



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 01:45 AM BST

PDB ID : 5AMA  
Title : Crystal structure of the Angiotensin-1 converting enzyme N-domain in complex with amyloid-beta 1-16  
Authors : Masuyer, G.; Larmuth, K.M.; Douglas, R.G.; Sturrock, E.D.; Acharya, K.R.  
Deposited on : 2015-03-10  
Resolution : 1.80 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](mailto: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.

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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

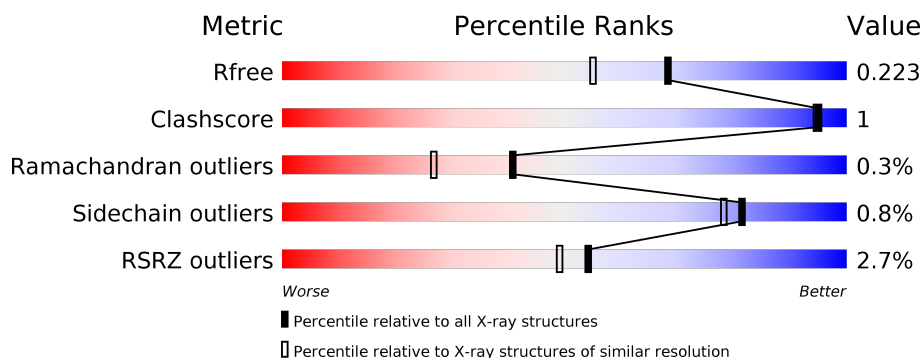
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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  $\geq 3$ , 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	629	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>5%</div> <div>5%</div> </div> <div>• •</div> </div>
1	B	629	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div>5%</div> </div> <div>• •</div> </div>
1	C	629	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>5%</div> <div>5%</div> </div> <div>• •</div> </div>
1	D	629	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div>5%</div> </div> <div>• •</div> </div>
2	E	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
2	F	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	H	2	 100%
2	K	2	 50% 50%
3	G	2	 50% 50%
3	J	2	 100%
3	M	2	 50% 50%
4	I	3	 33% 67%
5	L	4	 25% 75%
6	N	4	 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
2	NAG	E	2	-	-	-	X

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 22267 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 ANGIOTENSIN-CONVERTING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	603	Total	C	N	O	S	0	0	0
			4927	3165	846	897	19			
1	B	605	Total	C	N	O	S	0	1	0
			4939	3173	848	899	19			
1	C	609	Total	C	N	O	S	0	0	0
			4962	3189	852	902	19			
1	D	607	Total	C	N	O	S	0	1	0
			4941	3171	850	901	19			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	engineered mutation	UNP P12821
A	25	GLN	ASN	engineered mutation	UNP P12821
A	82	GLN	ASN	engineered mutation	UNP P12821
A	117	GLN	ASN	engineered mutation	UNP P12821
A	131	GLN	ASN	engineered mutation	UNP P12821
A	289	GLN	ASN	engineered mutation	UNP P12821
A	545	ARG	GLN	engineered mutation	UNP P12821
A	576	LEU	PRO	engineered mutation	UNP P12821
A	629	LEU	ARG	engineered mutation	UNP P12821
B	629	LEU	ARG	engineered mutation	UNP P12821
B	9	GLN	ASN	engineered mutation	UNP P12821
B	25	GLN	ASN	engineered mutation	UNP P12821
B	82	GLN	ASN	engineered mutation	UNP P12821
B	117	GLN	ASN	engineered mutation	UNP P12821
B	131	GLN	ASN	engineered mutation	UNP P12821
B	289	GLN	ASN	engineered mutation	UNP P12821
B	545	ARG	GLN	engineered mutation	UNP P12821
B	576	LEU	PRO	engineered mutation	UNP P12821
C	629	LEU	ARG	engineered mutation	UNP P12821
C	9	GLN	ASN	engineered mutation	UNP P12821
C	25	GLN	ASN	engineered mutation	UNP P12821

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Chain	Residue	Modelled	Actual	Comment	Reference
C	82	GLN	ASN	engineered mutation	UNP P12821
C	117	GLN	ASN	engineered mutation	UNP P12821
C	131	GLN	ASN	engineered mutation	UNP P12821
C	289	GLN	ASN	engineered mutation	UNP P12821
C	545	ARG	GLN	engineered mutation	UNP P12821
C	576	LEU	PRO	engineered mutation	UNP P12821
D	629	LEU	ARG	engineered mutation	UNP P12821
D	9	GLN	ASN	engineered mutation	UNP P12821
D	25	GLN	ASN	engineered mutation	UNP P12821
D	82	GLN	ASN	engineered mutation	UNP P12821
D	117	GLN	ASN	engineered mutation	UNP P12821
D	131	GLN	ASN	engineered mutation	UNP P12821
D	289	GLN	ASN	engineered mutation	UNP P12821
D	545	ARG	GLN	engineered mutation	UNP P12821
D	576	LEU	PRO	engineered mutation	UNP P12821

- 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	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



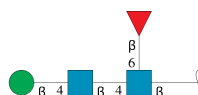
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	J	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	M	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 4 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.



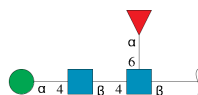
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



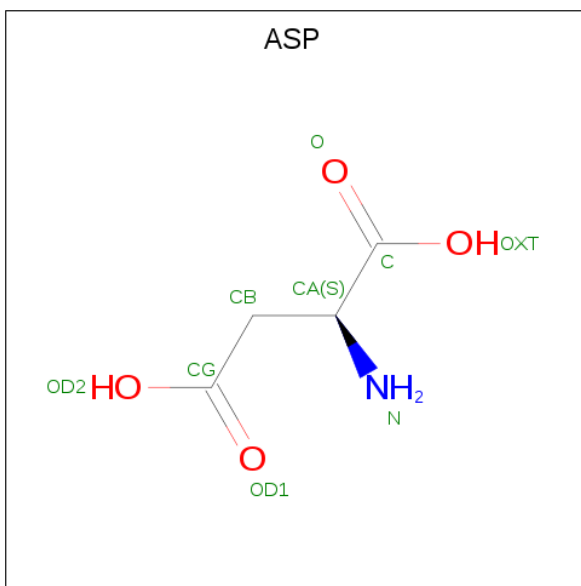
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	L	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



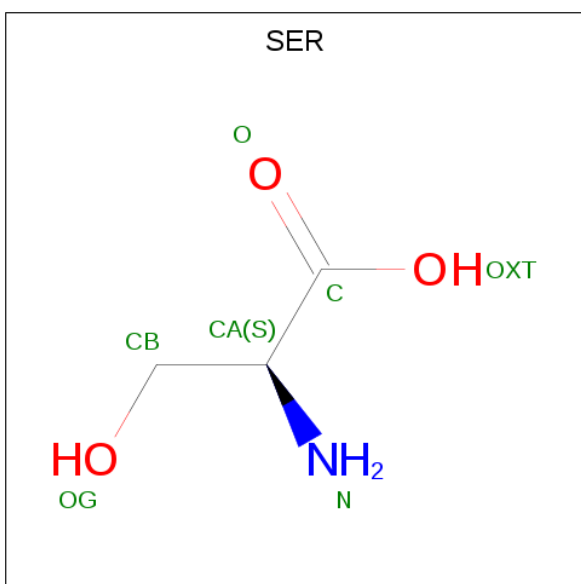
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	N	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 7 is ASPARTIC ACID (three-letter code: ASP) (formula:  $C_4H_7NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			8	4	1	3		
7	B	1	Total	C	N	O	0	0
			8	4	1	3		
7	C	1	Total	C	N	O	0	0
			8	4	1	3		
7	D	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 8 is SERINE (three-letter code: SER) (formula:  $C_3H_7NO_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 7 3 1 3	0	0
8	B	1	Total C N O 7 3 1 3	0	0
8	C	1	Total C N O 7 3 1 3	0	0
8	D	1	Total C N O 7 3 1 3	0	0

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

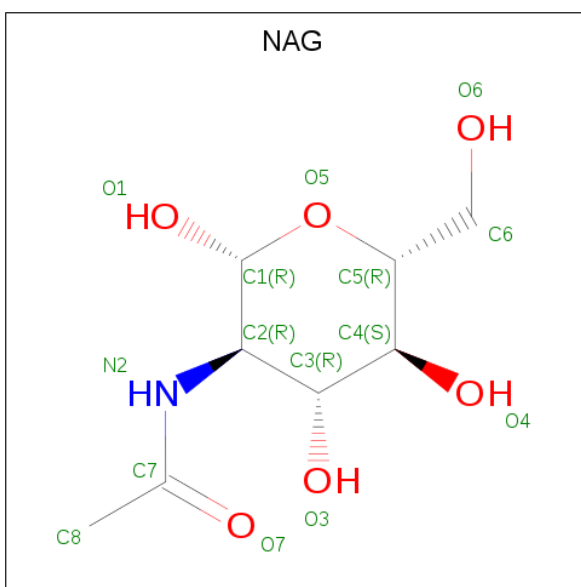
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Zn 1 1	0	0
9	A	1	Total Zn 1 1	0	0
9	D	1	Total Zn 1 1	0	0
9	C	1	Total Zn 1 1	0	0

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Cl 1 1	0	0
10	A	1	Total Cl 1 1	0	0
10	D	1	Total Cl 1 1	0	0
10	C	1	Total Cl 1 1	0	0

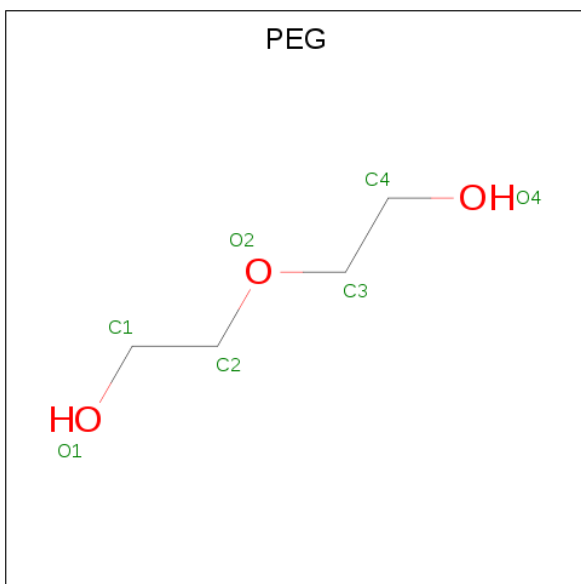
- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).





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

- Molecule 12 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



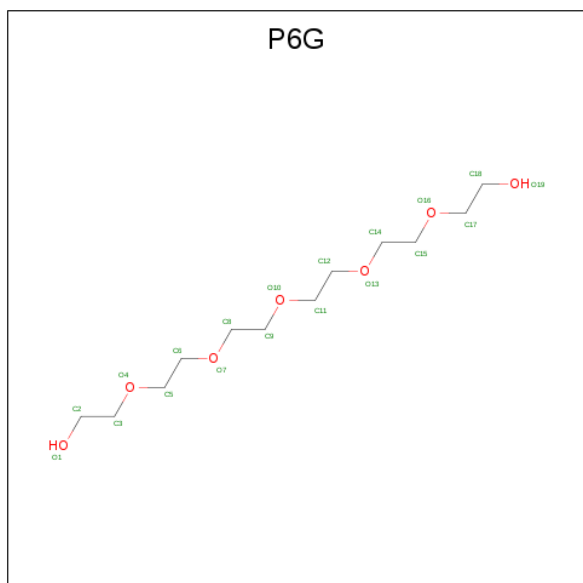
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			7	4	3		
12	A	1	Total	C	O	0	0
			7	4	3		
12	B	1	Total	C	O	0	0
			7	4	3		
12	B	1	Total	C	O	0	0
			7	4	3		
12	B	1	Total	C	O	0	0
			7	4	3		
12	C	1	Total	C	O	0	0
			7	4	3		
12	C	1	Total	C	O	0	0
			7	4	3		
12	D	1	Total	C	O	0	0
			7	4	3		
12	D	1	Total	C	O	0	0
			7	4	3		
12	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 13 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			19	12	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total C O 19 12 7	0	0
13	B	1	Total C O 19 12 7	0	0
13	C	1	Total C O 19 12 7	0	0
13	D	1	Total C O 19 12 7	0	0
13	D	1	Total C O 19 12 7	0	0

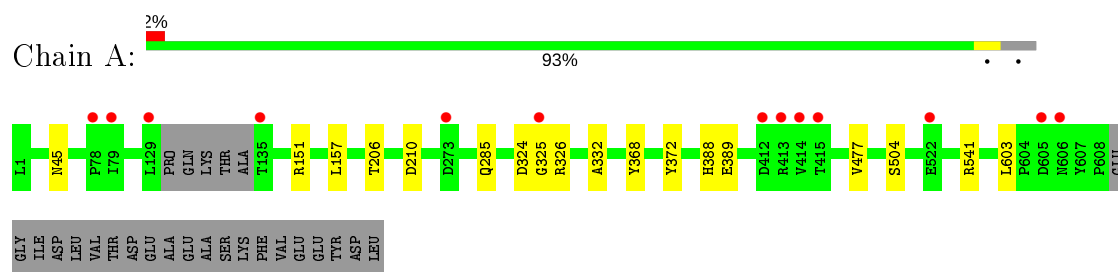
- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	424	Total O 424 424	0	0
14	A	1	Total O 1 1	0	0
14	B	482	Total O 482 482	0	0
14	B	1	Total O 1 1	0	0
14	C	515	Total O 515 515	0	0
14	D	467	Total O 467 467	0	0

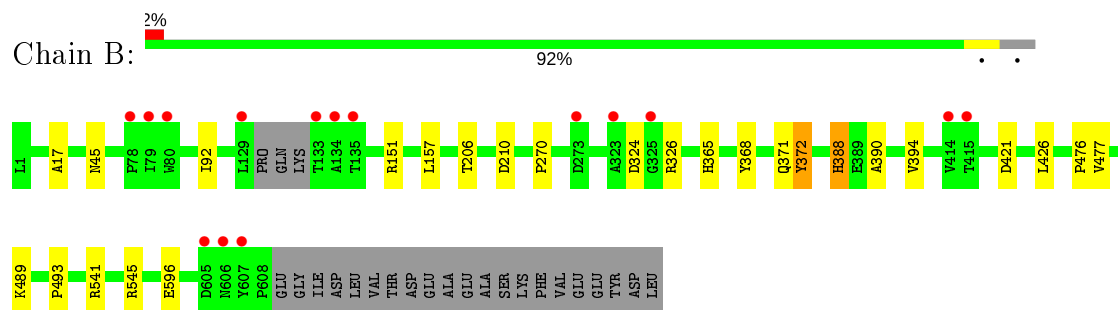
### 3 Residue-property plots [i](#)

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.

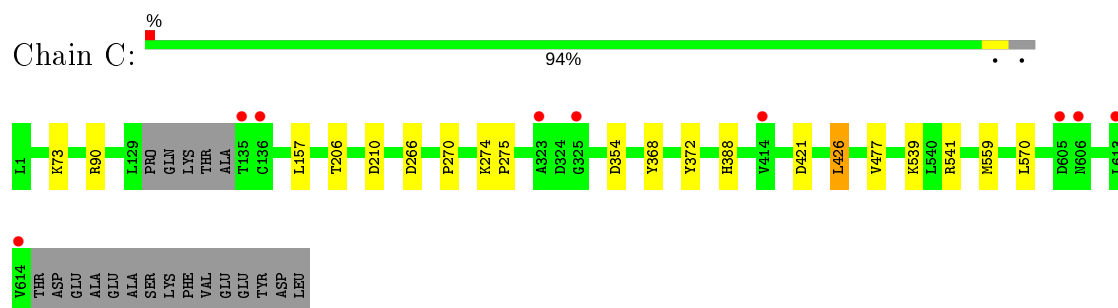
#### • Molecule 1: ANGIOTENSIN-CONVERTING ENZYME



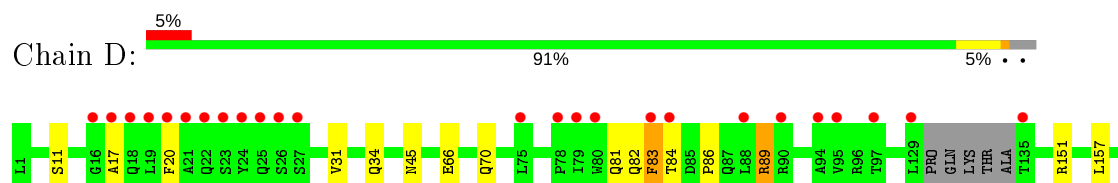
#### • Molecule 1: ANGIOTENSIN-CONVERTING ENZYME

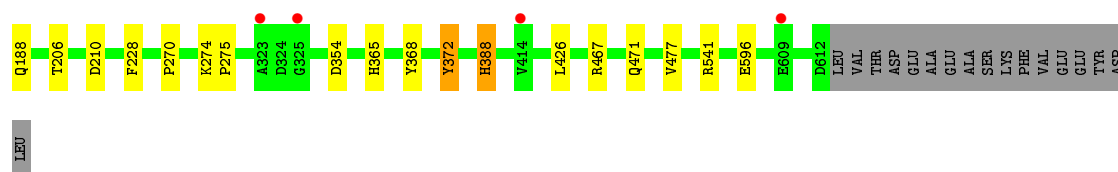


#### • Molecule 1: ANGIOTENSIN-CONVERTING ENZYME



#### • Molecule 1: ANGIOTENSIN-CONVERTING ENZYME





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

Chain E: 50%



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

Chain F: 50%



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

Chain H: 100%



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

Chain K: 50%



- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 50%



- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 100%



- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  50% 50%

MAG1  
FUC2

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

Chain I:  33% 67%

MAG1  
MAG2  
BOL3

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  25% 75%

MAG1  
MAG2  
BOL3  
FUL4

- Molecule 6: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  50% 50%

MAG1  
MAG2  
MAN3  
FUC4

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.34Å 101.73Å 114.14Å 85.09° 85.62° 81.30°	Depositor
Resolution (Å)	113.48 – 1.80 33.27 – 1.80	Depositor EDS
% Data completeness (in resolution range)	93.5 (113.48-1.80) 93.6 (33.27-1.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 1.81Å)	Xtrriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.187 , 0.218 0.194 , 0.223	Depositor DCC
$R_{free}$ test set	13921 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.8	Xtrriage
Anisotropy	0.299	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	22267	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.77 % 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 3.5050e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, FUC, P6G, FUL, PEG, 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	0.48	0/5082	0.68	4/6922 (0.1%)
1	B	0.51	0/5097	0.68	2/6943 (0.0%)
1	C	0.51	0/5117	0.70	5/6970 (0.1%)
1	D	0.52	0/5096	0.69	1/6940 (0.0%)
All	All	0.51	0/20392	0.69	12/27775 (0.0%)

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	D	0	2
All	All	0	3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	541	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	C	541	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	B	541	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	D	541	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	326	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	B	151	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	541	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	C	426	LEU	CA-CB-CG	-5.27	103.19	115.30
1	C	90	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	C	541	ARG	NE-CZ-NH2	-5.16	117.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	266	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	151	ARG	NE-CZ-NH1	5.09	122.85	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	325	GLY	Peptide
1	D	82	GLN	Peptide
1	D	83	PHE	Peptide

## 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	4927	0	4703	5	0
1	B	4939	0	4712	13	0
1	C	4962	0	4736	9	0
1	D	4941	0	4718	19	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	H	28	0	25	0	0
2	K	28	0	25	0	0
3	G	24	0	22	1	0
3	J	24	0	22	0	0
3	M	24	0	22	1	0
4	I	39	0	34	0	0
5	L	49	0	43	0	0
6	N	49	0	43	0	0
7	A	8	0	3	1	0
7	B	8	0	3	0	0
7	C	8	0	3	0	0
7	D	8	0	3	0	0
8	A	7	0	5	0	0
8	B	7	0	5	0	0
8	C	7	0	5	0	0
8	D	7	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
11	A	14	0	13	0	0
11	D	14	0	13	0	0
12	A	21	0	30	1	0
12	B	21	0	30	0	0
12	C	14	0	20	0	0
12	D	21	0	30	0	0
13	A	19	0	26	1	0
13	B	38	0	52	0	0
13	C	19	0	26	0	0
13	D	38	0	52	1	0
14	A	425	0	0	0	0
14	B	483	0	0	0	0
14	C	515	0	0	2	0
14	D	467	0	0	3	0
All	All	22267	0	19479	47	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 1.

All (47) 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:D:365:HIS:HD1	1:D:388:HIS:HD2	1.30	0.79
1:B:270:PRO:HD3	1:B:426:LEU:HD22	1.70	0.74
1:D:365:HIS:HD1	1:D:388:HIS:CD2	2.06	0.73
1:D:151:ARG:NH1	14:D:2138:HOH:O	2.16	0.72
1:D:467:ARG:HH11	1:D:471:GLN:HE22	1.37	0.72
1:B:365:HIS:HD1	1:B:388:HIS:CD2	2.11	0.69
1:C:206:THR:HG23	1:C:210:ASP:OD2	1.95	0.66
1:D:354:ASP:OD2	14:D:2317:HOH:O	2.14	0.64
1:D:206:THR:HG23	1:D:210:ASP:OD2	1.99	0.62
1:B:365:HIS:HD1	1:B:388:HIS:HD2	1.47	0.62
1:A:157:LEU:HD11	1:A:477:VAL:HG13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:THR:HG23	1:A:210:ASP:OD2	2.01	0.60
1:B:206:THR:HG23	1:B:210:ASP:OD2	2.02	0.60
1:D:157:LEU:HD11	1:D:477:VAL:HG13	1.84	0.58
1:D:270:PRO:HD3	1:D:426:LEU:HD23	1.87	0.57
1:C:539:LYS:HE3	1:C:559:MET:O	2.09	0.52
1:B:596:GLU:OE2	3:M:1:NAG:O7	2.29	0.51
1:B:157:LEU:HD11	1:B:477:VAL:HG13	1.93	0.50
1:D:372:TYR:OH	1:D:388:HIS:HE1	1.95	0.50
1:D:188[A]:GLN:NE2	14:D:2085:HOH:O	2.46	0.48
1:D:228:PHE:CZ	13:D:1201:P6G:H142	2.49	0.48
1:D:467:ARG:NH1	1:D:471:GLN:HE22	2.08	0.47
1:D:86:PRO:O	1:D:89:ARG:HD2	2.15	0.47
1:B:372:TYR:OH	1:B:388:HIS:HE1	1.97	0.47
1:D:270:PRO:HD3	1:D:426:LEU:CD2	2.44	0.47
1:C:157:LEU:HD11	1:C:477:VAL:HG13	1.97	0.47
1:B:324:ASP:OD1	1:B:326:ARG:HB2	2.16	0.46
1:D:66:GLU:O	1:D:70:GLN:HG2	2.16	0.46
1:B:17:ALA:HB1	1:B:92:ILE:HD11	1.97	0.45
12:A:1201:PEG:O4	13:A:1202:P6G:O19	2.35	0.45
1:C:270:PRO:HD3	1:C:426:LEU:HD22	1.99	0.44
1:D:31:VAL:O	1:D:34:GLN:HG3	2.17	0.44
1:D:596:GLU:OE2	3:G:1:NAG:O7	2.35	0.44
1:D:17:ALA:HA	1:D:20:PHE:HB3	1.99	0.44
1:C:274:LYS:HB3	1:C:275:PRO:CD	2.48	0.44
1:C:354:ASP:OD2	14:C:2286:HOH:O	2.21	0.43
1:A:389:GLU:HB2	1:A:504:SER:HB2	1.98	0.43
1:A:477:VAL:HG12	1:A:603:LEU:HD21	2.00	0.43
1:B:157:LEU:HD13	1:B:476:PRO:HB2	2.00	0.42
1:C:426:LEU:O	1:C:426:LEU:HG	2.17	0.42
1:B:371:GLN:HB3	1:B:545[B]:ARG:HG2	2.01	0.41
1:A:332:ALA:HB3	7:A:907:ASP:HB2	2.02	0.41
1:C:570:LEU:C	1:C:570:LEU:HD23	2.40	0.41
1:B:390:ALA:O	1:B:394:VAL:HG23	2.21	0.41
1:B:489:LYS:O	1:B:493:PRO:HD2	2.20	0.41
1:D:274:LYS:HB3	1:D:275:PRO:CD	2.51	0.40
1:C:73:LYS:NZ	14:C:2111:HOH:O	2.45	0.40

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	599/629 (95%)	588 (98%)	9 (2%)	2 (0%)	41	27
1	B	602/629 (96%)	593 (98%)	8 (1%)	1 (0%)	47	33
1	C	605/629 (96%)	595 (98%)	10 (2%)	0	100	100
1	D	604/629 (96%)	590 (98%)	10 (2%)	4 (1%)	22	10
All	All	2410/2516 (96%)	2366 (98%)	37 (2%)	7 (0%)	41	27

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	ASP
1	D	83	PHE
1	D	81	GLN
1	D	84	THR
1	D	45	ASN
1	A	45	ASN
1	B	45	ASN

### 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	518/541 (96%)	514 (99%)	4 (1%)	81	78
1	B	518/541 (96%)	514 (99%)	4 (1%)	81	78
1	C	520/541 (96%)	516 (99%)	4 (1%)	81	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	518/541 (96%)	513 (99%)	5 (1%)	76	71
All	All	2074/2164 (96%)	2057 (99%)	17 (1%)	81	78

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	285	GLN
1	A	368	TYR
1	A	372	TYR
1	A	388	HIS
1	B	368	TYR
1	B	372	TYR
1	B	388	HIS
1	B	421	ASP
1	C	368	TYR
1	C	372	TYR
1	C	388	HIS
1	C	421	ASP
1	D	11	SER
1	D	89	ARG
1	D	368	TYR
1	D	372	TYR
1	D	388	HIS

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

Mol	Chain	Res	Type
1	B	217	GLN
1	B	388	HIS
1	C	117	GLN
1	D	9	GLN
1	D	87	GLN
1	D	203	ASN
1	D	371	GLN
1	D	388	HIS
1	D	471	GLN
1	D	491	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 ⓘ

25 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	E	1	1,2	14,14,15	0.42	0	17,19,21	1.16	2 (11%)
2	NAG	E	2	2	14,14,15	0.50	0	17,19,21	0.96	0
2	NAG	F	1	1,2	14,14,15	0.34	0	17,19,21	0.79	0
2	NAG	F	2	2	14,14,15	0.45	0	17,19,21	0.98	1 (5%)
3	NAG	G	1	1,3	14,14,15	0.75	0	17,19,21	1.55	5 (29%)
3	FUC	G	2	3	10,10,11	0.69	0	14,14,16	1.48	1 (7%)
2	NAG	H	1	1,2	14,14,15	0.49	0	17,19,21	0.87	1 (5%)
2	NAG	H	2	2	14,14,15	0.53	0	17,19,21	1.29	1 (5%)
4	NAG	I	1	1,4	14,14,15	0.41	0	17,19,21	0.92	1 (5%)
4	NAG	I	2	4	14,14,15	0.33	0	17,19,21	0.64	0
4	BMA	I	3	4	11,11,12	0.40	0	15,15,17	1.18	2 (13%)
3	NAG	J	1	1,3	14,14,15	0.69	0	17,19,21	1.61	4 (23%)
3	FUC	J	2	3	10,10,11	0.71	0	14,14,16	2.01	2 (14%)
2	NAG	K	1	1,2	14,14,15	0.49	0	17,19,21	0.96	2 (11%)
2	NAG	K	2	2	14,14,15	0.35	0	17,19,21	0.93	0
5	NAG	L	1	1,5	14,14,15	0.64	0	17,19,21	1.09	1 (5%)
5	NAG	L	2	5	14,14,15	0.43	0	17,19,21	1.06	1 (5%)
5	BMA	L	3	5	11,11,12	0.40	0	15,15,17	0.69	0
5	FUL	L	4	5	10,10,11	0.68	0	14,14,16	1.14	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	M	1	1,3	14,14,15	0.72	0	17,19,21	1.69	5 (29%)
3	FUC	M	2	3	10,10,11	0.60	0	14,14,16	1.21	1 (7%)
6	NAG	N	1	1,6	14,14,15	0.46	0	17,19,21	0.89	0
6	NAG	N	2	6	14,14,15	0.48	0	17,19,21	0.75	0
6	MAN	N	3	6	11,11,12	0.57	0	15,15,17	1.62	5 (33%)
6	FUC	N	4	6	10,10,11	0.48	0	14,14,16	1.18	2 (14%)

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	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	FUC	G	2	3	-	-	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	BMA	I	3	4	-	2/2/19/22	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	J	2	3	-	-	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
5	NAG	L	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	L	2	5	-	0/6/23/26	0/1/1/1
5	BMA	L	3	5	-	2/2/19/22	0/1/1/1
5	FUL	L	4	5	-	-	0/1/1/1
3	NAG	M	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	M	2	3	-	-	0/1/1/1
6	NAG	N	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	N	2	6	-	0/6/23/26	0/1/1/1
6	MAN	N	3	6	-	0/2/19/22	0/1/1/1
6	FUC	N	4	6	-	-	0/1/1/1

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	2	FUC	C1-C2-C3	5.90	116.92	109.67
3	G	2	FUC	O5-C1-C2	-4.32	104.11	110.77
3	J	2	FUC	O5-C1-C2	3.80	116.64	110.77
3	M	1	NAG	O5-C5-C6	3.44	112.60	107.20
3	J	1	NAG	C4-C3-C2	3.38	115.97	111.02
4	I	3	BMA	O5-C5-C6	3.27	112.33	107.20
6	N	3	MAN	O5-C5-C6	3.10	112.06	107.20
3	M	1	NAG	C2-N2-C7	-3.03	118.59	122.90
2	E	1	NAG	C1-O5-C5	2.77	115.95	112.19
6	N	3	MAN	C3-C4-C5	2.77	115.18	110.24
2	H	2	NAG	O5-C1-C2	-2.68	107.05	111.29
3	G	1	NAG	O7-C7-N2	-2.61	117.16	121.95
6	N	3	MAN	C1-C2-C3	2.57	112.83	109.67
2	E	1	NAG	O5-C1-C2	-2.56	107.25	111.29
3	G	1	NAG	C1-C2-N2	-2.55	106.14	110.49
3	M	1	NAG	O7-C7-N2	-2.55	117.27	121.95
5	L	2	NAG	C2-N2-C7	2.45	126.39	122.90
3	J	1	NAG	O5-C5-C6	2.42	111.00	107.20
6	N	3	MAN	C1-O5-C5	2.41	115.45	112.19
4	I	1	NAG	O4-C4-C3	-2.37	104.86	110.35
3	M	1	NAG	C8-C7-N2	2.35	120.08	116.10
5	L	4	FUL	C1-O5-C5	2.33	118.06	112.78
3	J	1	NAG	C2-N2-C7	2.33	126.22	122.90
4	I	3	BMA	C1-O5-C5	2.29	115.29	112.19
2	K	1	NAG	O5-C1-C2	-2.28	107.69	111.29
3	J	1	NAG	C1-C2-N2	-2.27	106.61	110.49
2	K	1	NAG	C1-O5-C5	2.26	115.25	112.19
6	N	4	FUC	C3-C4-C5	2.23	113.24	109.77
3	G	1	NAG	C6-C5-C4	2.16	118.07	113.00
3	M	1	NAG	O4-C4-C3	-2.15	105.39	110.35
3	G	1	NAG	O6-C6-C5	2.13	118.58	111.29
3	M	2	FUC	C1-C2-C3	2.11	112.26	109.67
5	L	1	NAG	C1-C2-N2	-2.08	106.93	110.49
3	G	1	NAG	C8-C7-N2	2.08	119.62	116.10
2	F	2	NAG	C2-N2-C7	2.07	125.85	122.90
2	H	1	NAG	C1-O5-C5	2.03	114.95	112.19
6	N	4	FUC	O5-C1-C2	-2.03	107.64	110.77
6	N	3	MAN	C2-C3-C4	2.01	114.37	110.89

There are no chirality outliers.

All (12) torsion outliers are listed below:



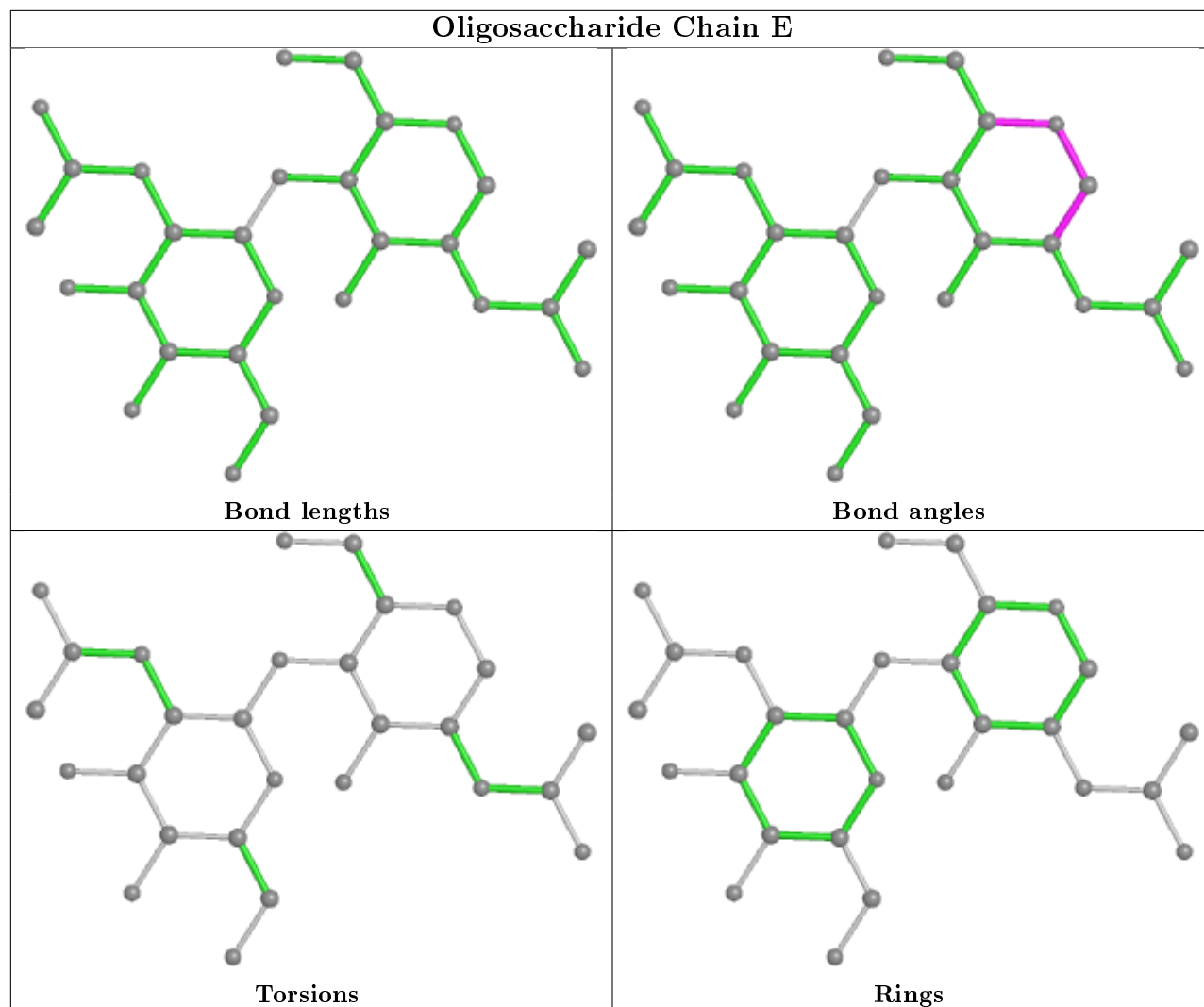
Mol	Chain	Res	Type	Atoms
5	L	3	BMA	C4-C5-C6-O6
5	L	3	BMA	O5-C5-C6-O6
4	I	3	BMA	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
4	I	3	BMA	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6

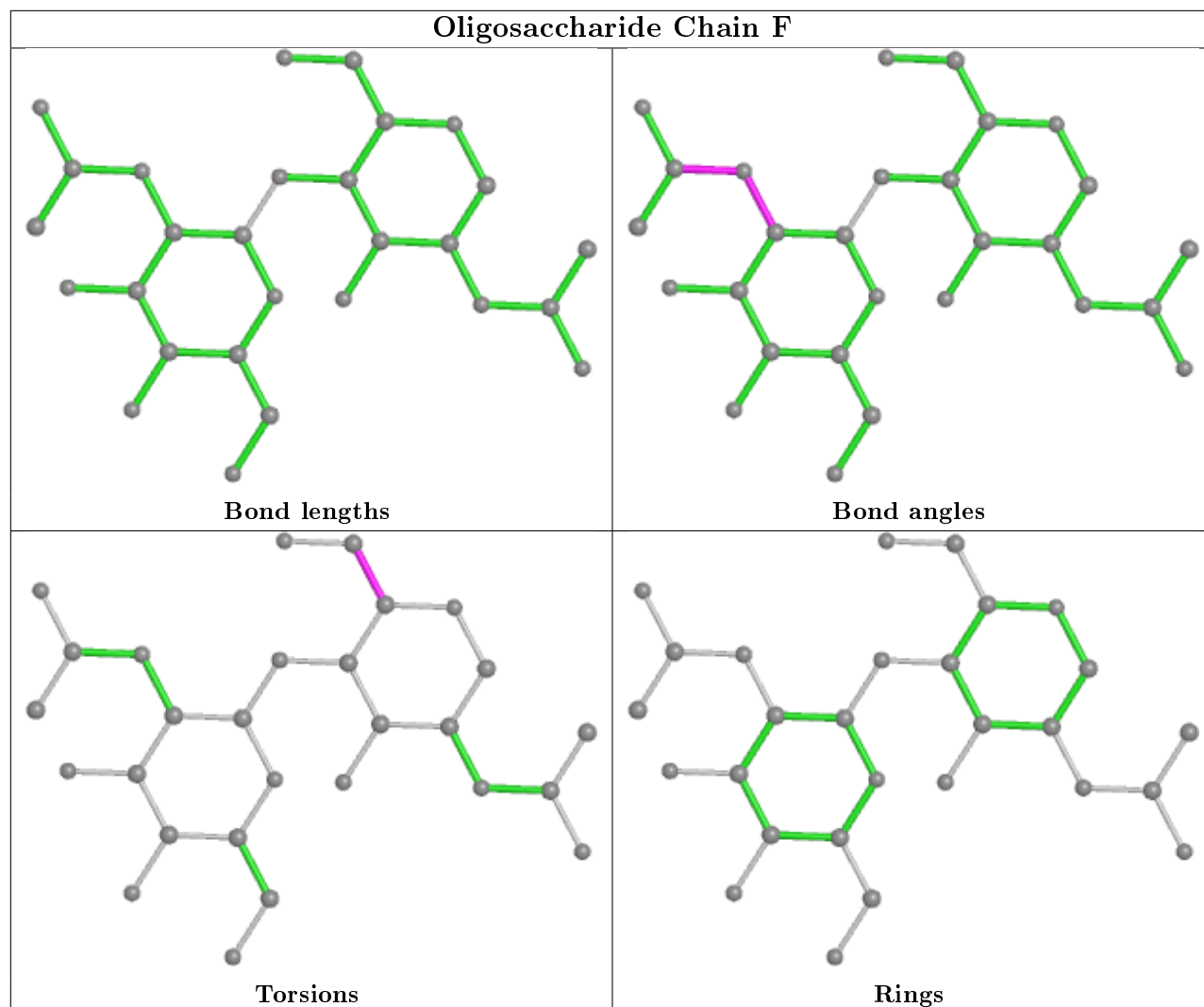
There are no ring outliers.

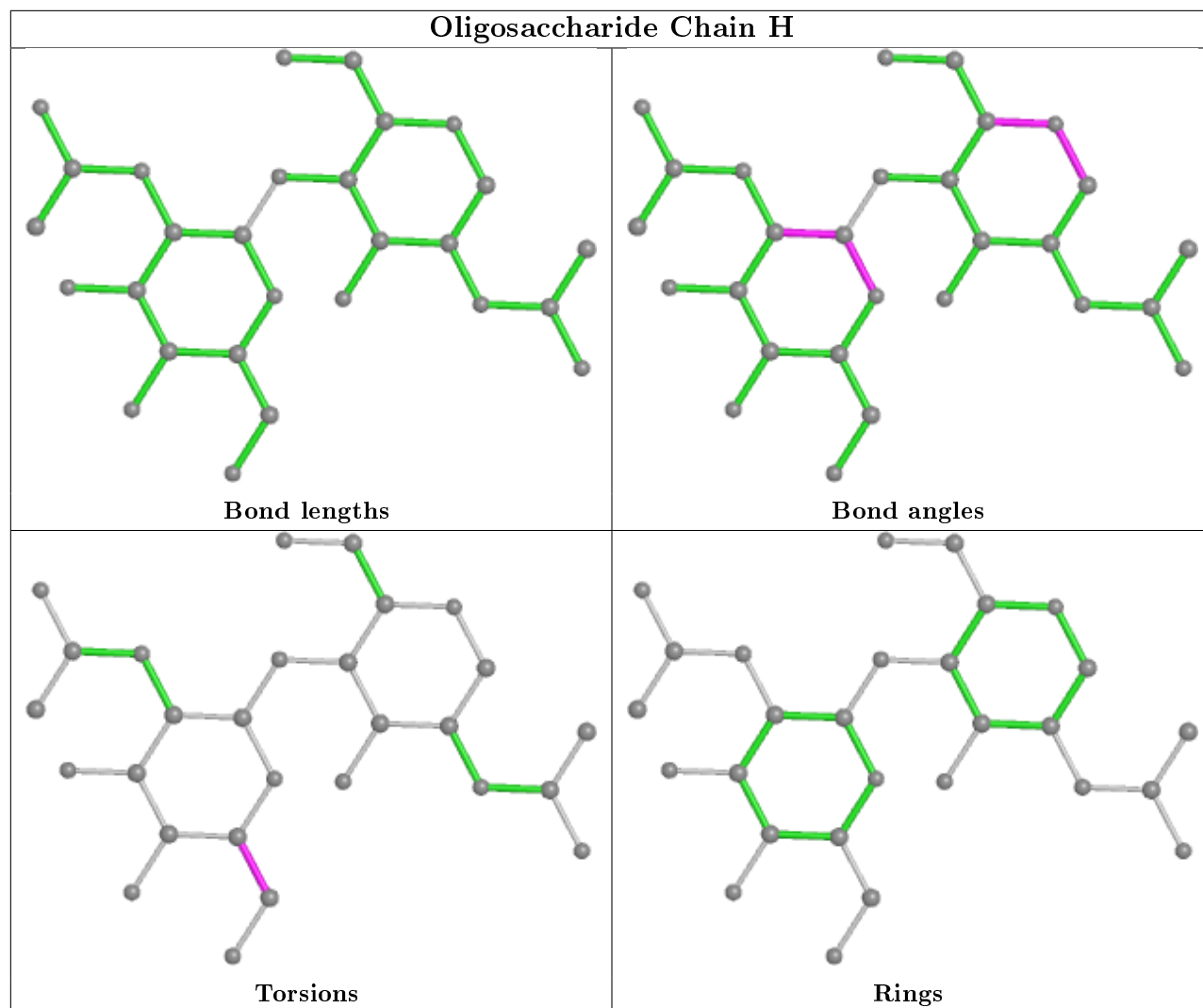
2 monomers are involved in 2 short contacts:

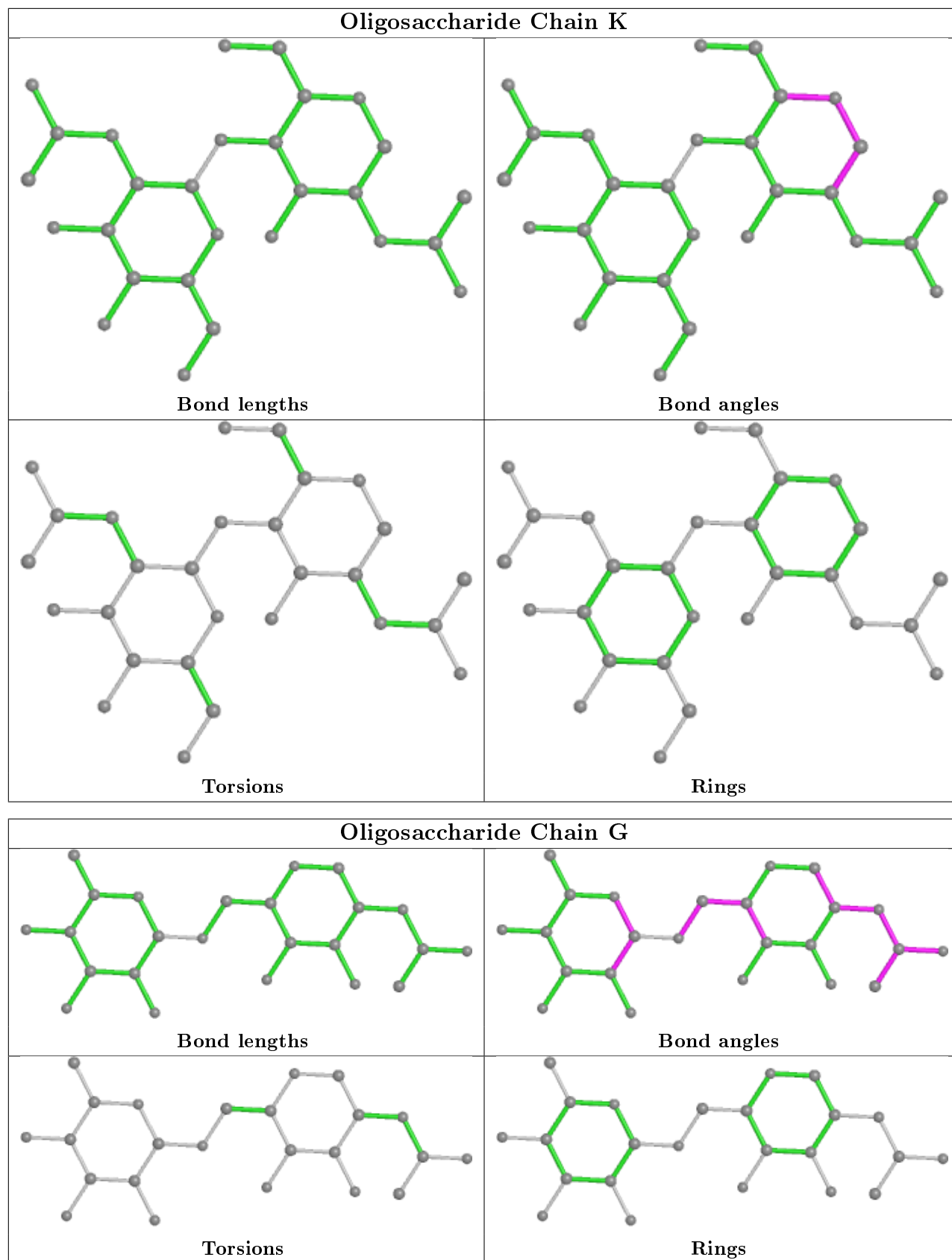
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	1	NAG	1	0
3	G	1	NAG	1	0

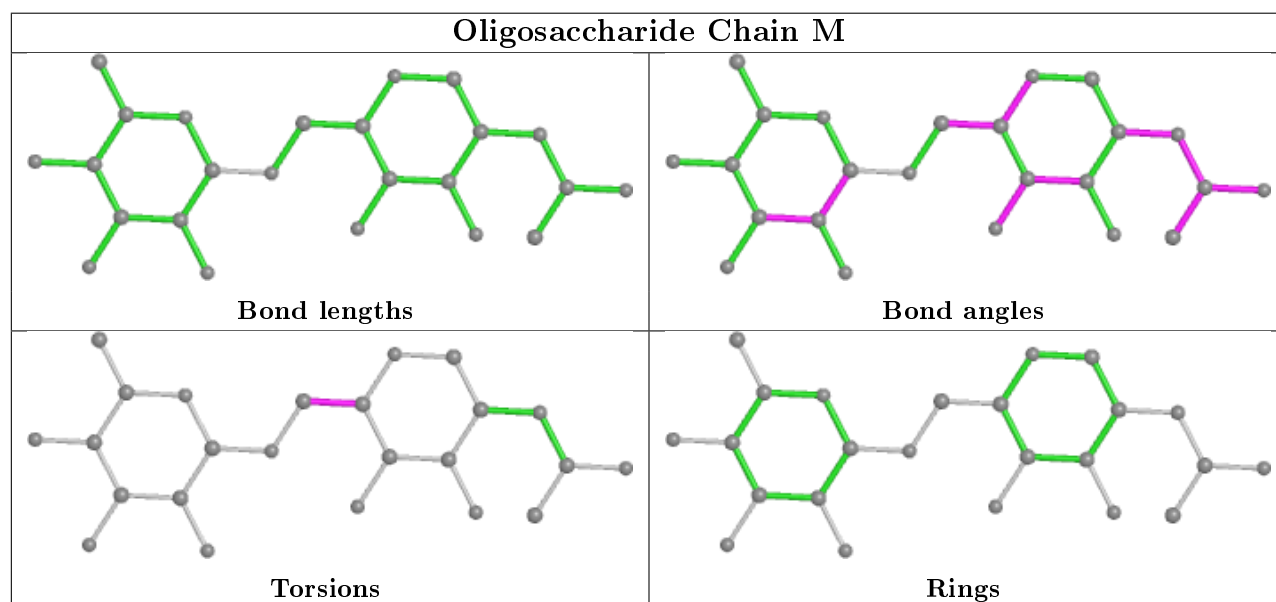
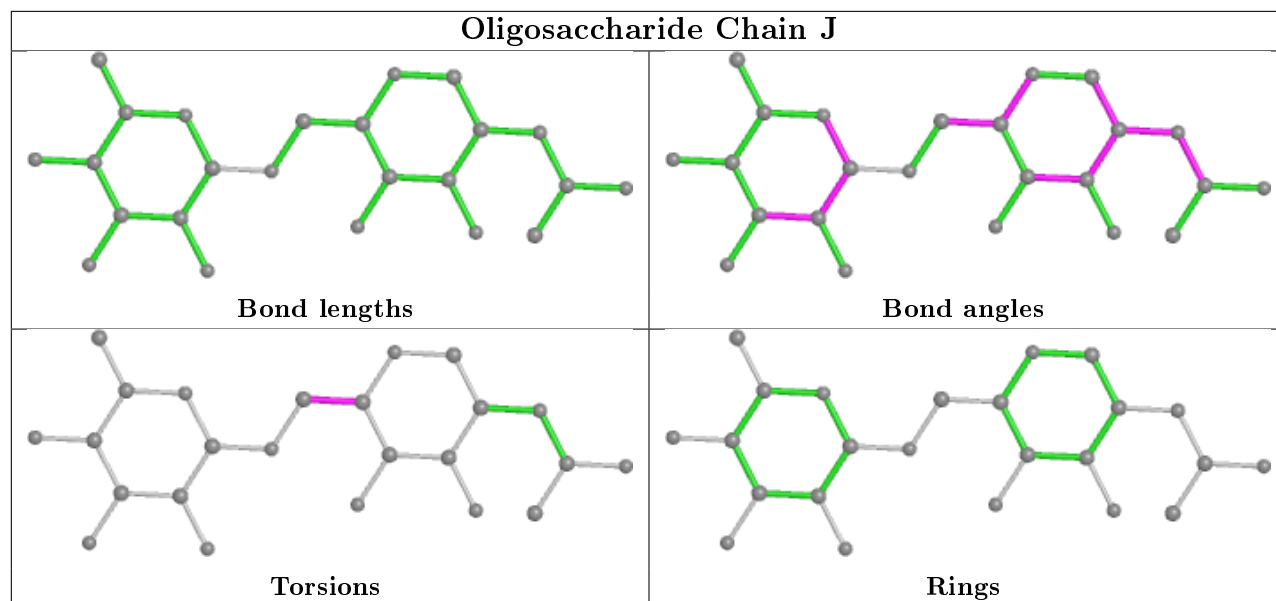
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

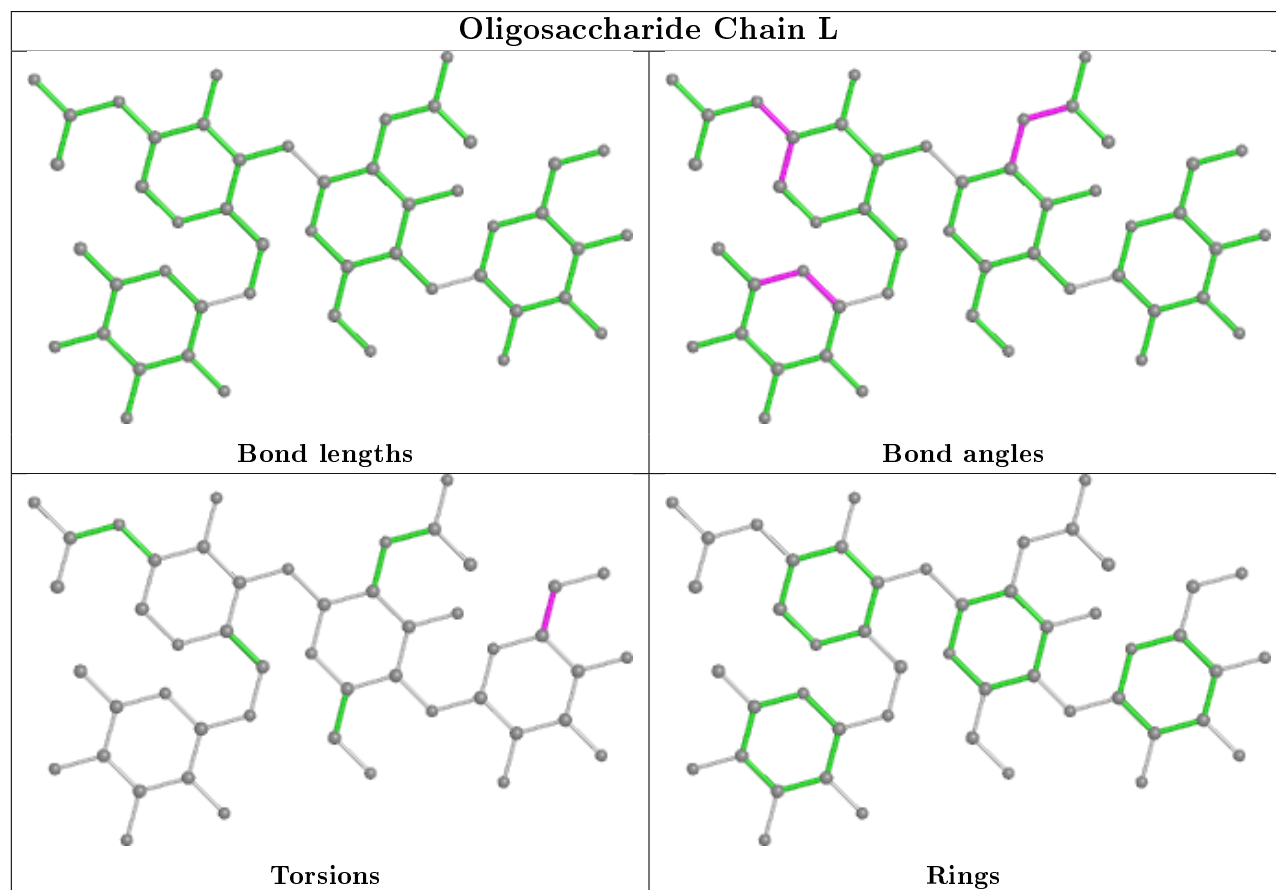
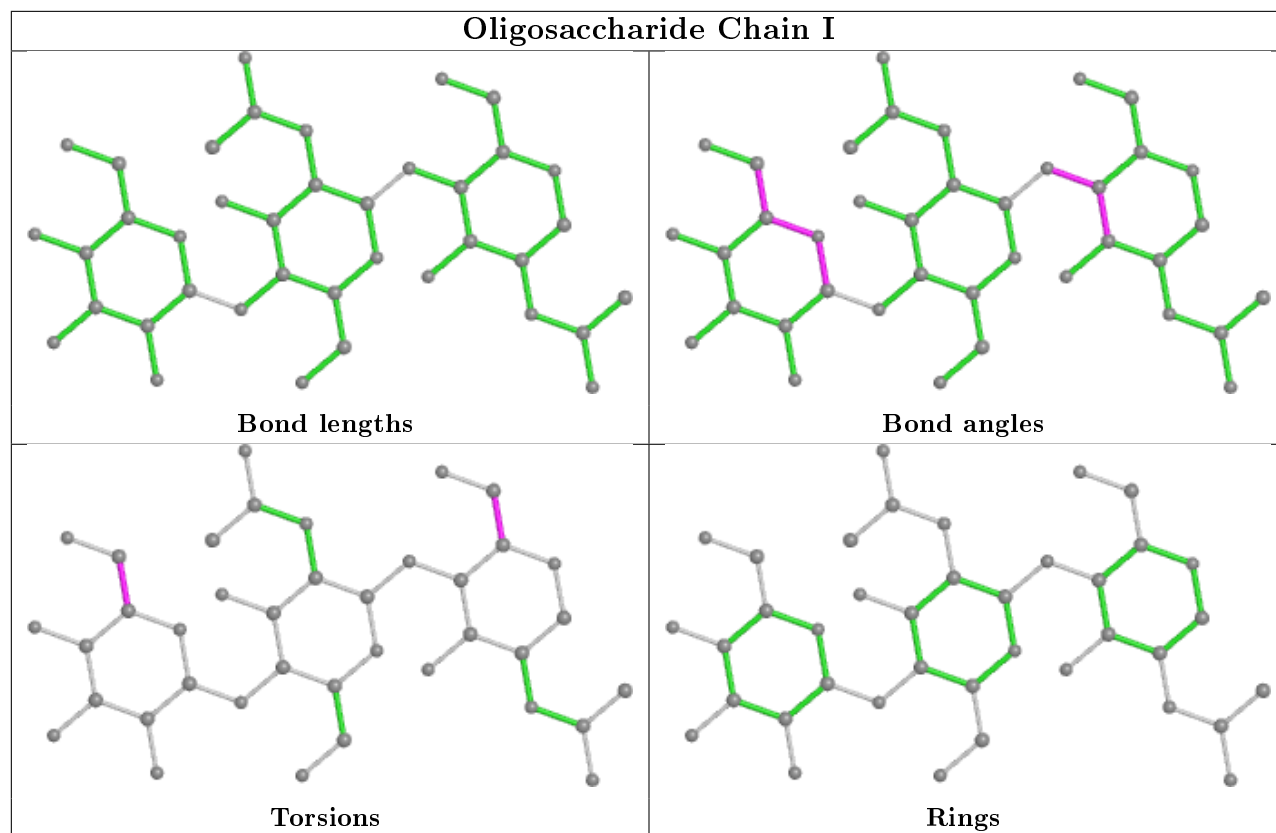


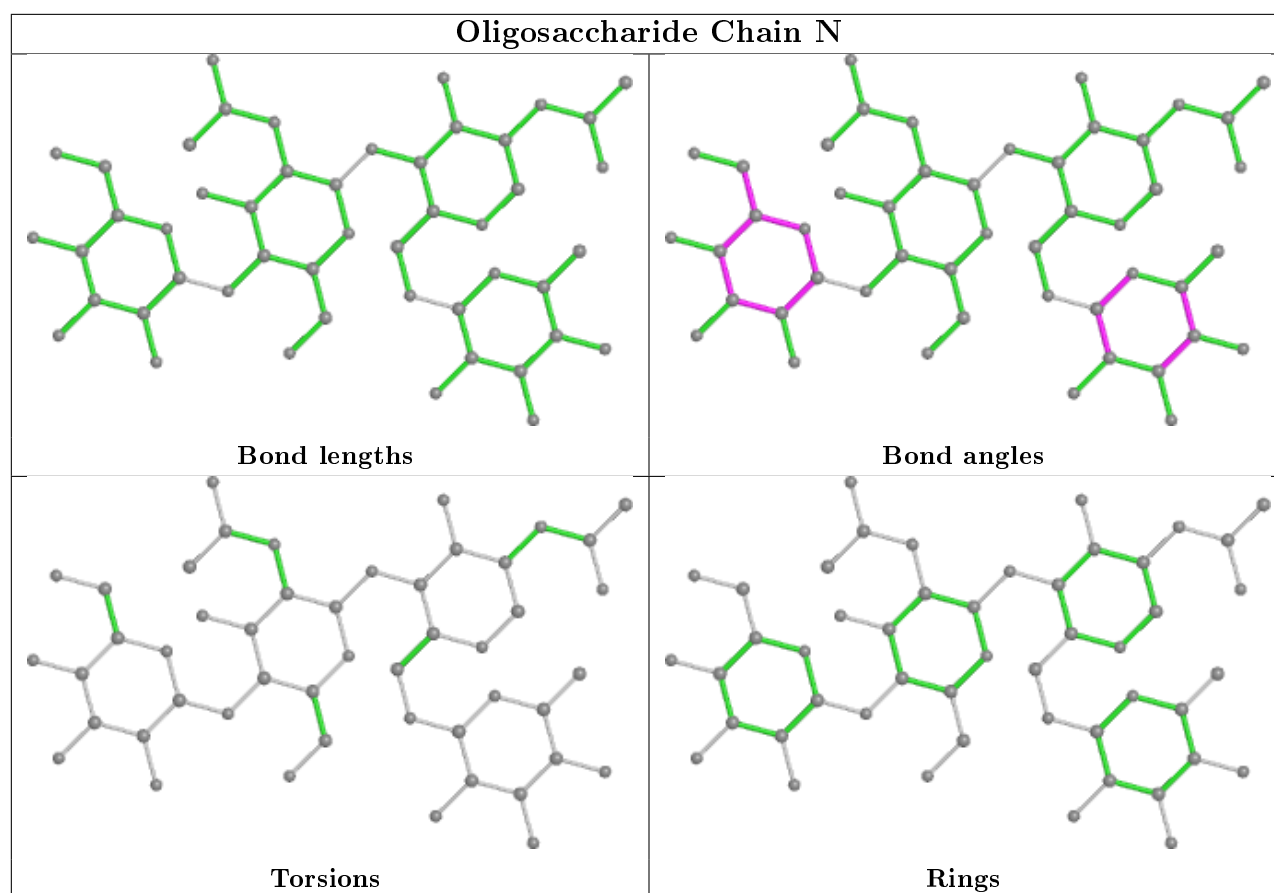












## 5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 8 are monoatomic - leaving 27 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	$\# Z  > 2$
13	P6G	B	1203	-	18,18,18	0.67	0	17,17,17	0.90	0
12	PEG	B	1201	-	6,6,6	0.52	0	5,5,5	0.37	0
12	PEG	A	1201	-	6,6,6	0.44	0	5,5,5	0.39	0
12	PEG	D	1205	-	6,6,6	0.51	0	5,5,5	0.22	0
12	PEG	D	1200	-	6,6,6	0.40	0	5,5,5	0.34	0
13	P6G	B	1204	-	18,18,18	0.54	0	17,17,17	0.52	0
13	P6G	C	1202	-	18,18,18	0.52	0	17,17,17	0.40	0
13	P6G	A	1202	-	18,18,18	0.46	0	17,17,17	0.42	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	NAG	A	1100	1	14,14,15	0.45	0	17,19,21	1.02	2 (11%)
11	NAG	D	1102	1	14,14,15	0.54	0	17,19,21	1.14	0
13	P6G	D	1203	-	18,18,18	0.52	0	17,17,17	0.35	0
13	P6G	D	1201	-	18,18,18	0.61	0	17,17,17	0.94	1 (5%)
12	PEG	B	1200	-	6,6,6	0.42	0	5,5,5	0.38	0
12	PEG	A	1204	-	6,6,6	0.40	0	5,5,5	0.40	0
12	PEG	C	1201	-	6,6,6	0.48	0	5,5,5	0.42	0
12	PEG	C	1200	-	6,6,6	0.42	0	5,5,5	0.29	0
12	PEG	B	1202	-	6,6,6	0.46	0	5,5,5	0.31	0
12	PEG	A	1200	-	6,6,6	0.43	0	5,5,5	0.42	0
12	PEG	D	1202	-	6,6,6	0.47	0	5,5,5	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	P6G	B	1203	-	-	12/16/16/16	-
12	PEG	B	1201	-	-	1/4/4/4	-
12	PEG	A	1201	-	-	1/4/4/4	-
12	PEG	D	1205	-	-	2/4/4/4	-
12	PEG	D	1200	-	-	2/4/4/4	-
13	P6G	B	1204	-	-	10/16/16/16	-
13	P6G	C	1202	-	-	7/16/16/16	-
13	P6G	A	1202	-	-	5/16/16/16	-
11	NAG	A	1100	1	-	0/6/23/26	0/1/1/1
11	NAG	D	1102	1	-	0/6/23/26	0/1/1/1
13	P6G	D	1203	-	-	5/16/16/16	-
13	P6G	D	1201	-	-	8/16/16/16	-
12	PEG	B	1200	-	-	3/4/4/4	-
12	PEG	A	1204	-	-	2/4/4/4	-
12	PEG	C	1201	-	-	1/4/4/4	-
12	PEG	C	1200	-	-	2/4/4/4	-
12	PEG	B	1202	-	-	3/4/4/4	-
12	PEG	A	1200	-	-	3/4/4/4	-
12	PEG	D	1202	-	-	1/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1100	NAG	O5-C5-C6	2.54	111.18	107.20
13	D	1201	P6G	O16-C17-C18	2.44	120.79	110.07
11	A	1100	NAG	O5-C5-C4	-2.04	105.86	110.83

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	B	1204	P6G	O16-C17-C18-O19
13	B	1203	P6G	O7-C8-C9-O10
13	B	1204	P6G	O10-C11-C12-O13
13	D	1201	P6G	O4-C5-C6-O7
13	D	1201	P6G	O7-C8-C9-O10
12	A	1204	PEG	O1-C1-C2-O2
13	B	1203	P6G	C15-C14-O13-C12
12	D	1205	PEG	O2-C3-C4-O4
13	D	1201	P6G	O1-C2-C3-O4
13	D	1203	P6G	O10-C11-C12-O13
12	A	1201	PEG	O2-C3-C4-O4
13	A	1202	P6G	O16-C17-C18-O19
12	B	1201	PEG	O1-C1-C2-O2
12	B	1200	PEG	O2-C3-C4-O4
13	D	1203	P6G	O1-C2-C3-O4
12	D	1205	PEG	O1-C1-C2-O2
13	B	1203	P6G	O16-C17-C18-O19
12	B	1200	PEG	O1-C1-C2-O2
13	C	1202	P6G	O10-C11-C12-O13
12	B	1202	PEG	O2-C3-C4-O4
13	A	1202	P6G	O10-C11-C12-O13
13	D	1201	P6G	C8-C9-O10-C11
13	B	1203	P6G	O1-C2-C3-O4
12	D	1200	PEG	O1-C1-C2-O2
12	D	1200	PEG	O2-C3-C4-O4
12	C	1200	PEG	O1-C1-C2-O2
12	C	1200	PEG	O2-C3-C4-O4
12	B	1202	PEG	O1-C1-C2-O2
12	C	1201	PEG	O1-C1-C2-O2
13	B	1204	P6G	O13-C14-C15-O16
13	C	1202	P6G	O4-C5-C6-O7
13	A	1202	P6G	O13-C14-C15-O16
13	B	1204	P6G	O4-C5-C6-O7

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Mol	Chain	Res	Type	Atoms
12	A	1200	PEG	O1-C1-C2-O2
13	B	1203	P6G	C6-C5-O4-C3
13	B	1203	P6G	C14-C15-O16-C17
13	B	1204	P6G	C11-C12-O13-C14
12	B	1200	PEG	C4-C3-O2-C2
13	C	1202	P6G	C9-C8-O7-C6
13	B	1203	P6G	C2-C3-O4-C5
13	B	1204	P6G	C8-C9-O10-C11
12	A	1200	PEG	O2-C3-C4-O4
12	A	1200	PEG	C1-C2-O2-C3
13	C	1202	P6G	C8-C9-O10-C11
13	D	1201	P6G	C9-C8-O7-C6
13	D	1201	P6G	O13-C14-C15-O16
13	B	1203	P6G	C5-C6-O7-C8
13	D	1201	P6G	C2-C3-O4-C5
12	D	1202	PEG	O2-C3-C4-O4
13	D	1203	P6G	C15-C14-O13-C12
13	C	1202	P6G	C15-C14-O13-C12
12	A	1204	PEG	C1-C2-O2-C3
13	C	1202	P6G	C6-C5-O4-C3
12	B	1202	PEG	C1-C2-O2-C3
13	B	1204	P6G	C9-C8-O7-C6
13	B	1203	P6G	C8-C9-O10-C11
13	D	1203	P6G	C14-C15-O16-C17
13	C	1202	P6G	O7-C8-C9-O10
13	B	1204	P6G	C2-C3-O4-C5
13	A	1202	P6G	C8-C9-O10-C11
13	A	1202	P6G	O7-C8-C9-O10
13	B	1204	P6G	O1-C2-C3-O4
13	D	1203	P6G	O7-C8-C9-O10
13	D	1201	P6G	O10-C11-C12-O13
13	B	1203	P6G	O13-C14-C15-O16
13	B	1203	P6G	C18-C17-O16-C15
13	B	1203	P6G	O4-C5-C6-O7
13	B	1204	P6G	C5-C6-O7-C8

There are no ring outliers.

3 monomers are involved in 2 short contacts:

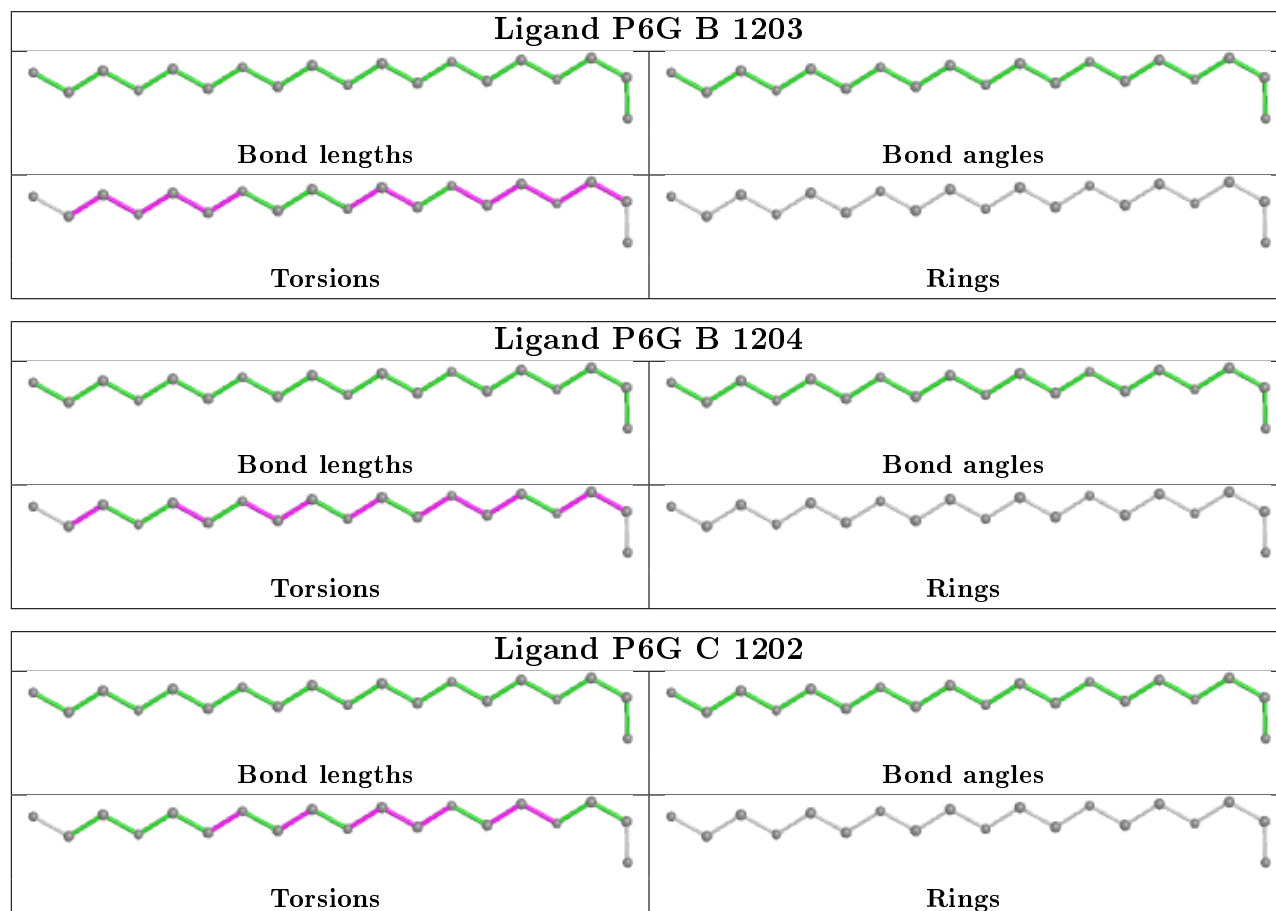
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	1201	PEG	1	0
13	A	1202	P6G	1	0

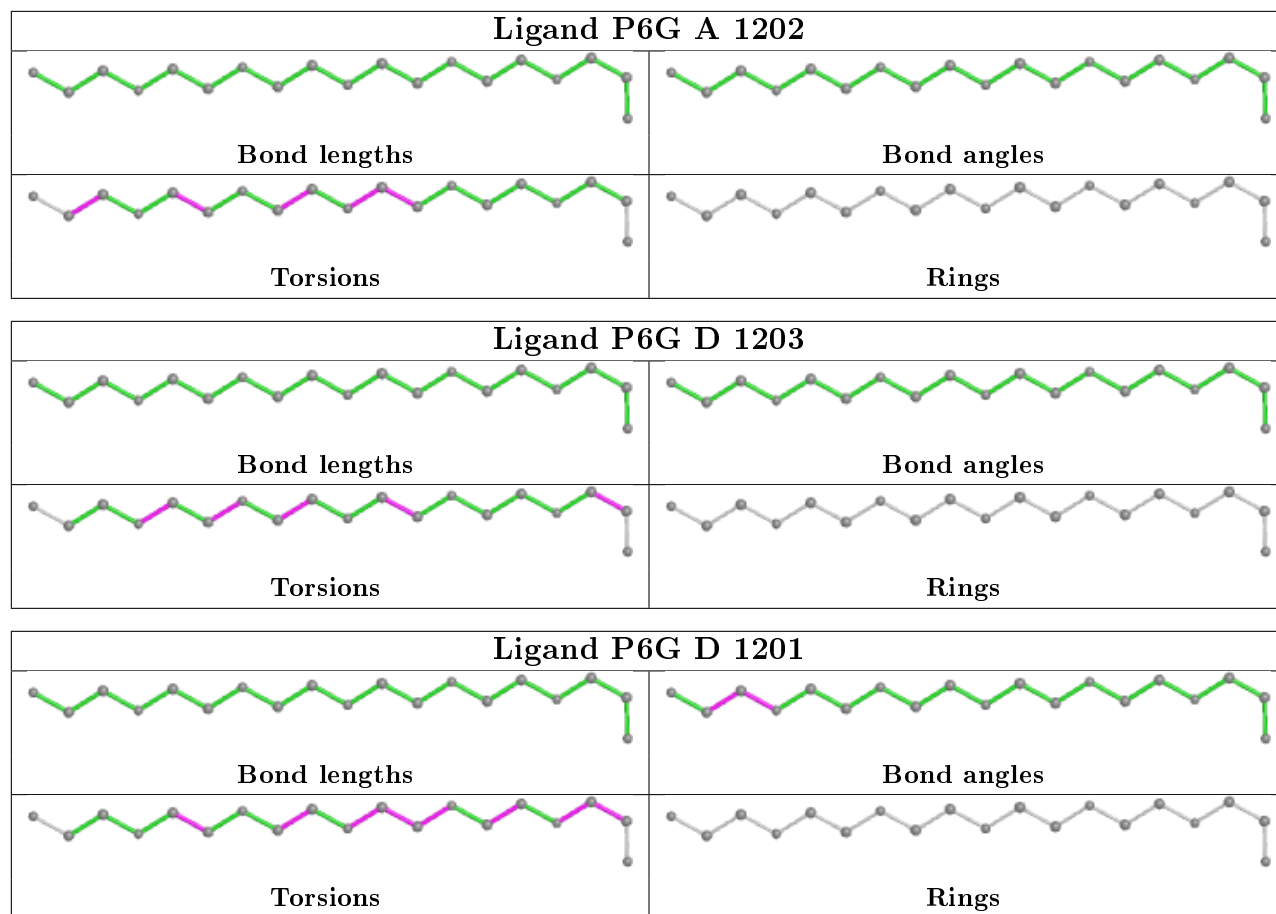
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	D	1201	P6G	1	0

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.





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	603/629 (95%)	-0.22	13 (2%) 62 57	14, 24, 42, 69	0
1	B	605/629 (96%)	-0.21	15 (2%) 57 52	12, 21, 37, 69	0
1	C	609/629 (96%)	-0.35	9 (1%) 73 70	12, 19, 35, 59	0
1	D	607/629 (96%)	-0.14	29 (4%) 30 25	12, 20, 43, 60	0
All	All	2424/2516 (96%)	-0.23	66 (2%) 54 49	12, 21, 41, 69	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	135	THR	7.0
1	A	415	THR	6.6
1	B	134	ALA	6.4
1	D	88	LEU	6.1
1	B	325	GLY	5.7
1	C	325	GLY	5.4
1	D	19	LEU	5.1
1	D	80	TRP	4.9
1	D	325	GLY	4.8
1	D	79	ILE	4.7
1	A	606	ASN	4.4
1	D	78	PRO	4.2
1	B	606	ASN	4.1
1	D	84	THR	4.1
1	D	135	THR	4.0
1	C	606	ASN	3.9
1	D	23	SER	3.8
1	B	129	LEU	3.6
1	A	414	VAL	3.6
1	B	415	THR	3.6
1	A	413	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	609	GLU	3.5
1	A	78	PRO	3.5
1	C	135	THR	3.5
1	D	24	TYR	3.5
1	A	135	THR	3.4
1	D	25	GLN	3.3
1	C	414	VAL	3.2
1	B	133	THR	3.2
1	D	16	GLY	3.1
1	B	80	TRP	3.1
1	B	607	TYR	3.0
1	B	78	PRO	3.0
1	D	18	GLN	2.9
1	D	21	ALA	2.8
1	B	605	ASP	2.8
1	A	605	ASP	2.8
1	D	95	VAL	2.8
1	D	22	GLN	2.7
1	A	412	ASP	2.6
1	A	325	GLY	2.6
1	D	83	PHE	2.6
1	A	522	GLU	2.6
1	D	17	ALA	2.5
1	B	273	ASP	2.5
1	D	323	ALA	2.5
1	D	94	ALA	2.5
1	B	414	VAL	2.5
1	D	20	PHE	2.5
1	D	26	SER	2.5
1	D	129	LEU	2.4
1	A	129	LEU	2.4
1	B	323	ALA	2.4
1	D	27	SER	2.3
1	D	414	VAL	2.3
1	D	90	ARG	2.3
1	C	613	LEU	2.2
1	B	79	ILE	2.2
1	C	614	VAL	2.2
1	A	273	ASP	2.2
1	C	136	CYS	2.2
1	A	79	ILE	2.1
1	C	605	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	97	THR	2.1
1	C	323	ALA	2.0
1	D	75	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

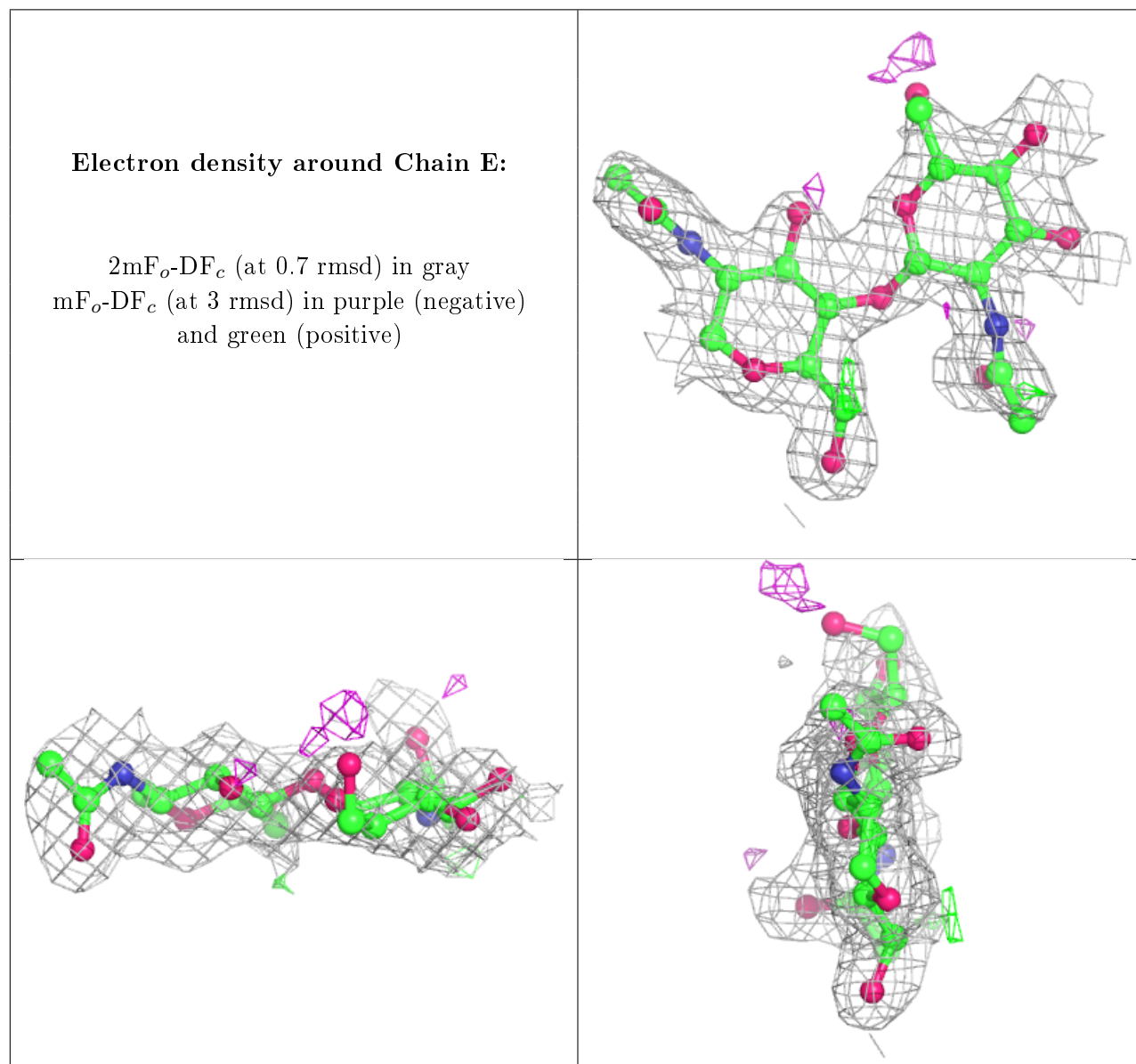
## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	FUC	J	2	10/11	0.57	0.38	54,58,61,62	0
6	MAN	N	3	11/12	0.64	0.26	61,63,65,65	0
3	FUC	G	2	10/11	0.69	0.25	43,47,48,49	0
3	FUC	M	2	10/11	0.70	0.29	50,54,56,56	0
2	NAG	H	2	14/15	0.70	0.39	56,59,61,61	0
2	NAG	E	2	14/15	0.71	0.42	54,59,60,61	0
5	FUL	L	4	10/11	0.72	0.19	44,48,50,50	0
3	NAG	G	1	14/15	0.79	0.13	29,34,39,40	0
2	NAG	K	2	14/15	0.80	0.30	40,44,48,49	0
3	NAG	M	1	14/15	0.80	0.14	30,35,40,44	0
2	NAG	F	2	14/15	0.81	0.33	65,66,68,68	0
2	NAG	H	1	14/15	0.82	0.26	37,39,44,50	0
4	BMA	I	3	11/12	0.83	0.30	60,63,64,65	0
2	NAG	F	1	14/15	0.83	0.26	61,63,66,69	0
6	NAG	N	2	14/15	0.85	0.16	42,49,53,57	0
6	FUC	N	4	10/11	0.85	0.17	40,42,45,45	0
5	BMA	L	3	11/12	0.86	0.18	40,42,45,47	0
3	NAG	J	1	14/15	0.87	0.15	32,38,43,46	0
4	NAG	I	2	14/15	0.87	0.23	47,49,52,56	0
2	NAG	E	1	14/15	0.88	0.21	34,37,41,47	0
5	NAG	L	2	14/15	0.91	0.14	32,34,39,41	0
2	NAG	K	1	14/15	0.92	0.15	28,31,33,36	0
6	NAG	N	1	14/15	0.92	0.10	31,34,36,38	0
5	NAG	L	1	14/15	0.94	0.09	27,29,32,37	0
4	NAG	I	1	14/15	0.95	0.13	38,40,43,43	0

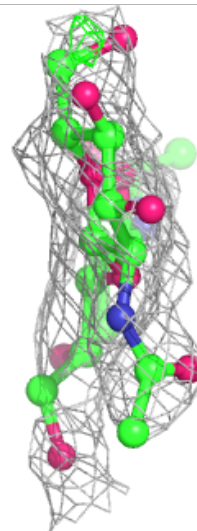
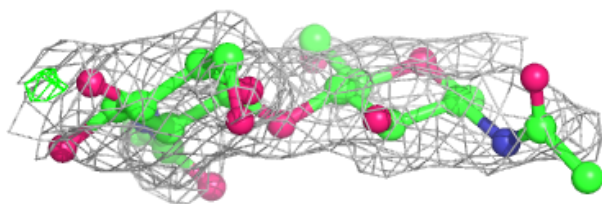
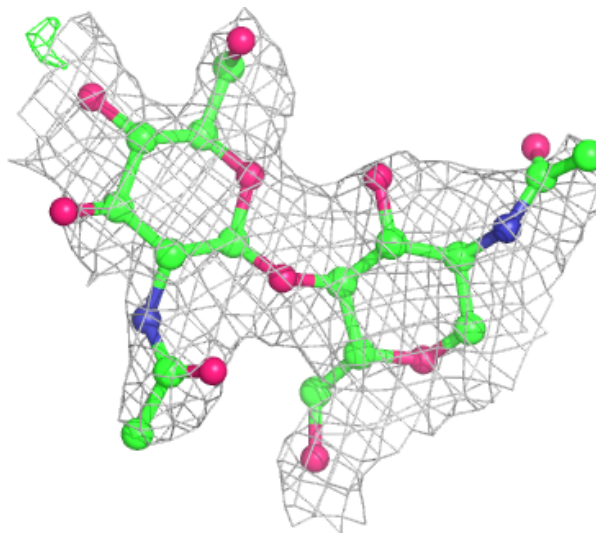


The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



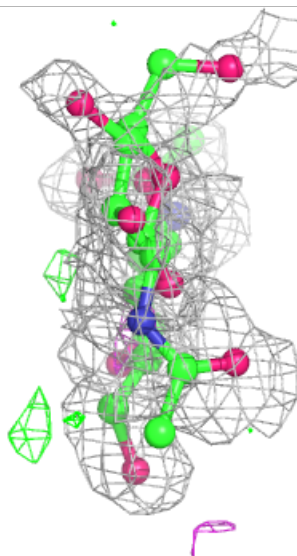
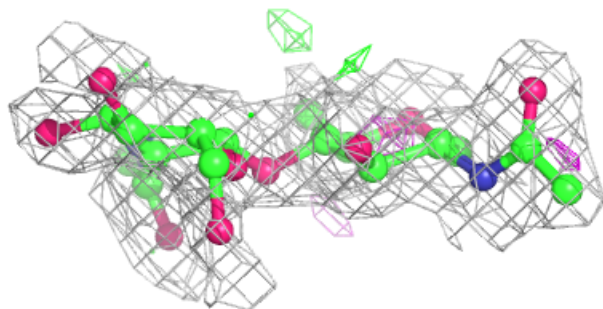
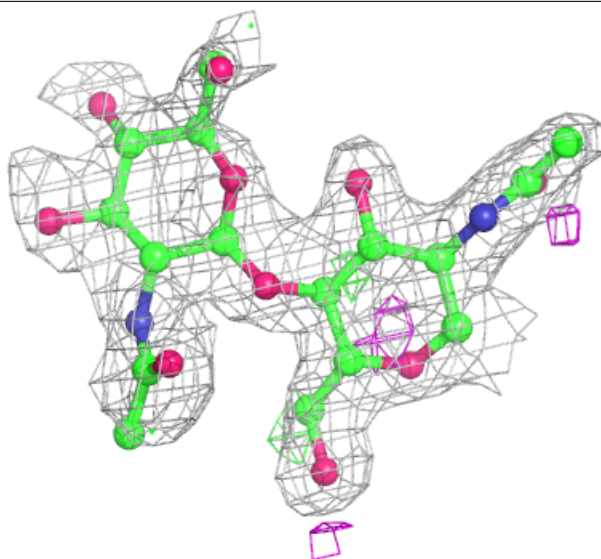
**Electron density around Chain F:**

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



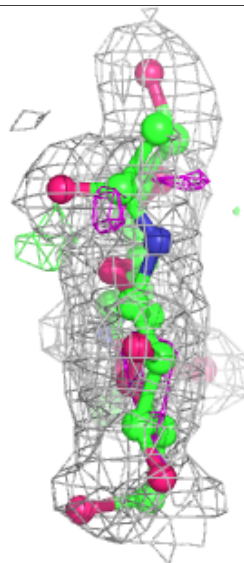
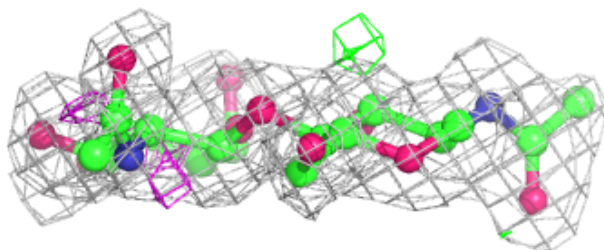
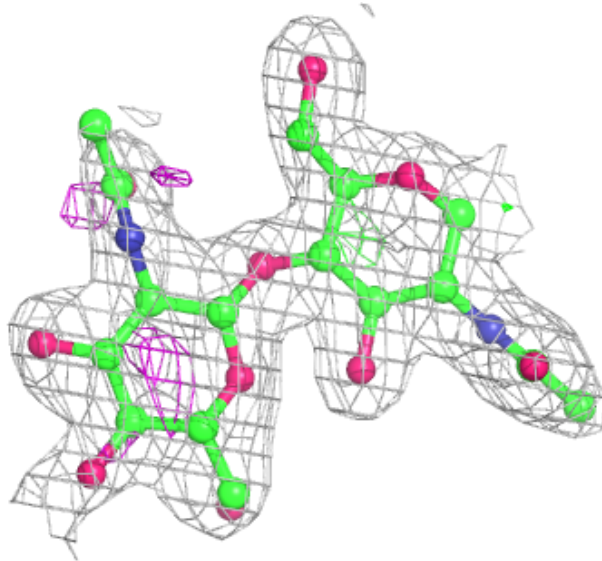
**Electron density around Chain H:**

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



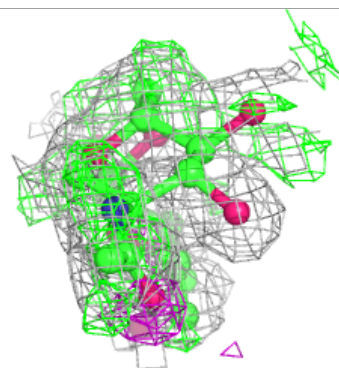
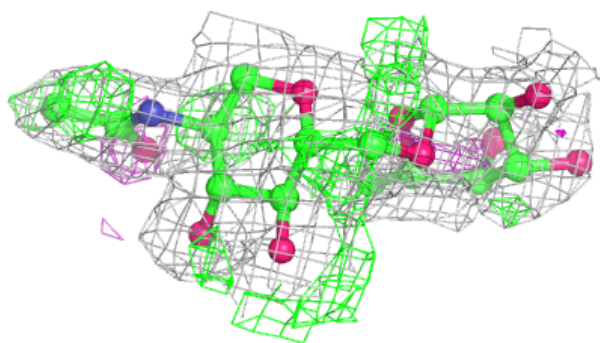
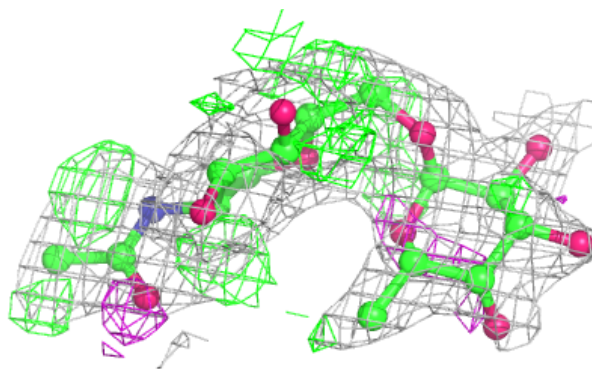
**Electron density around Chain K:**

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

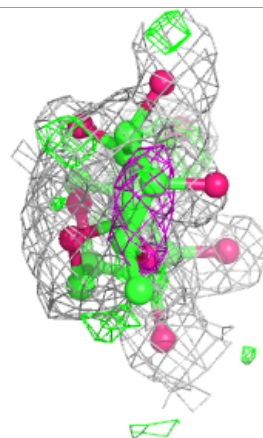
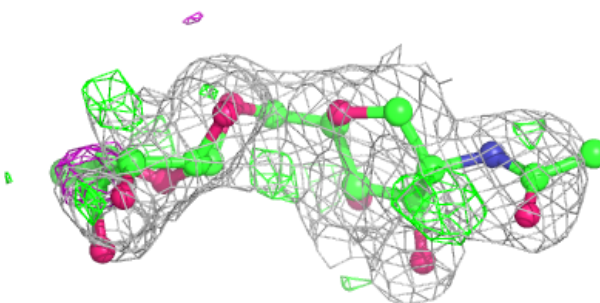
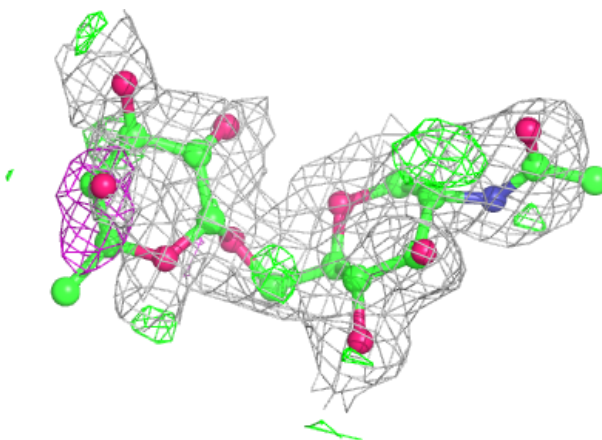


**Electron density around Chain G:**

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

**Electron density around Chain J:**

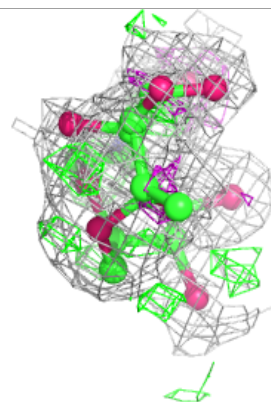
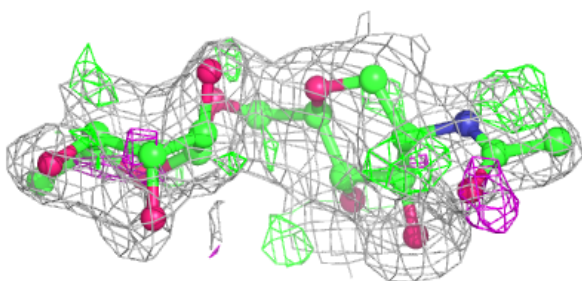
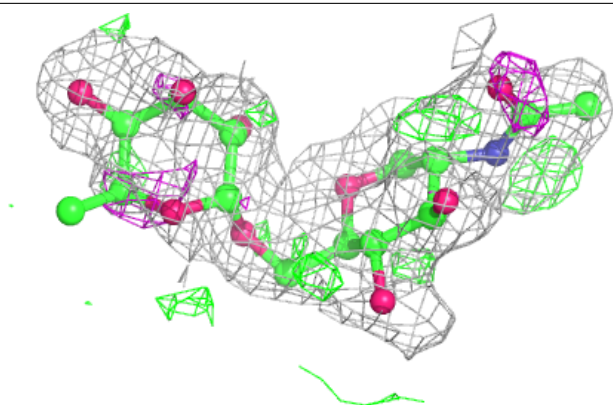
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



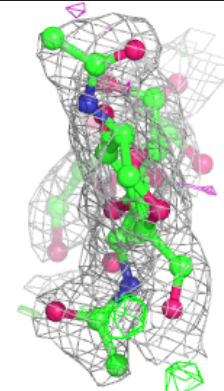
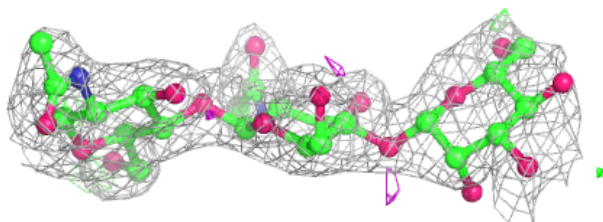
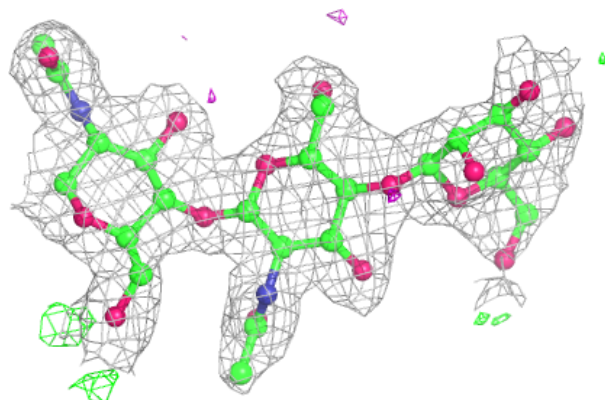


**Electron density around Chain M:**

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

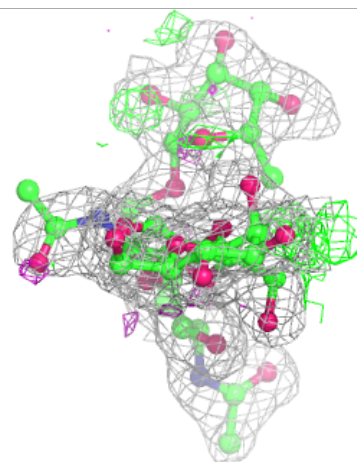
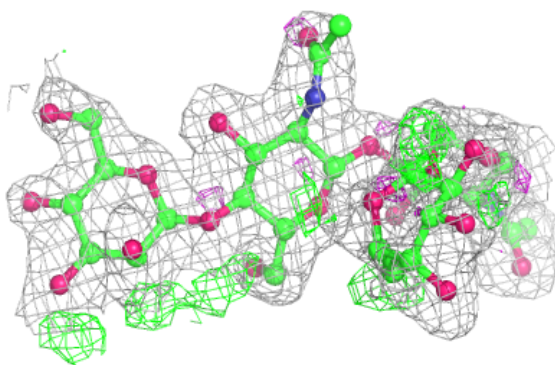
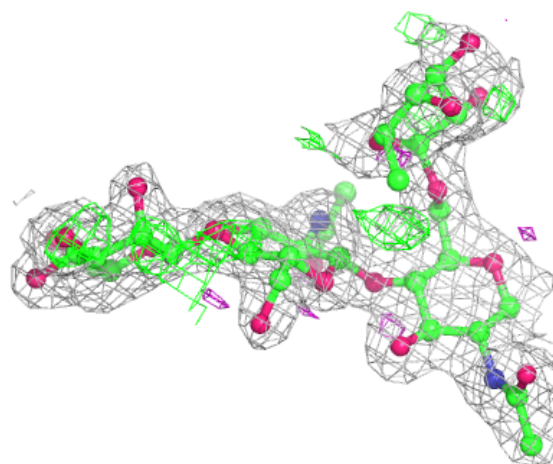
**Electron density around Chain I:**

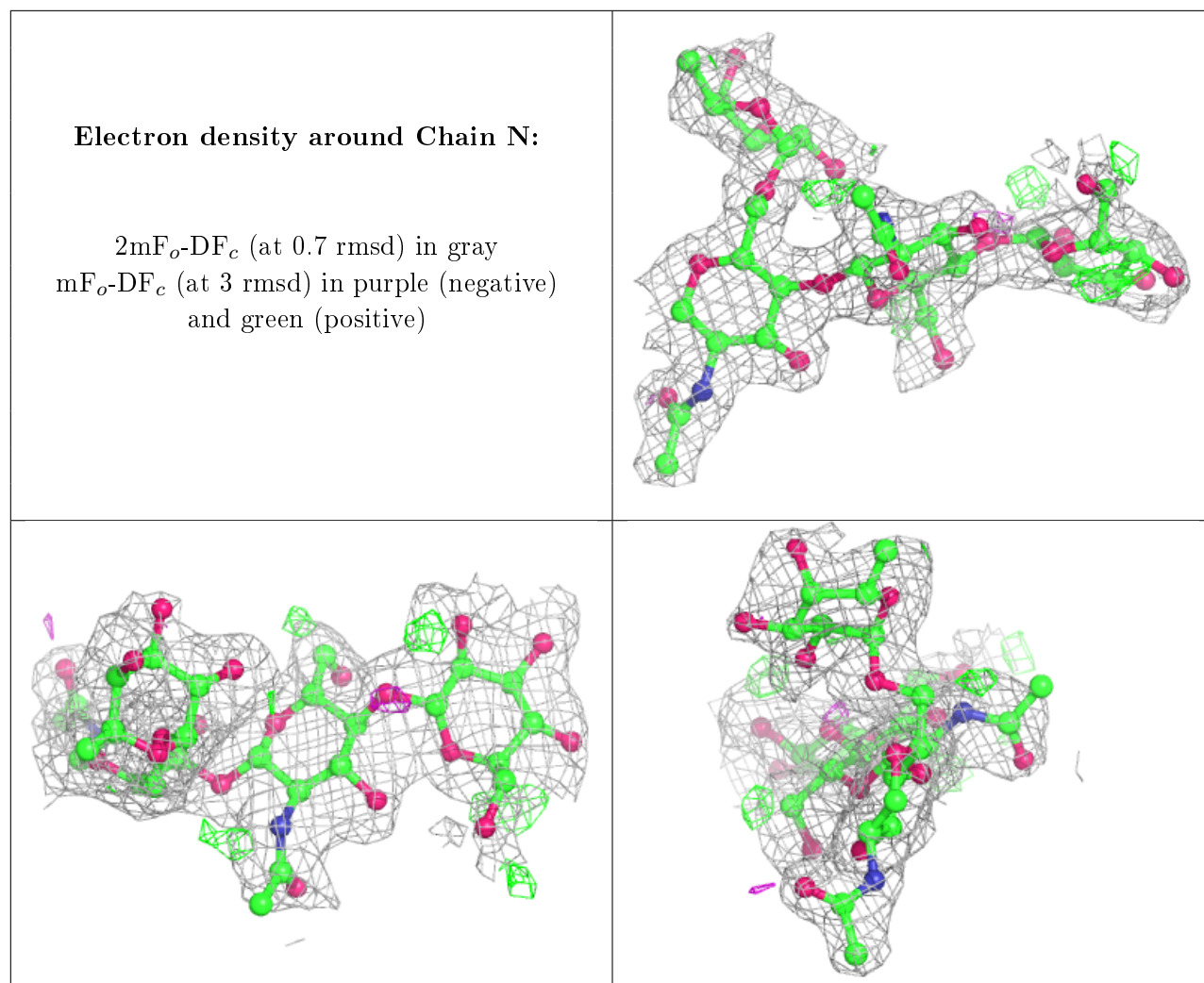
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain L:**

$2mF_o-DF_c$  (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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
13	P6G	C	1202	19/19	0.66	0.25	44,57,61,63	0
12	PEG	B	1201	7/7	0.72	0.18	45,46,47,48	0
11	NAG	D	1102	14/15	0.74	0.26	36,37,40,40	0
13	P6G	B	1204	19/19	0.74	0.27	48,55,65,66	0
13	P6G	D	1203	19/19	0.77	0.21	44,56,64,64	0
12	PEG	D	1205	7/7	0.79	0.20	43,44,48,49	0
13	P6G	B	1203	19/19	0.79	0.16	36,39,47,47	0
11	NAG	A	1100	14/15	0.80	0.17	37,42,47,50	0
12	PEG	B	1202	7/7	0.81	0.18	41,41,42,43	0

*Continued on next page...*



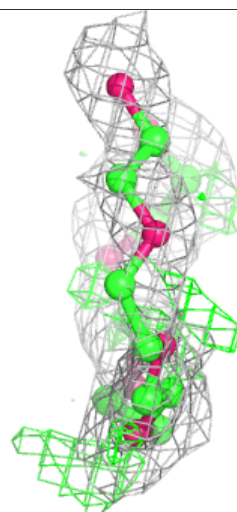
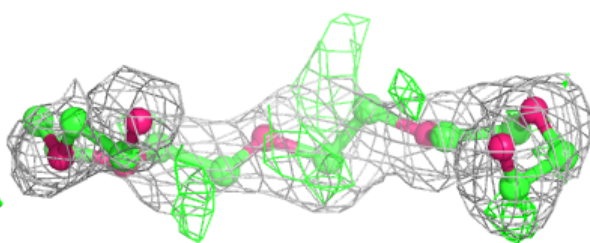
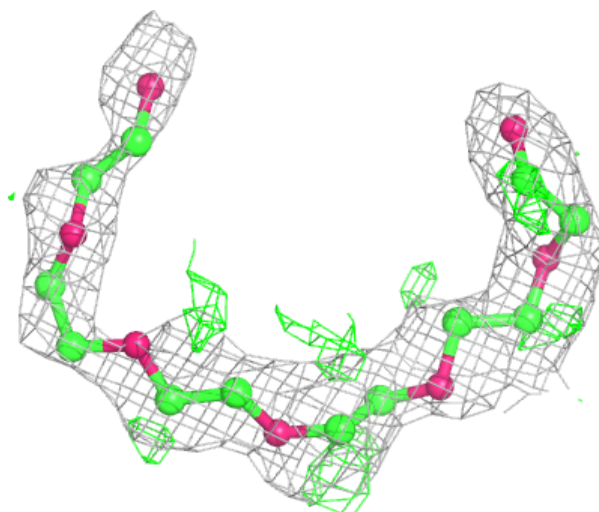
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
12	PEG	D	1200	7/7	0.82	0.15	51,51,53,55	0
12	PEG	A	1204	7/7	0.84	0.22	40,40,43,44	0
12	PEG	A	1200	7/7	0.85	0.18	53,53,54,54	0
12	PEG	C	1200	7/7	0.86	0.13	44,45,48,49	0
13	P6G	A	1202	19/19	0.86	0.12	33,39,43,44	0
7	ASP	B	907	8/9	0.86	0.17	22,27,36,37	0
13	P6G	D	1201	19/19	0.86	0.14	27,30,42,43	0
12	PEG	B	1200	7/7	0.87	0.19	61,61,62,63	0
12	PEG	D	1202	7/7	0.87	0.14	48,48,49,50	0
12	PEG	A	1201	7/7	0.87	0.15	40,42,45,46	0
12	PEG	C	1201	7/7	0.88	0.17	38,39,43,44	0
7	ASP	C	907	8/9	0.90	0.13	18,23,29,31	0
7	ASP	D	907	8/9	0.91	0.14	20,25,36,37	0
7	ASP	A	907	8/9	0.91	0.16	21,26,36,37	0
8	SER	B	908	7/7	0.94	0.15	18,20,23,25	0
8	SER	C	908	7/7	0.95	0.08	17,19,21,23	0
8	SER	A	908	7/7	0.95	0.10	20,22,24,26	0
8	SER	D	908	7/7	0.97	0.09	20,21,22,25	0
9	ZN	B	1001	1/1	1.00	0.05	17,17,17,17	0
10	CL	A	1002	1/1	1.00	0.07	18,18,18,18	0
10	CL	B	1002	1/1	1.00	0.06	16,16,16,16	0
10	CL	C	1002	1/1	1.00	0.06	14,14,14,14	0
10	CL	D	1002	1/1	1.00	0.05	15,15,15,15	0
9	ZN	C	1001	1/1	1.00	0.04	15,15,15,15	0
9	ZN	A	1001	1/1	1.00	0.04	18,18,18,18	0
9	ZN	D	1001	1/1	1.00	0.04	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.

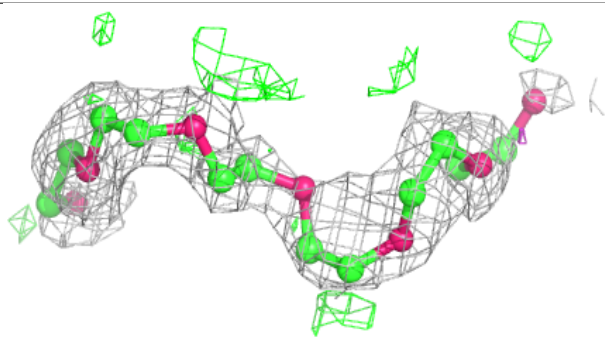
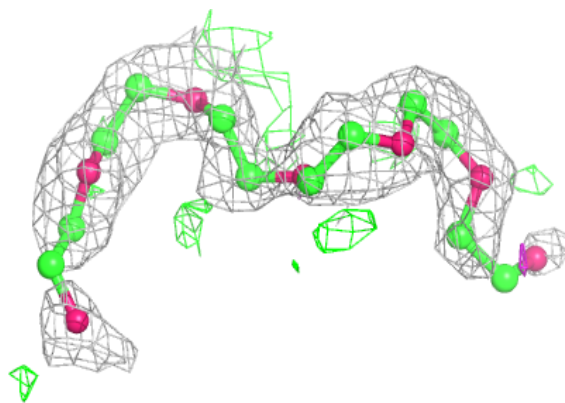
**Electron density around P6G C 1202:**

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



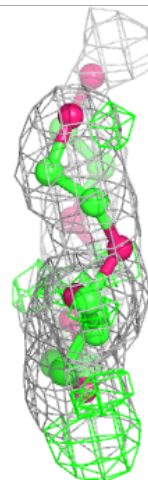
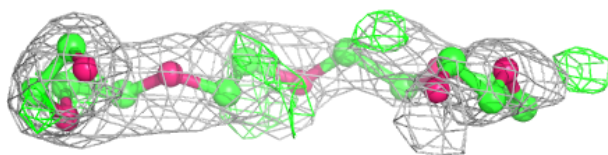
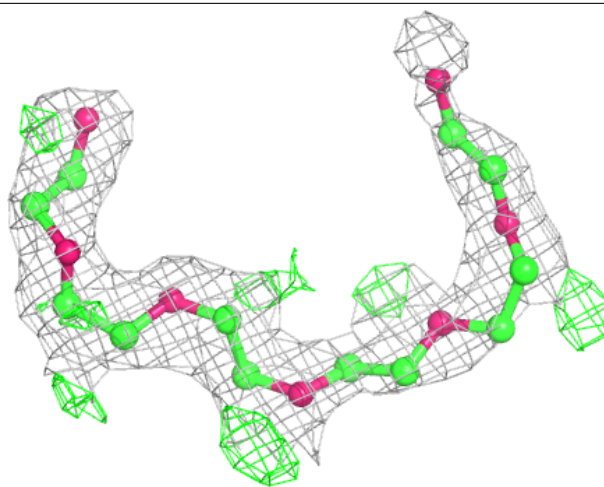
**Electron density around P6G B 1204:**

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



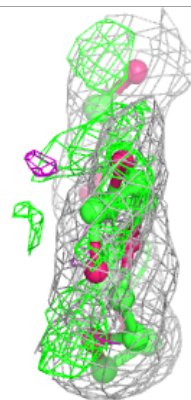
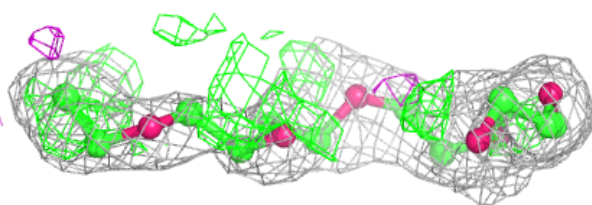
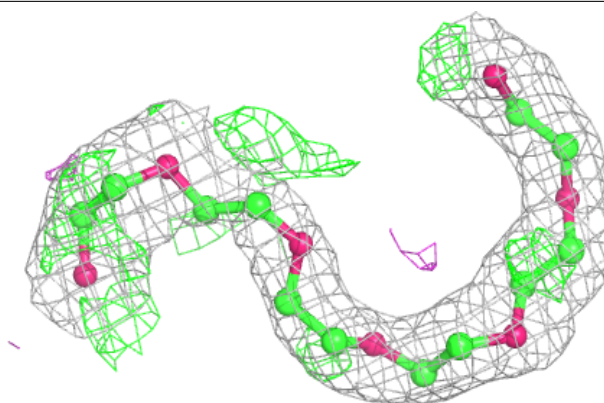
**Electron density around P6G D 1203:**

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

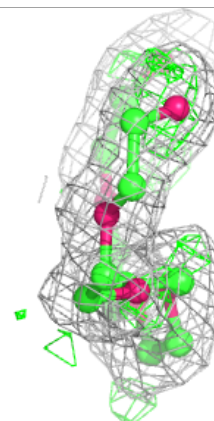
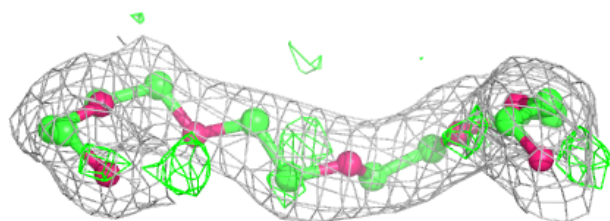
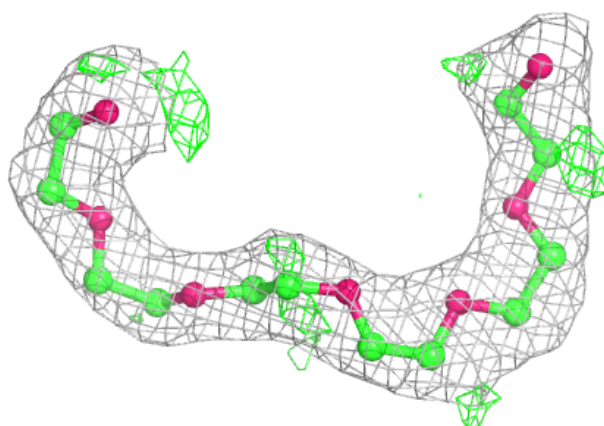


**Electron density around P6G B 1203:**

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

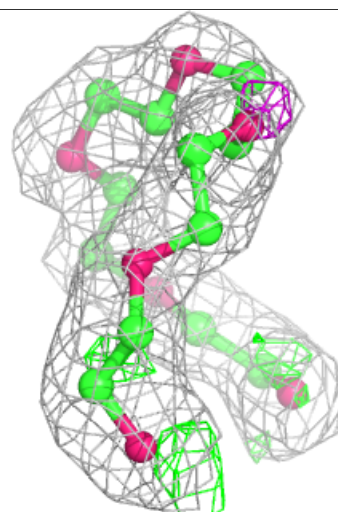
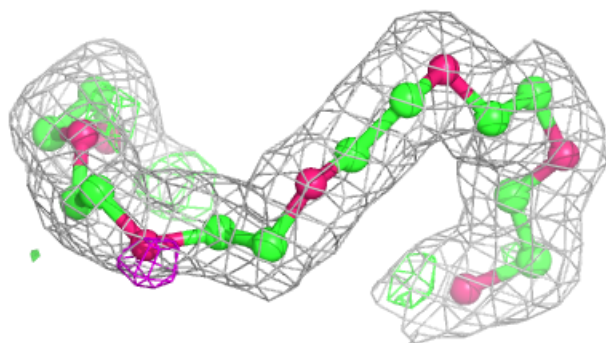
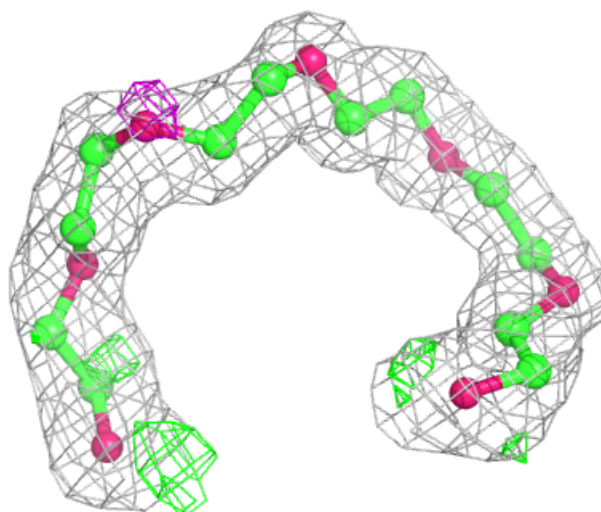
**Electron density around P6G A 1202:**

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



**Electron density around P6G D 1201:**

$2mF_o-DF_c$  (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.