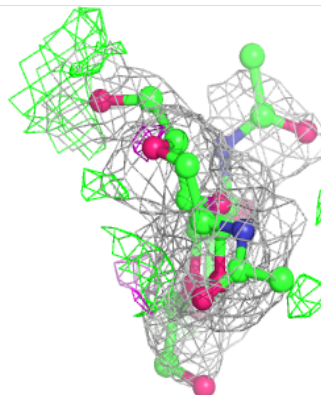
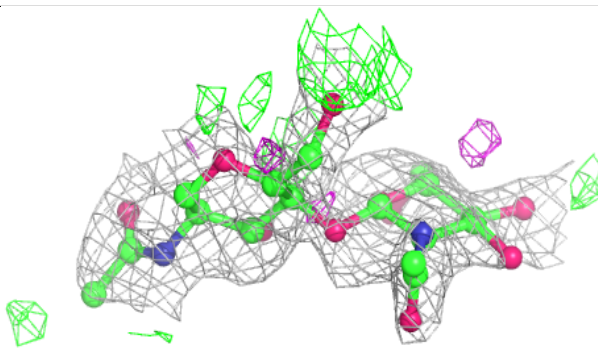
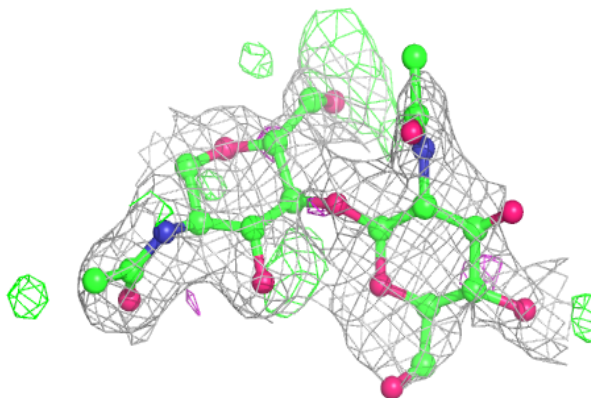
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

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

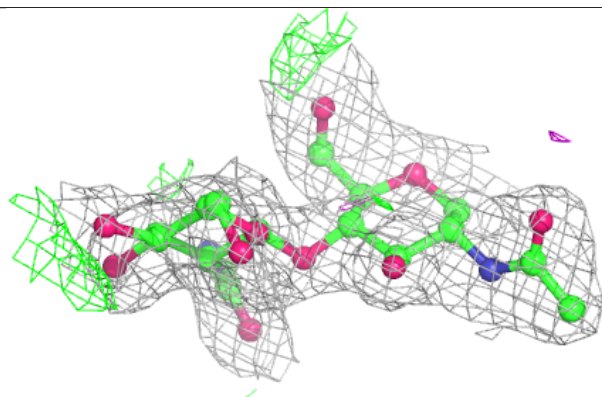
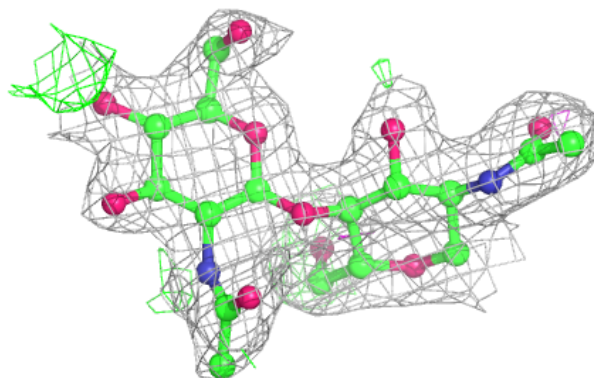
**Electron density around Chain C:**

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

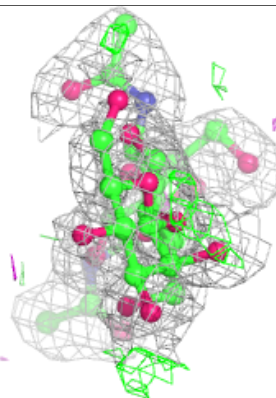
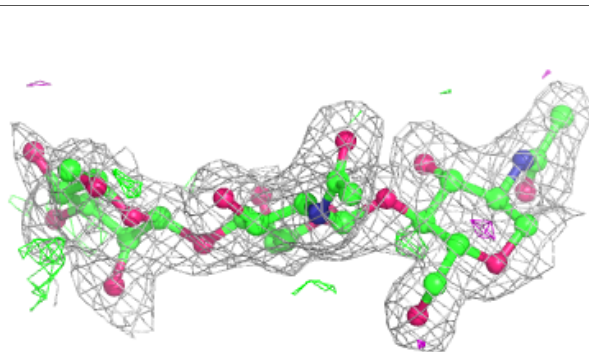
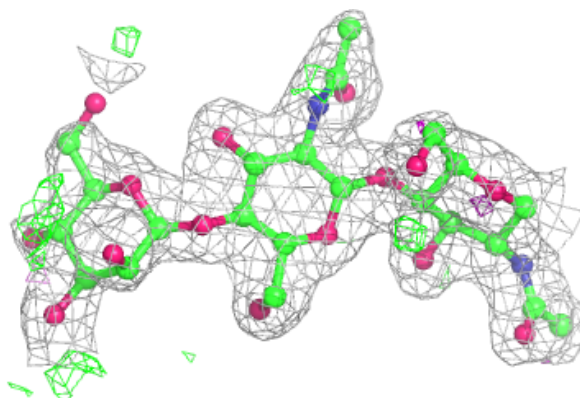


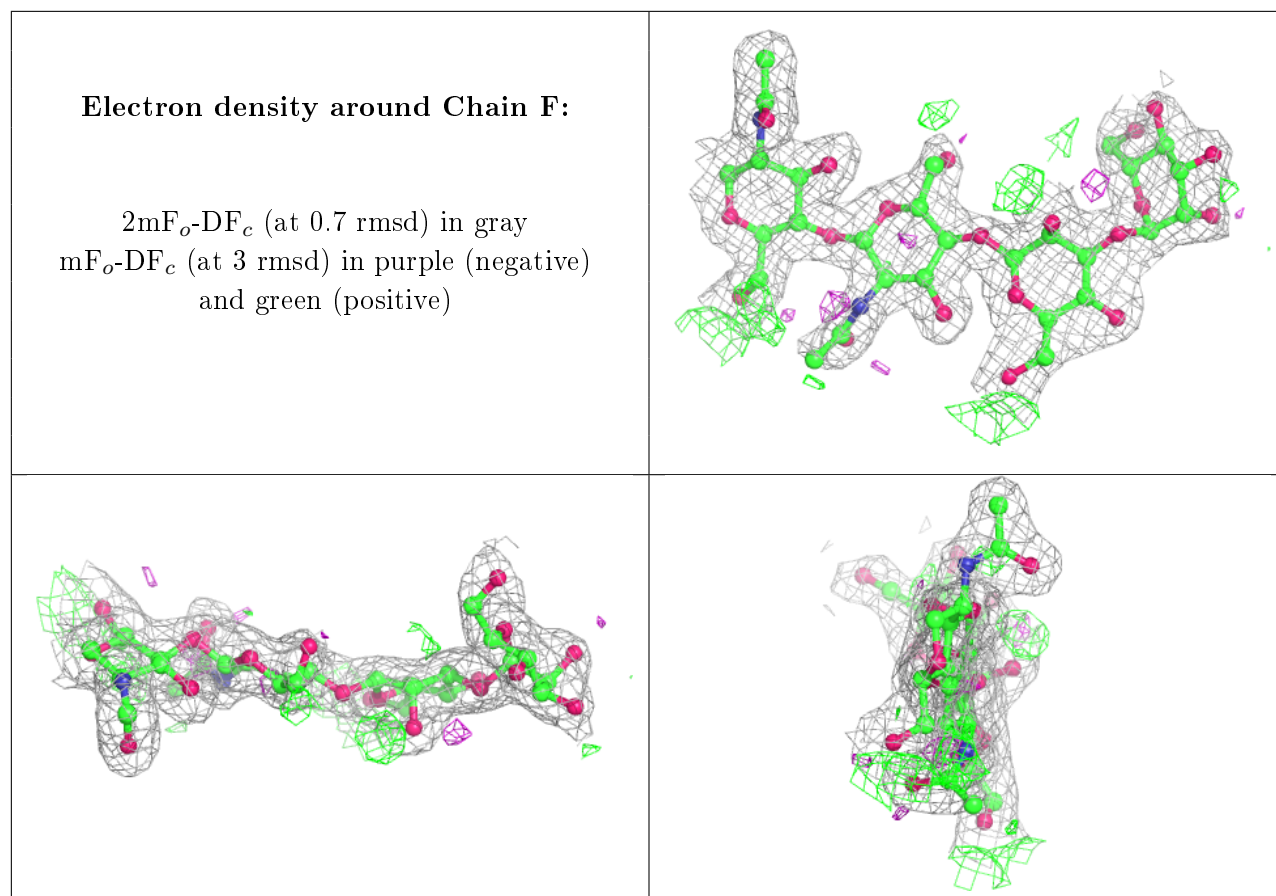
Electron density around Chain D:

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

**Electron density around Chain E:**

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





6.4 Ligands ⓘ

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

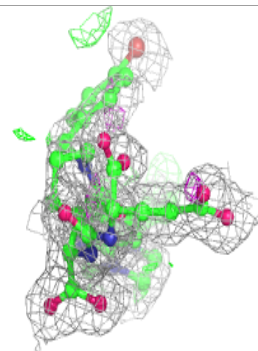
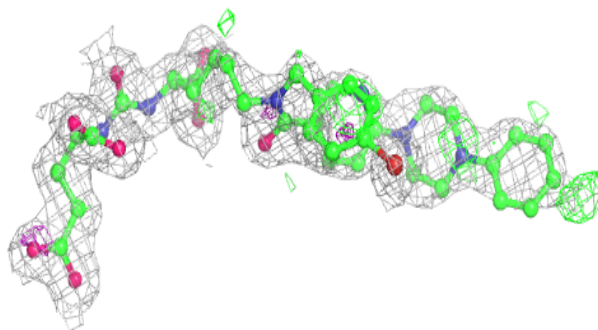
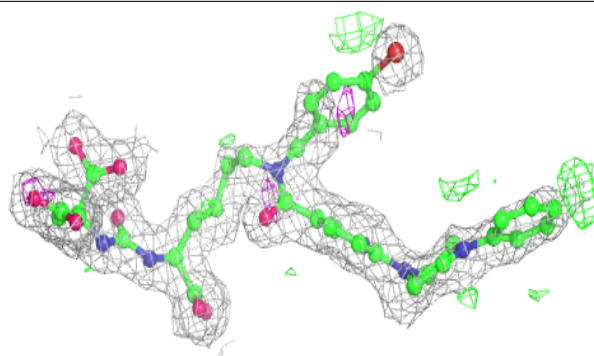
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	NAG	A	1311	14/15	0.74	0.20	60,71,80,86	0
8	NAG	A	1312	14/15	0.91	0.16	33,43,52,55	0
9	686	A	1320[C]	50/83	0.94	0.16	18,39,58,61	50
9	686	A	1320[B]	38/83	0.94	0.16	14,23,30,36	38
9	686	A	1320[A]	50/83	0.94	0.16	19,37,53,56	50
5	ZN	A	1301	1/1	1.00	0.08	19,19,19,19	0
5	ZN	A	1302	1/1	1.00	0.07	20,20,20,20	0
6	CL	A	1303	1/1	1.00	0.11	20,20,20,20	0
7	CA	A	1304	1/1	1.00	0.06	17,17,17,17	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.

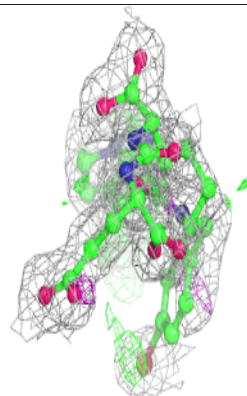
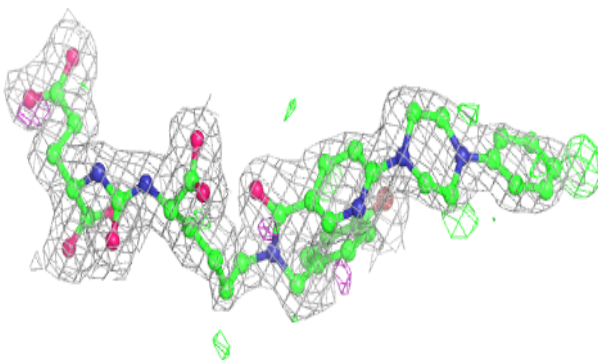
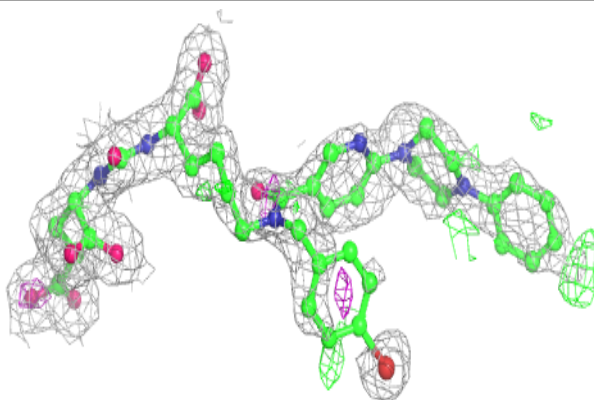
Electron density around 686 A 1320 (C):

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



Electron density around 686 A 1320 (A):

$2mF_o-DF_c$ (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.