



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 6, 2022 – 04:37 pm BST

PDB ID : 6TAV  
Title : Crystal structure of endopeptidase-induced alpha2-macroglobulin  
Authors : Gomis-Ruth, F.X.; Duquerroy, S.; Trapani, S.; Marrero, A.; Goulas, T.; Guevara, T.; Andersen, G.A.; Sottrup-Jensen, L.; Navaza, J.  
Deposited on : 2019-10-30  
Resolution : 4.20 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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.27  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

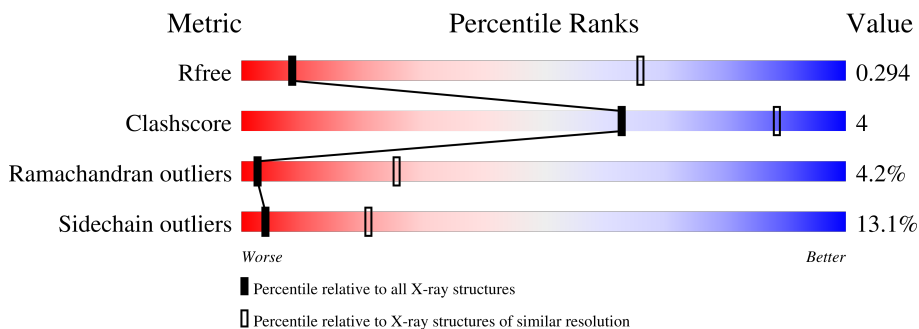
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.20 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	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1474	74% (green), 20% (yellow), 6% (orange), 0% (red), 0% (grey)
1	B	1474	66% (green), 18% (yellow), 14% (orange), 2% (red), 2% (grey)
1	C	1474	67% (green), 18% (yellow), 14% (orange), 2% (red), 2% (grey)
1	D	1474	65% (green), 20% (yellow), 14% (orange), 2% (red), 2% (grey)
2	E	4	50% (yellow), 50% (orange)
2	G	4	50% (yellow), 50% (orange)
2	J	4	25% (green), 75% (yellow)

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Mol	Chain	Length	Quality of chain
2	O	4	 75% 25%
2	V	4	 25% 75%
3	F	3	 33% 67%
3	I	3	 33% 67%
3	M	3	 33% 67%
3	R	3	 67% 33%
4	H	2	 50% 50%
4	K	2	 50% 50%
4	L	2	 50% 50%
4	N	2	 100%
4	P	2	 50% 50%
4	Q	2	 50% 50%
4	S	2	 50% 50%
4	T	2	 50% 50%
4	U	2	 50% 50%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 82015 atoms, of which 40382 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 Alpha-2-macroglobulin.

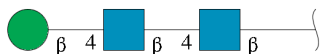
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	1416	Total 21976	C 7027	H 10926	N 1849	O 2125	S 49	10926	0	0
1	B	1273	Total 19741	C 6312	H 9812	N 1665	O 1909	S 43	9812	0	0
1	C	1274	Total 19770	C 6315	H 9834	N 1668	O 1910	S 43	9834	0	0
1	D	1271	Total 19716	C 6298	H 9810	N 1664	O 1901	S 43	9810	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	4	Total 50	C 28	N 2	O 20	0	0	0
2	G	4	Total 50	C 28	N 2	O 20	0	0	0
2	J	4	Total 50	C 28	N 2	O 20	0	0	0
2	O	4	Total 50	C 28	N 2	O 20	0	0	0
2	V	4	Total 50	C 28	N 2	O 20	0	0	0

- 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
			Total	C	N	O			
3	F	3	39	22	2	15	0	0	0
3	I	3	39	22	2	15	0	0	0
3	M	3	39	22	2	15	0	0	0
3	R	3	39	22	2	15	0	0	0

- Molecule 4 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
			Total	C	N	O			
4	H	2	28	16	2	10	0	0	0
4	K	2	28	16	2	10	0	0	0
4	L	2	28	16	2	10	0	0	0
4	N	2	28	16	2	10	0	0	0
4	P	2	28	16	2	10	0	0	0
4	Q	2	28	16	2	10	0	0	0
4	S	2	28	16	2	10	0	0	0
4	T	2	28	16	2	10	0	0	0
4	U	2	28	16	2	10	0	0	0

- Molecule 5 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>).

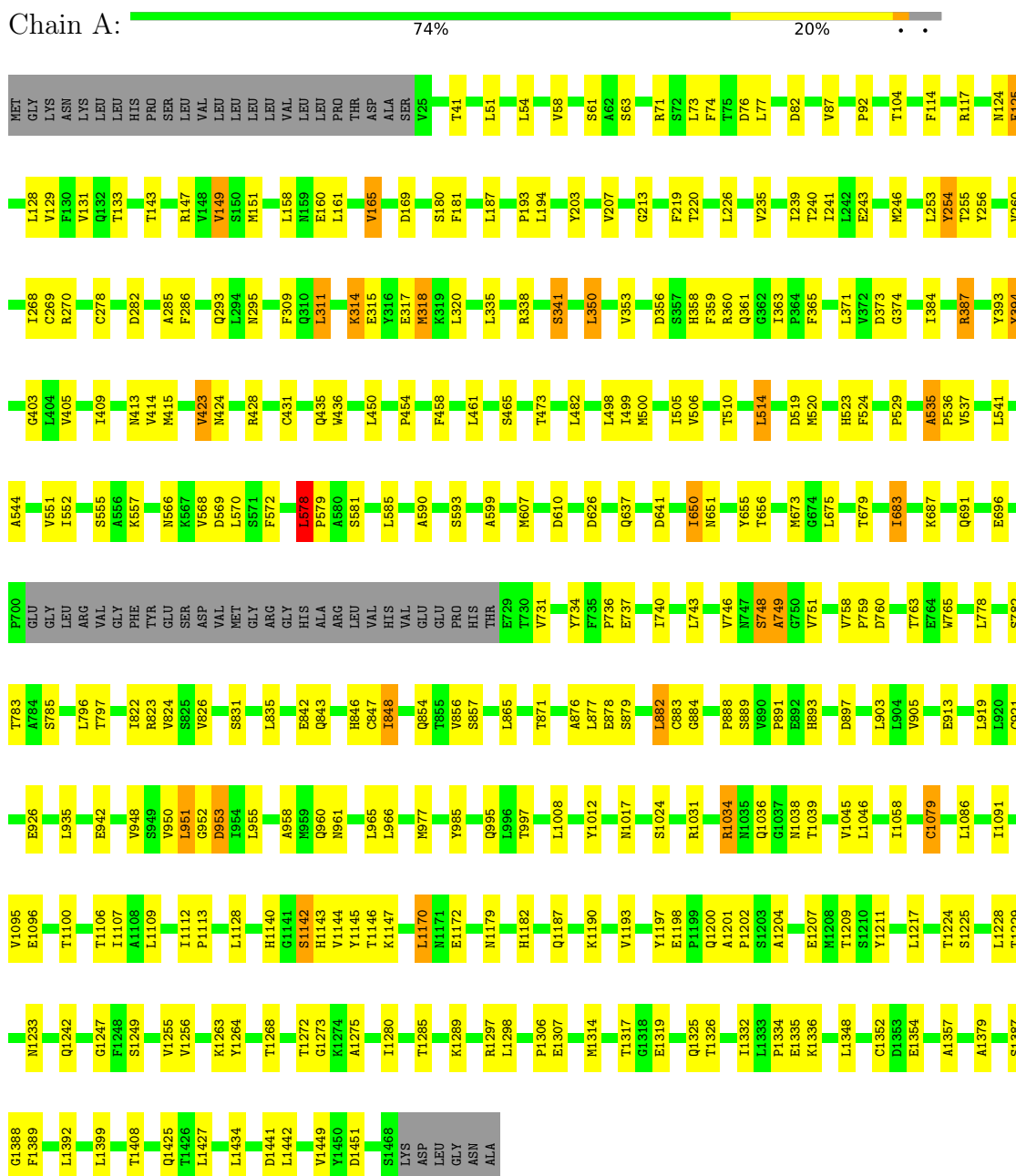


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
	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

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

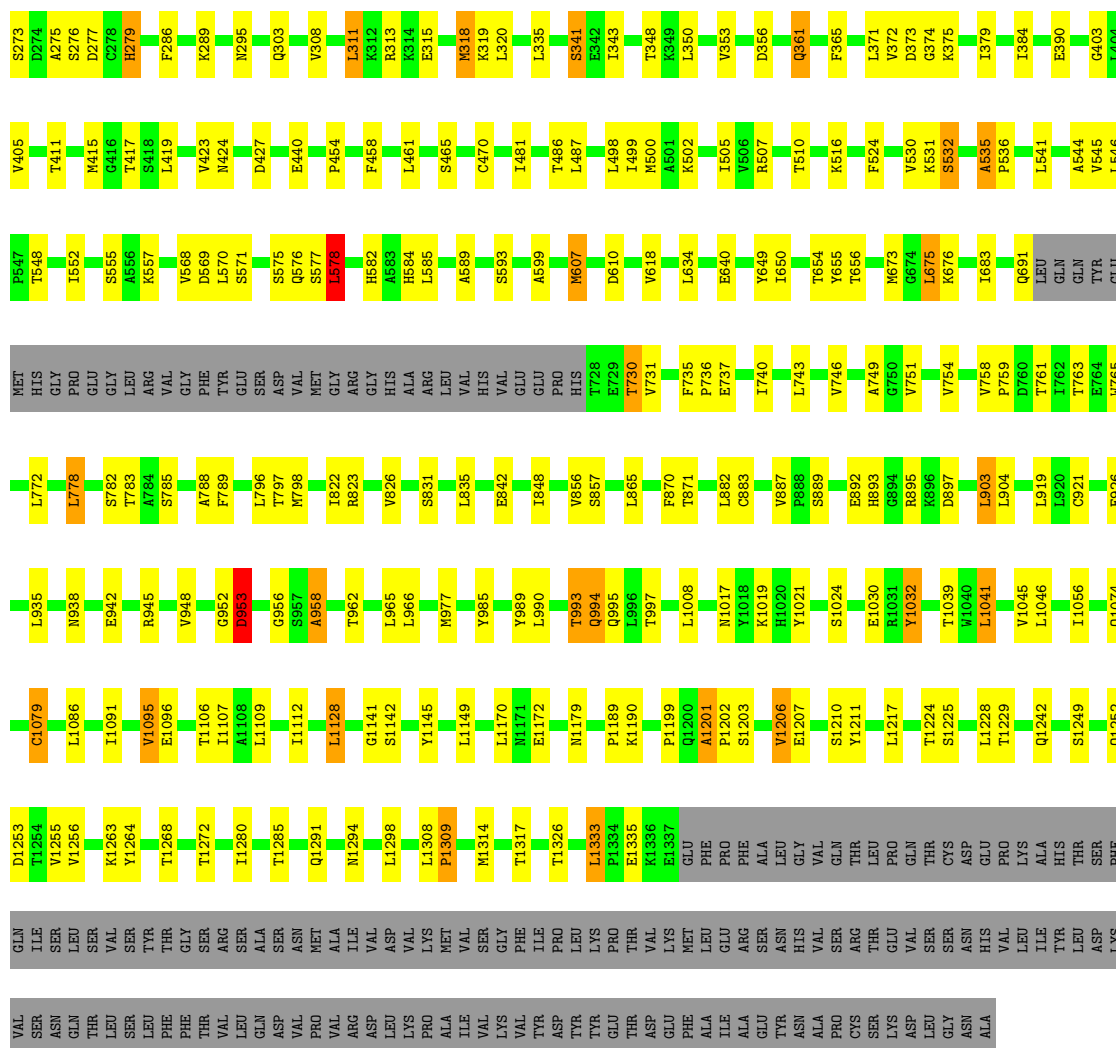
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Alpha-2-macroglobulin



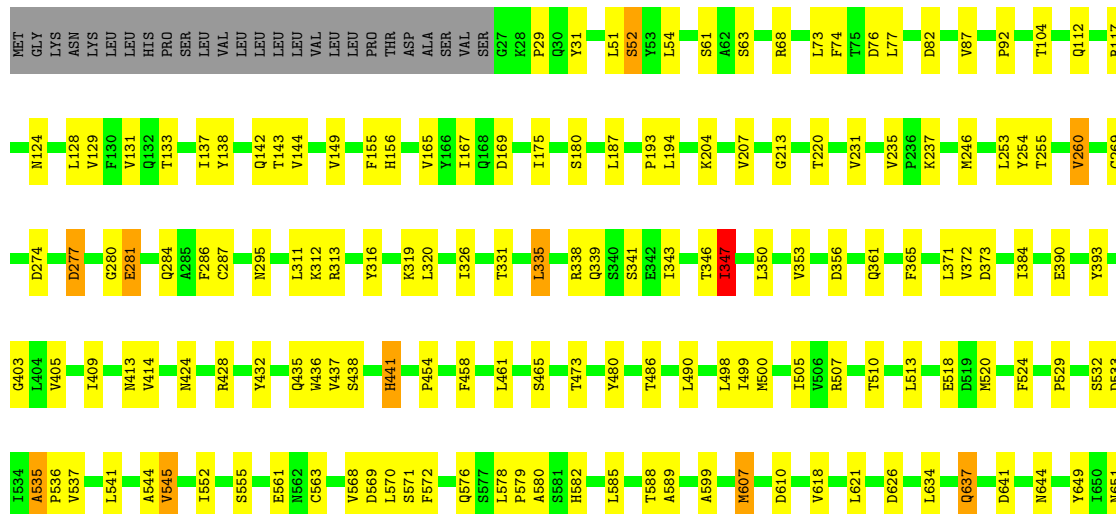


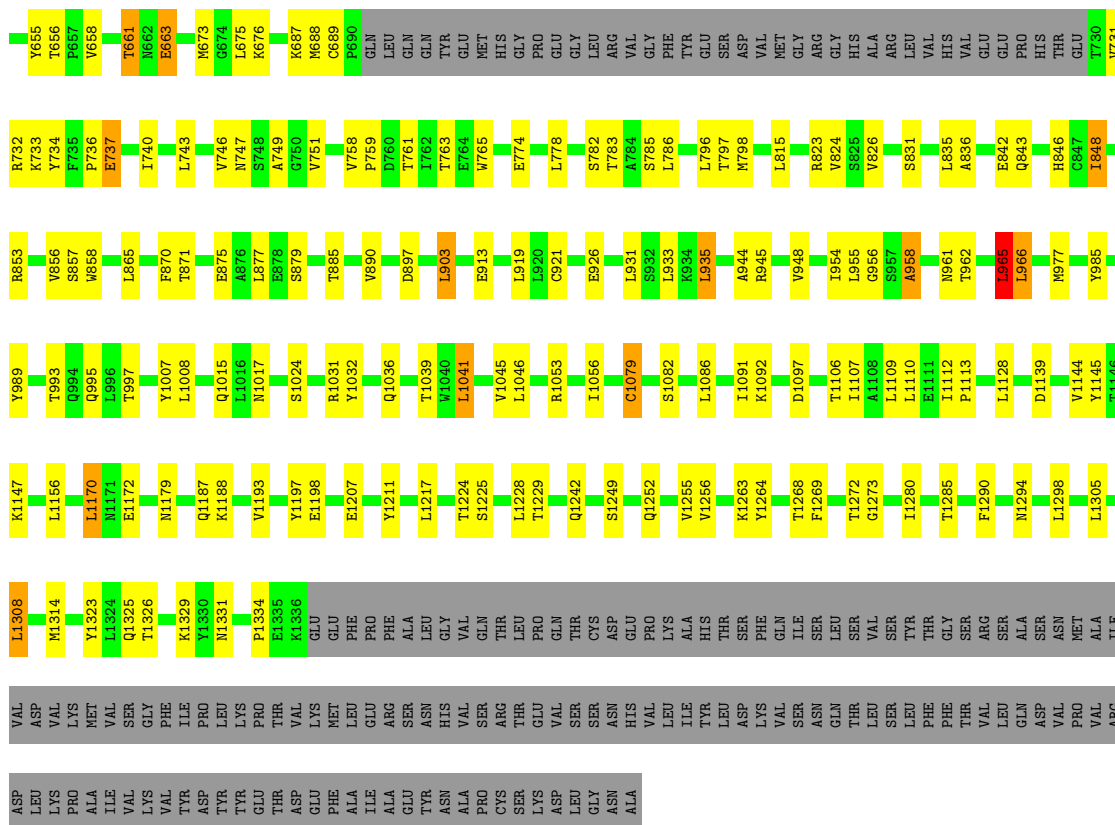




● Molecule 1: Alpha-2-macroglobulin

Chain D:  65% 20% 14%





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

Chain E: 50%

MAG1  
MAG2  
BNA3  
MAN4

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

Chain G: 50%


MAG1  
MAG2  
BNA3  
MAN4

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

Chain J: 25%

MAG1  
MAG2  
BNA3  
MAN4

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

Chain O:  75% 25%

MAG1  
MAG2  
BMA3  
MAM4

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

Chain V:  25% 75%

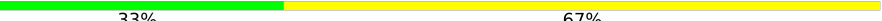
MAG1  
MAG2  
BMA3  
MAM4

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

Chain F:  33% 67%

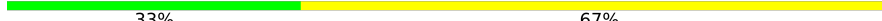
MAG1  
MAG2  
BMA3

- Molecule 3: 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  
BMA3

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

Chain M:  33% 67%

MAG1  
MAG2  
BMA3

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

Chain R:  67% 33%

MAG1  
MAG2  
BMA3

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

Chain H:  50% 50%

MAG1  
BMA3

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

Chain K:  50% 50%

MAG1  
MAG2

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

Chain L:  50% 50%

MAG1  
MAG2

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

Chain N:  100%

MAG1  
MAG2

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

Chain P:  50% 50%


MAG1  
MAG2

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

Chain Q:  50% 50%

MAG1  
MAG2

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

Chain S:  50% 50%

MAG1  
MAG2

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

Chain T:  50% 50%

MAG1  
MAG2

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

Chain U: 

MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.80Å 260.30Å 281.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.24 – 4.20 95.86 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (34.24-4.20) 99.2 (95.86-4.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.03 (at 4.15Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.235 , 0.282 0.268 , 0.294	Depositor DCC
$R_{free}$ test set	834 reflections (1.19%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	221.9	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.78	EDS
Total number of atoms	82015	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	256.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, BMA

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	0.58	0/11297	0.75	1/15352 (0.0%)
1	B	0.54	0/10149	0.72	0/13786
1	C	0.56	0/10156	0.74	2/13798 (0.0%)
1	D	0.53	0/10126	0.74	0/13757
All	All	0.55	0/41728	0.74	3/56693 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	952	GLY	C-N-CA	6.84	138.81	121.70
1	C	953	ASP	N-CA-C	5.73	126.47	111.00
1	A	952	GLY	C-N-CA	5.60	135.70	121.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	11050	10926	10934	88	0
1	B	9929	9812	9818	83	0
1	C	9936	9834	9836	91	0
1	D	9906	9810	9812	97	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	50	0	43	1	0
2	G	50	0	43	1	0
2	J	50	0	43	0	0
2	O	50	0	43	0	0
2	V	50	0	43	0	0
3	F	39	0	34	0	0
3	I	39	0	34	0	0
3	M	39	0	34	0	0
3	R	39	0	34	1	0
4	H	28	0	25	0	0
4	K	28	0	25	0	0
4	L	28	0	25	0	0
4	N	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	S	28	0	25	1	0
4	T	28	0	25	0	0
4	U	28	0	25	0	0
5	A	42	0	39	0	0
5	B	14	0	13	0	0
5	C	56	0	52	0	0
5	D	42	0	39	0	0
All	All	41633	40382	41119	353	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (353) 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:1147:LYS:HB3	1:D:1170:LEU:HD21	1.54	0.90
1:D:77:LEU:HD22	1:D:87:VAL:HG11	1.53	0.89
1:C:77:LEU:HD22	1:C:87:VAL:HG11	1.55	0.89
1:A:77:LEU:HD22	1:A:87:VAL:HG11	1.56	0.87
1:C:535:ALA:HB1	1:C:536:PRO:CD	2.20	0.71
1:B:679:THR:HG21	1:B:683:ILE:HD12	1.73	0.70
1:A:1399:LEU:HB2	1:A:1408:THR:HG21	1.73	0.70
1:A:1095:VAL:HG21	1:A:1145:TYR:CE2	2.27	0.69
1:C:165:VAL:HG22	1:C:207:VAL:HG12	1.73	0.69
1:C:384:ILE:CD1	1:C:405:VAL:HG21	2.23	0.69
1:D:384:ILE:CD1	1:D:405:VAL:HG21	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:VAL:HG22	1:D:207:VAL:HG12	1.76	0.68
1:A:384:ILE:CD1	1:A:405:VAL:HG21	2.24	0.67
1:D:935:LEU:HD11	1:D:1308:LEU:HD13	1.76	0.66
1:D:312:LYS:HD3	1:D:437:VAL:HG21	1.78	0.66
1:C:231:VAL:HG13	1:C:335:LEU:HB2	1.79	0.65
1:D:826:VAL:HG11	1:D:856:VAL:HG21	1.79	0.65
1:B:658:VAL:HG12	1:C:656:THR:CG2	2.27	0.64
1:B:658:VAL:HG12	1:C:656:THR:HG22	1.79	0.64
1:C:962:THR:HG22	1:C:990:LEU:HD21	1.80	0.64
1:C:1145:TYR:CE2	1:C:1149:LEU:HD11	2.32	0.64
1:A:1106:THR:HG21	1:A:1128:LEU:HD11	1.80	0.64
1:D:1106:THR:HG21	1:D:1128:LEU:HD11	1.80	0.63
1:D:962:THR:O	1:D:965:LEU:HD22	1.99	0.63
1:C:758:VAL:HG11	1:C:765:TRP:CZ2	2.33	0.63
1:D:758:VAL:HG11	1:D:765:TRP:CZ2	2.34	0.62
1:D:138:TYR:CZ	1:D:144:VAL:HG23	2.35	0.61
1:A:1100:THR:CG2	1:A:1146:THR:HG22	2.30	0.61
1:B:535:ALA:HB1	1:B:536:PRO:CD	2.30	0.61
1:B:499:ILE:HD11	1:B:507:ARG:HB2	1.83	0.61
1:D:535:ALA:HB1	1:D:536:PRO:CD	2.30	0.61
1:A:1211:TYR:CE2	1:A:1256:VAL:HG11	2.36	0.60
1:B:758:VAL:HG11	1:B:765:TRP:CZ2	2.36	0.60
1:A:656:THR:HG22	1:D:658:VAL:HG12	1.82	0.60
1:D:1211:TYR:CE2	1:D:1256:VAL:HG11	2.37	0.60
1:A:239:ILE:HD11	1:A:243:GLU:HG2	1.83	0.60
1:A:535:ALA:HB1	1:A:536:PRO:CD	2.31	0.60
1:D:1147:LYS:CB	1:D:1170:LEU:HD21	2.30	0.59
1:A:1100:THR:HG22	1:A:1146:THR:HG22	1.84	0.59
1:B:535:ALA:HB1	1:B:536:PRO:HD3	1.83	0.59
1:B:350:LEU:HD21	1:B:443:GLU:HA	1.83	0.59
1:B:365:PHE:CE1	1:B:409:ILE:HD13	2.38	0.59
1:A:656:THR:CG2	1:D:658:VAL:HG12	2.33	0.59
1:A:826:VAL:HG11	1:A:856:VAL:HG21	1.84	0.58
1:C:1211:TYR:CE2	1:C:1256:VAL:HG11	2.37	0.58
1:B:166:TYR:CE1	1:B:206:VAL:HG13	2.38	0.58
1:B:1211:TYR:CE2	1:B:1256:VAL:HG11	2.39	0.58
1:B:268:ILE:HD12	1:B:320:LEU:HD21	1.86	0.58
1:A:498:LEU:HD22	1:A:505:ILE:HD11	1.84	0.58
1:A:535:ALA:HB1	1:A:536:PRO:HD3	1.84	0.58
1:D:578:LEU:O	1:D:580:ALA:N	2.36	0.58
1:D:535:ALA:HB1	1:D:536:PRO:HD3	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:572:PHE:CZ	1:D:786:LEU:HD22	2.39	0.57
1:D:836:ALA:HB1	1:D:858:TRP:CE3	2.39	0.57
1:C:498:LEU:HD22	1:C:505:ILE:HD11	1.86	0.57
1:D:1046:LEU:HG	1:D:1112:ILE:HD11	1.87	0.57
1:A:977:MET:CE	1:A:1045:VAL:HG22	2.34	0.57
1:C:73:LEU:HD11	1:C:92:PRO:CD	2.34	0.57
1:C:977:MET:CE	1:C:1045:VAL:HG22	2.34	0.57
1:B:151:MET:CE	1:B:778:LEU:HD13	2.35	0.57
1:C:371:LEU:HD22	1:C:379:ILE:HG22	1.85	0.57
1:D:977:MET:CE	1:D:1045:VAL:HG22	2.35	0.57
1:D:498:LEU:HD22	1:D:505:ILE:HD11	1.86	0.57
1:C:870:PHE:CE1	1:C:903:LEU:HD21	2.39	0.57
1:B:498:LEU:HD22	1:B:505:ILE:HD11	1.87	0.57
1:B:73:LEU:HD11	1:B:92:PRO:CD	2.35	0.57
1:B:977:MET:CE	1:B:1045:VAL:HG22	2.34	0.57
1:C:958:ALA:HB2	1:C:989:TYR:OH	2.05	0.57
1:B:599:ALA:HB3	1:B:740:ILE:HG22	1.87	0.56
1:D:966:LEU:HD13	1:D:1007:TYR:CD2	2.39	0.56
1:A:73:LEU:HD11	1:A:92:PRO:CD	2.35	0.56
1:D:73:LEU:HD11	1:D:92:PRO:CD	2.35	0.56
1:C:1046:LEU:HG	1:C:1112:ILE:HD11	1.87	0.56
1:D:260:VAL:HB	1:D:326:ILE:HD11	1.87	0.56
1:A:824:VAL:HG12	1:A:848:ILE:HD11	1.88	0.56
1:D:870:PHE:CE1	1:D:903:LEU:HD21	2.40	0.56
1:B:1046:LEU:HG	1:B:1112:ILE:HD11	1.87	0.56
1:A:129:VAL:HG23	1:A:149:VAL:O	2.06	0.55
1:C:546:LEU:HB3	1:C:548:THR:HG22	1.88	0.55
1:C:650:ILE:HD12	1:C:655:TYR:CD2	2.41	0.55
1:A:1095:VAL:HG21	1:A:1145:TYR:CD2	2.41	0.55
1:C:570:LEU:HD21	1:C:585:LEU:HD21	1.88	0.55
1:A:578:LEU:HD13	1:A:579:PRO:HD2	1.89	0.55
1:A:1182:HIS:HB2	1:A:1209:THR:HG21	1.87	0.55
1:A:551:VAL:HG21	1:A:683:ILE:HD11	1.89	0.54
1:A:1046:LEU:HG	1:A:1112:ILE:HD11	1.88	0.54
1:A:235:VAL:HG21	1:A:320:LEU:HD22	1.89	0.54
1:C:350:LEU:HD11	1:C:423:VAL:HG12	1.88	0.54
1:A:1012:TYR:CE1	1:A:1058:ILE:HG23	2.43	0.54
1:C:235:VAL:HG21	1:C:320:LEU:HD22	1.89	0.54
1:B:235:VAL:HG21	1:B:320:LEU:HD22	1.90	0.54
1:A:1147:LYS:HB3	1:A:1170:LEU:HD21	1.89	0.53
1:B:1063:ILE:HD12	1:D:68:ARG:NH2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:589:ALA:HB3	1:C:746:VAL:HG21	1.90	0.53
1:D:931:LEU:HD11	1:D:933:LEU:HD21	1.90	0.53
1:A:537:VAL:HG21	1:A:626:ASP:CG	2.29	0.53
1:D:746:VAL:HG22	1:D:751:VAL:HG12	1.90	0.53
1:B:537:VAL:HG21	1:B:626:ASP:CG	2.28	0.53
1:B:962:THR:HG22	1:B:990:LEU:HD21	1.90	0.53
1:C:882:LEU:HD13	1:C:887:VAL:HG13	1.90	0.53
1:C:584:HIS:NE2	1:C:754:VAL:HG22	2.23	0.53
1:C:458:PHE:CZ	1:C:481:ILE:HD12	2.44	0.53
1:D:537:VAL:HG21	1:D:626:ASP:CG	2.29	0.53
1:C:224:PHE:CD2	1:C:607:MET:CE	2.92	0.52
1:D:848:ILE:N	1:D:848:ILE:HD12	2.25	0.52
2:E:1:NAG:H3	2:E:2:NAG:N2	2.25	0.52
1:A:371:LEU:HD12	1:A:423:VAL:HG21	1.90	0.52
1:D:919:LEU:HD22	1:D:1228:LEU:CD1	2.40	0.52
1:D:758:VAL:HG13	1:D:761:THR:CG2	2.40	0.52
1:B:824:VAL:HG23	1:B:875:GLU:C	2.30	0.52
1:C:1206:VAL:CG1	1:C:1253:ASP:OD2	2.57	0.52
1:C:151:MET:CE	1:C:778:LEU:HD13	2.39	0.51
1:A:965:LEU:HD11	1:A:1247:GLY:CA	2.40	0.51
1:B:1314:MET:HG2	1:B:1324:LEU:HD13	1.92	0.51
1:A:254:TYR:CD2	1:A:255:THR:HG22	2.45	0.51
1:C:52:SER:OG	1:C:545:VAL:HG21	2.10	0.51
1:C:318:MET:SD	1:C:318:MET:N	2.84	0.51
1:B:151:MET:HE2	1:B:778:LEU:HD13	1.93	0.51
1:C:104:THR:HG22	1:C:117:ARG:CB	2.41	0.51
1:C:361:GLN:HA	1:C:411:THR:HB	1.92	0.51
1:B:241:ILE:HD11	1:B:344:THR:O	2.11	0.51
1:B:1095:VAL:HG12	1:B:1095:VAL:O	2.11	0.51
1:D:104:THR:HG22	1:D:117:ARG:CB	2.40	0.51
1:C:570:LEU:HD23	1:C:571:SER:N	2.27	0.50
1:C:746:VAL:HG22	1:C:751:VAL:HG12	1.94	0.50
1:A:919:LEU:HD22	1:A:1228:LEU:CD1	2.42	0.50
1:B:758:VAL:HG13	1:B:761:THR:HG22	1.93	0.50
1:B:104:THR:HG22	1:B:117:ARG:CB	2.41	0.50
1:D:961:ASN:O	1:D:965:LEU:HB2	2.11	0.50
1:C:758:VAL:HG13	1:C:761:THR:CG2	2.41	0.50
1:A:823:ARG:O	1:A:876:ALA:HA	2.11	0.50
1:B:231:VAL:O	1:B:335:LEU:HD22	2.12	0.50
1:A:104:THR:HG22	1:A:117:ARG:HB2	1.93	0.49
1:C:578:LEU:HD23	1:C:578:LEU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:ILE:HD11	1:C:507:ARG:HB2	1.94	0.49
1:A:977:MET:HE3	1:A:1045:VAL:HG22	1.94	0.49
1:B:1191:ALA:HB3	1:B:1192:PRO:HD3	1.95	0.49
1:C:535:ALA:HB1	1:C:536:PRO:HD3	1.94	0.49
1:D:138:TYR:CE2	1:D:144:VAL:HG23	2.47	0.49
1:B:919:LEU:HD22	1:B:1228:LEU:CD1	2.41	0.49
1:C:1207:GLU:HB3	1:C:1253:ASP:HB3	1.93	0.49
1:D:589:ALA:HB3	1:D:746:VAL:HG21	1.95	0.49
1:A:360:ARG:HB2	1:A:363:ILE:CG2	2.43	0.49
1:D:499:ILE:HD11	1:D:507:ARG:HB2	1.94	0.49
1:D:570:LEU:HD21	1:D:585:LEU:HD21	1.95	0.49
1:D:1308:LEU:O	1:D:1308:LEU:HD12	2.12	0.49
1:B:823:ARG:HD3	1:B:846:HIS:N	2.28	0.48
1:B:661:THR:CG2	1:C:655:TYR:HB2	2.44	0.48
1:D:962:THR:HA	1:D:965:LEU:HD13	1.96	0.48
1:C:155:PHE:CE1	1:C:618:VAL:HG12	2.49	0.48
1:A:203:TYR:HB2	1:A:219:PHE:CE1	2.48	0.48
1:B:340:SER:O	1:B:341:SER:C	2.51	0.48
1:A:359:PHE:CZ	1:A:450:LEU:HB3	2.48	0.48
1:A:268:ILE:HD12	1:A:320:LEU:HD21	1.95	0.48
1:A:384:ILE:HD13	1:A:405:VAL:HG21	1.96	0.48
1:D:568:VAL:HG23	1:D:588:THR:O	2.13	0.48
1:D:384:ILE:HD13	1:D:405:VAL:HG21	1.95	0.48
1:C:384:ILE:HD13	1:C:405:VAL:HG21	1.94	0.48
1:A:1145:TYR:CD2	1:A:1146:THR:HG23	2.49	0.48
1:B:461:LEU:HD12	1:B:542:ILE:HG22	1.95	0.48
1:D:231:VAL:HB	1:D:335:LEU:HB2	1.96	0.47
1:B:985:TYR:CE1	1:B:1255:VAL:HG13	2.49	0.47
1:B:165:VAL:HB	1:B:207:VAL:HG12	1.96	0.47
1:D:235:VAL:HG21	1:D:320:LEU:HD22	1.96	0.47
1:A:578:LEU:HD13	1:A:579:PRO:CD	2.44	0.47
1:B:823:ARG:HH22	1:B:843:GLN:NE2	2.13	0.47
1:D:985:TYR:CE1	1:D:1255:VAL:HG13	2.49	0.47
1:A:241:ILE:HA	1:A:311:LEU:HD11	1.96	0.47
1:C:919:LEU:HD22	1:C:1228:LEU:CD1	2.44	0.47
1:A:514:LEU:O	1:A:514:LEU:HD23	2.14	0.47
1:A:882:LEU:HD23	1:A:884:GLY:O	2.14	0.47
1:A:985:TYR:CE1	1:A:1255:VAL:HG13	2.50	0.47
1:B:104:THR:HG22	1:B:117:ARG:HB2	1.96	0.47
1:B:798:MET:SD	1:B:903:LEU:HD22	2.54	0.47
1:C:985:TYR:CE1	1:C:1255:VAL:HG13	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1199:PRO:O	1:C:1203:SER:HB3	2.15	0.47
1:D:326:ILE:HG22	1:D:331:THR:HB	1.97	0.47
1:D:758:VAL:HG13	1:D:761:THR:HG22	1.96	0.47
1:A:544:ALA:HB3	1:A:552:ILE:HG13	1.97	0.47
1:B:1109:LEU:HA	1:B:1112:ILE:HD12	1.96	0.47
1:B:758:VAL:HG13	1:B:761:THR:CG2	2.45	0.47
1:D:561:GLU:HG3	1:D:563:CYS:SG	2.54	0.47
1:D:958:ALA:HB1	1:D:995:GLN:OE1	2.15	0.47
1:D:798:MET:SD	1:D:903:LEU:HD22	2.55	0.46
1:D:1041:LEU:O	1:D:1045:VAL:HG23	2.15	0.46
1:C:675:LEU:HD12	1:C:675:LEU:O	2.16	0.46
1:C:761:THR:HB	1:C:788:ALA:HB3	1.96	0.46
1:C:231:VAL:HG13	1:C:335:LEU:CB	2.45	0.46
1:C:772:LEU:CD2	1:C:778:LEU:HD12	2.45	0.46
1:C:1225:SER:O	1:C:1229:THR:HG23	2.15	0.46
1:A:758:VAL:HG11	1:A:765:TRP:CH2	2.51	0.46
1:C:165:VAL:CG2	1:C:207:VAL:HG12	2.45	0.46
1:C:350:LEU:N	1:C:350:LEU:HD12	2.31	0.46
1:A:350:LEU:N	1:A:350:LEU:HD12	2.31	0.46
1:C:50:LEU:HD21	1:C:52:SER:OG	2.16	0.46
2:G:1:NAG:H4	2:G:2:NAG:N2	2.31	0.46
1:B:407:PHE:CE2	1:B:409:ILE:HD11	2.51	0.45
1:A:104:THR:HG22	1:A:117:ARG:CB	2.46	0.45
1:B:531:LYS:O	1:B:532:SER:CB	2.63	0.45
1:C:1109:LEU:HA	1:C:1112:ILE:HD12	1.98	0.45
1:C:1203:SER:HA	1:C:1206:VAL:HG12	1.97	0.45
1:C:798:MET:SD	1:C:903:LEU:HD22	2.56	0.45
1:D:1225:SER:O	1:D:1229:THR:HG23	2.15	0.45
1:B:409:ILE:HD12	1:B:409:ILE:N	2.32	0.45
1:D:155:PHE:CE1	1:D:618:VAL:HG12	2.52	0.45
1:D:661:THR:HG21	1:D:663:GLU:CD	2.36	0.45
1:B:977:MET:HE3	1:B:1045:VAL:HG22	1.98	0.45
1:D:347:ILE:HG22	1:D:441:HIS:CE1	2.50	0.45
1:A:748:SER:O	1:A:749:ALA:HB2	2.17	0.45
1:C:535:ALA:HB1	1:C:536:PRO:HD2	1.98	0.45
1:B:268:ILE:HD11	1:B:270:ARG:NH2	2.32	0.45
1:B:589:ALA:HB3	1:B:746:VAL:HG21	1.99	0.45
1:C:531:LYS:O	1:C:532:SER:CB	2.65	0.45
1:D:1110:LEU:HB3	1:D:1156:LEU:HG	1.98	0.45
1:C:29:PRO:HA	1:C:53:TYR:HB2	1.98	0.45
1:A:270:ARG:HD3	1:A:309:PHE:CG	2.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:826:VAL:HG23	1:A:826:VAL:O	2.16	0.45
1:B:584:HIS:CE1	1:B:754:VAL:HG22	2.52	0.45
1:B:870:PHE:O	1:B:900:ILE:HG23	2.17	0.45
1:D:961:ASN:O	1:D:965:LEU:CB	2.65	0.45
1:D:1109:LEU:HA	1:D:1112:ILE:HD12	1.98	0.45
1:C:599:ALA:HB3	1:C:740:ILE:HG22	1.99	0.44
1:A:423:VAL:HG22	1:A:424:ASN:H	1.81	0.44
1:A:1200:GLN:O	1:A:1204:ALA:HB2	2.17	0.44
1:B:939:VAL:HG12	1:B:1332:ILE:HG22	2.00	0.44
1:C:384:ILE:HD12	1:C:405:VAL:HG21	1.99	0.44
1:C:535:ALA:CB	1:C:536:PRO:CD	2.95	0.44
1:D:231:VAL:HB	1:D:335:LEU:CB	2.47	0.44
1:D:544:ALA:HB3	1:D:552:ILE:HG13	1.99	0.44
1:A:1225:SER:O	1:A:1229:THR:HG23	2.18	0.44
1:D:143:THR:HG22	1:D:193:PRO:HA	1.99	0.44
1:C:1201:ALA:HB3	1:C:1202:PRO:CD	2.47	0.44
1:D:1106:THR:HG21	1:D:1128:LEU:CD1	2.47	0.44
1:D:281:GLU:CB	1:D:284:GLN:HB3	2.48	0.44
1:A:254:TYR:CE2	1:A:255:THR:HG22	2.52	0.44
1:C:1041:LEU:O	1:C:1045:VAL:HG23	2.18	0.44
3:R:1:NAG:H62	3:R:2:NAG:C7	2.47	0.44
1:C:977:MET:HE3	1:C:1045:VAL:HG22	1.99	0.44
1:C:143:THR:HG22	1:C:193:PRO:HA	2.00	0.44
1:D:269:CYS:HA	1:D:287:CYS:HB3	2.00	0.44
1:D:824:VAL:HG23	1:D:875:GLU:O	2.17	0.44
1:D:826:VAL:HG23	1:D:826:VAL:O	2.17	0.44
1:D:958:ALA:HB2	1:D:989:TYR:OH	2.17	0.44
1:A:1264:TYR:CE2	1:A:1268:THR:HG21	2.53	0.43
1:C:61:SER:HB2	1:C:74:PHE:CE1	2.53	0.43
1:C:1211:TYR:CZ	1:C:1256:VAL:HG11	2.53	0.43
1:B:658:VAL:HG12	1:C:656:THR:HG21	2.00	0.43
1:A:147:ARG:HB2	1:A:187:LEU:HD11	2.00	0.43
1:A:384:ILE:HD12	1:A:405:VAL:HG21	2.00	0.43
1:B:151:MET:HE1	1:B:778:LEU:HD13	2.00	0.43
1:C:1106:THR:HG21	1:C:1128:LEU:HD21	2.00	0.43
1:D:167:ILE:O	1:D:175:ILE:HG22	2.18	0.43
1:D:977:MET:HE2	1:D:1045:VAL:HG22	2.00	0.43
1:D:52:SER:HB3	1:D:545:VAL:HG21	2.00	0.43
1:B:650:ILE:HG23	1:B:651:ASN:N	2.33	0.43
1:A:599:ALA:HB3	1:A:740:ILE:HG22	2.01	0.43
1:A:746:VAL:HA	1:A:751:VAL:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1264:TYR:CE2	1:C:1268:THR:HG21	2.53	0.43
1:A:1211:TYR:CZ	1:A:1256:VAL:HG11	2.54	0.43
1:D:599:ALA:HB3	1:D:740:ILE:HG22	2.00	0.43
1:A:143:THR:HG22	1:A:193:PRO:HA	2.00	0.43
1:A:822:ILE:HG22	1:A:889:SER:CB	2.49	0.43
1:A:1106:THR:HG21	1:A:1128:LEU:CD1	2.46	0.43
1:A:1399:LEU:CB	1:A:1408:THR:HG21	2.46	0.43
1:B:34:LEU:HB3	1:B:675:LEU:HD13	2.00	0.43
1:B:119:THR:O	1:B:676:LYS:NZ	2.51	0.43
1:B:1225:SER:O	1:B:1229:THR:HG23	2.18	0.43
1:C:371:LEU:HD23	1:C:372:VAL:N	2.33	0.43
1:C:544:ALA:HB3	1:C:552:ILE:HG13	2.01	0.43
1:C:758:VAL:HG13	1:C:761:THR:HG22	1.99	0.43
1:C:826:VAL:O	1:C:826:VAL:HG23	2.18	0.43
1:D:977:MET:HE1	1:D:1015:GLN:HG2	2.00	0.43
1:D:1211:TYR:CZ	1:D:1256:VAL:HG11	2.54	0.43
1:A:269:CYS:O	1:A:318:MET:HB2	2.19	0.43
1:A:570:LEU:HD21	1:A:585:LEU:HD21	1.99	0.43
1:A:1095:VAL:HG23	1:A:1100:THR:HG21	2.01	0.43
1:B:338:ARG:HD3	1:B:340:SER:HB2	2.01	0.43
1:B:826:VAL:HG23	1:B:826:VAL:O	2.17	0.43
1:D:966:LEU:HD13	1:D:1007:TYR:HD2	1.84	0.43
1:D:1264:TYR:CE2	1:D:1268:THR:HG21	2.53	0.43
1:B:1264:TYR:CE2	1:B:1268:THR:HG21	2.54	0.43
1:D:61:SER:HB2	1:D:74:PHE:CE1	2.54	0.43
1:D:480:TYR:CE2	1:D:513:LEU:HD21	2.53	0.43
1:D:585:LEU:C	1:D:585:LEU:HD23	2.39	0.43
1:D:965:LEU:O	1:D:966:LEU:O	2.37	0.43
1:B:1185:ARG:HB3	1:B:1186:PRO:CD	2.49	0.42
1:A:948:VAL:HG12	1:A:1326:THR:HG23	2.01	0.42
1:A:950:VAL:C	1:A:951:LEU:HD23	2.39	0.42
1:B:61:SER:HB2	1:B:74:PHE:CE1	2.54	0.42
1:A:650:ILE:O	1:A:655:TYR:CD2	2.72	0.42
1:C:167:ILE:O	1:C:175:ILE:HG22	2.19	0.42
1:B:882:LEU:HB3	1:B:886:GLU:O	2.20	0.42
1:A:482:LEU:HD22	1:A:482:LEU:N	2.34	0.42
1:B:138:TYR:CZ	1:B:144:VAL:HG23	2.55	0.42
1:B:143:THR:HG22	1:B:193:PRO:HA	2.01	0.42
1:B:364:PRO:HB3	1:B:410:ASN:HA	2.01	0.42
1:D:944:ALA:HA	1:D:1329:LYS:O	2.20	0.42
1:C:502:LYS:CG	1:C:535:ALA:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1323:TYR:CE2	1:D:1325:GLN:HB2	2.54	0.42
1:A:566:ASN:OD1	1:A:590:ALA:HB2	2.20	0.42
1:C:948:VAL:HG12	1:C:1326:THR:HG23	2.01	0.42
1:D:948:VAL:HG12	1:D:1326:THR:HG23	2.02	0.42
1:B:352:PHE:CD1	1:B:355:VAL:HG11	2.54	0.42
1:B:977:MET:HE2	1:B:1045:VAL:HG22	2.01	0.42
1:D:473:THR:HG22	1:D:529:PRO:HB3	2.02	0.42
1:A:535:ALA:CB	1:A:536:PRO:CD	2.98	0.42
1:D:977:MET:HE3	1:D:1045:VAL:HG22	2.01	0.42
1:A:61:SER:HB2	1:A:74:PHE:CE1	2.54	0.41
1:B:167:ILE:O	1:B:175:ILE:HG22	2.19	0.41
1:B:1018:TYR:HB3	1:B:1029:GLY:HA2	2.01	0.41
1:C:286:PHE:CD2	1:C:308:VAL:O	2.73	0.41
1:A:77:LEU:HD22	1:A:87:VAL:CG1	2.37	0.41
1:B:329:GLU:HA	1:B:811:LYS:HE2	2.02	0.41
1:C:1308:LEU:HB3	1:C:1309:PRO:HD3	2.02	0.41
1:D:129:VAL:O	1:D:621:LEU:HD21	2.20	0.41
1:A:165:VAL:HB	1:A:207:VAL:HG12	2.02	0.41
1:B:1041:LEU:O	1:B:1045:VAL:HG23	2.21	0.41
1:B:1191:ALA:HB3	1:B:1192:PRO:CD	2.51	0.41
1:A:235:VAL:CG2	1:A:320:LEU:HD22	2.51	0.41
1:A:393:TYR:CG	1:A:409:ILE:HG22	2.55	0.41
1:D:29:PRO:HD3	4:S:1:NAG:HN2	1.84	0.41
1:A:1201:ALA:HB3	1:A:1202:PRO:HD3	2.02	0.41
1:B:473:THR:HG22	1:B:529:PRO:HB3	2.03	0.41
1:A:387:ARG:HD3	1:A:394:TYR:CE1	2.56	0.41
1:B:350:LEU:HD23	1:B:350:LEU:N	2.36	0.41
1:B:1211:TYR:CZ	1:B:1256:VAL:HG11	2.56	0.41
1:D:1308:LEU:HD12	1:D:1308:LEU:C	2.41	0.41
1:B:135:LYS:CE	1:B:604:VAL:HG11	2.51	0.41
1:B:666:MET:CG	1:B:683:ILE:HG23	2.51	0.41
1:C:958:ALA:HB1	1:C:995:GLN:OE1	2.21	0.41
1:D:137:ILE:CD1	1:D:607:MET:HG2	2.51	0.41
1:D:384:ILE:HD12	1:D:405:VAL:HG21	1.99	0.41
1:D:535:ALA:CB	1:D:536:PRO:CD	2.98	0.41
1:D:954:ILE:HD12	1:D:1269:PHE:CE2	2.56	0.41
1:C:137:ILE:CD1	1:C:607:MET:HG2	2.51	0.41
1:A:679:THR:HG21	1:A:683:ILE:HD13	2.03	0.40
1:B:418:SER:HA	1:B:447:THR:HG22	2.03	0.40
1:C:977:MET:HE2	1:C:1045:VAL:HG22	2.01	0.40
1:A:239:ILE:HD12	1:A:240:THR:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1379:ALA:HA	1:A:1451:ASP:HA	2.03	0.40
1:B:578:LEU:O	1:B:580:ALA:N	2.54	0.40
1:B:948:VAL:HG12	1:B:1326:THR:HG23	2.02	0.40
1:D:903:LEU:HD23	1:D:903:LEU:N	2.36	0.40
1:C:275:ALA:HB3	1:D:436:TRP:HE1	1.85	0.40
1:C:318:MET:SD	1:C:341:SER:O	2.80	0.40
1:D:393:TYR:CG	1:D:409:ILE:HG22	2.57	0.40
1:A:655:TYR:H	1:D:661:THR:HG23	1.87	0.40
1:C:470:CYS:HA	1:C:530:VAL:HG12	2.01	0.40
1:C:993:THR:O	1:C:994:GLN:HB2	2.21	0.40
1:A:473:THR:HG22	1:A:529:PRO:HB3	2.03	0.40
1:B:1333:LEU:N	1:B:1334:PRO:CD	2.84	0.40
1:C:1095:VAL:O	1:C:1095:VAL:HG12	2.22	0.40
1:C:1128:LEU:N	1:C:1128:LEU:HD13	2.37	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	1412/1474 (96%)	1184 (84%)	168 (12%)	60 (4%)	3	26
1	B	1269/1474 (86%)	1064 (84%)	146 (12%)	59 (5%)	2	24
1	C	1270/1474 (86%)	1082 (85%)	141 (11%)	47 (4%)	3	28
1	D	1267/1474 (86%)	1068 (84%)	145 (11%)	54 (4%)	2	25
All	All	5218/5896 (88%)	4398 (84%)	600 (12%)	220 (4%)	3	26

All (220) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	282	ASP
1	A	286	PHE
1	A	374	GLY
1	A	535	ALA
1	A	578	LEU
1	A	749	ALA
1	A	953	ASP
1	A	966	LEU
1	A	1079	CYS
1	A	1144	VAL
1	A	1348	LEU
1	A	1387	SER
1	B	328	GLU
1	B	340	SER
1	B	413	ASN
1	B	424	ASN
1	B	535	ALA
1	B	736	PRO
1	B	749	ALA
1	B	959	MET
1	B	966	LEU
1	B	1079	CYS
1	B	1088	ASN
1	B	1187	GLN
1	C	311	LEU
1	C	424	ASN
1	C	578	LEU
1	C	730	THR
1	C	736	PRO
1	C	749	ALA
1	C	895	ARG
1	C	1032	TYR
1	C	1201	ALA
1	D	286	PHE
1	D	435	GLN
1	D	532	SER
1	D	535	ALA
1	D	582	HIS
1	D	736	PRO
1	D	749	ALA
1	D	965	LEU
1	D	966	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	1079	CYS
1	D	1193	VAL
1	D	1294	ASN
1	A	213	GLY
1	A	314	LYS
1	A	338	ARG
1	A	651	ASN
1	A	687	LYS
1	A	748	SER
1	A	891	PRO
1	A	1038	ASN
1	A	1140	HIS
1	A	1193	VAL
1	A	1249	SER
1	A	1273	GLY
1	A	1334	PRO
1	A	1357	ALA
1	B	56	GLU
1	B	213	GLY
1	B	310	GLN
1	B	313	ARG
1	B	341	SER
1	B	414	VAL
1	B	438	SER
1	B	439	GLU
1	B	491	LYS
1	B	532	SER
1	B	582	HIS
1	B	638	ASP
1	B	639	ASN
1	B	688	MET
1	B	883	CYS
1	B	961	ASN
1	B	962	THR
1	B	1031	ARG
1	B	1249	SER
1	B	1285	THR
1	C	180	SER
1	C	213	GLY
1	C	374	GLY
1	C	516	LYS
1	C	532	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	582	HIS
1	C	892	GLU
1	C	953	ASP
1	C	958	ALA
1	C	966	LEU
1	C	1079	CYS
1	C	1096	GLU
1	C	1249	SER
1	C	1285	THR
1	D	180	SER
1	D	213	GLY
1	D	338	ARG
1	D	390	GLU
1	D	579	PRO
1	D	842	GLU
1	D	955	LEU
1	D	956	GLY
1	D	958	ALA
1	D	1031	ARG
1	D	1144	VAL
1	D	1249	SER
1	D	1273	GLY
1	D	1285	THR
1	A	180	SER
1	A	285	ALA
1	A	423	VAL
1	A	454	PRO
1	A	581	SER
1	A	641	ASP
1	A	783	THR
1	A	842	GLU
1	A	888	PRO
1	A	893	HIS
1	A	1298	LEU
1	B	338	ARG
1	B	454	PRO
1	B	581	SER
1	B	640	GLU
1	B	730	THR
1	B	783	THR
1	B	1197	TYR
1	C	55	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	454	PRO
1	C	783	THR
1	C	1294	ASN
1	D	274	ASP
1	D	414	VAL
1	D	424	ASN
1	D	454	PRO
1	D	637	GLN
1	D	641	ASP
1	D	651	ASN
1	D	655	TYR
1	D	689	CYS
1	D	783	THR
1	A	254	TYR
1	A	341	SER
1	A	403	GLY
1	A	1031	ARG
1	A	1272	THR
1	A	1285	THR
1	A	1297	ARG
1	A	1307	GLU
1	A	1352	CYS
1	B	180	SER
1	B	254	TYR
1	B	429	SER
1	B	487	LEU
1	B	580	ALA
1	B	958	ALA
1	B	1336	LYS
1	C	279	HIS
1	C	390	GLU
1	C	403	GLY
1	C	535	ALA
1	C	640	GLU
1	C	994	GLN
1	C	1141	GLY
1	D	281	GLU
1	D	687	LYS
1	D	759	PRO
1	D	885	THR
1	D	1032	TYR
1	D	1053	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	1097	ASP
1	D	1334	PRO
1	A	607	MET
1	A	736	PRO
1	A	1034	ARG
1	A	1142	SER
1	A	1275	ALA
1	A	1335	GLU
1	B	53	TYR
1	B	520	MET
1	B	607	MET
1	B	686	PRO
1	B	759	PRO
1	B	994	GLN
1	B	1309	PRO
1	C	254	TYR
1	C	415	MET
1	C	607	MET
1	C	649	TYR
1	C	735	PHE
1	C	1309	PRO
1	D	403	GLY
1	D	607	MET
1	D	1198	GLU
1	A	414	VAL
1	A	759	PRO
1	A	958	ALA
1	B	579	PRO
1	B	1305	LEU
1	C	487	LEU
1	D	254	TYR
1	D	277	ASP
1	D	737	GLU
1	D	1197	TYR
1	A	1306	PRO
1	B	1084	GLY
1	C	1189	PRO
1	A	1388	GLY
1	B	1189	PRO
1	C	1091	ILE
1	C	1095	VAL
1	D	1113	PRO

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Mol	Chain	Res	Type
1	A	1113	PRO
1	A	1449	VAL
1	B	1113	PRO
1	C	956	GLY
1	C	1333	LEU
1	D	280	GLY
1	D	347	ILE
1	B	268	ILE
1	C	759	PRO

### 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	1241/1290 (96%)	1075 (87%)	166 (13%)	4	20
1	B	1110/1290 (86%)	971 (88%)	139 (12%)	4	22
1	C	1112/1290 (86%)	967 (87%)	145 (13%)	4	21
1	D	1108/1290 (86%)	957 (86%)	151 (14%)	3	20
All	All	4571/5160 (89%)	3970 (87%)	601 (13%)	4	21

All (601) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	51	LEU
1	A	54	LEU
1	A	58	VAL
1	A	63	SER
1	A	71	ARG
1	A	76	ASP
1	A	82	ASP
1	A	114	PHE
1	A	124	ASN
1	A	125	GLU
1	A	128	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	131	VAL
1	A	133	THR
1	A	149	VAL
1	A	151	MET
1	A	158	LEU
1	A	160	GLU
1	A	161	LEU
1	A	165	VAL
1	A	169	ASP
1	A	181	PHE
1	A	194	LEU
1	A	220	THR
1	A	226	LEU
1	A	246	MET
1	A	253	LEU
1	A	256	TYR
1	A	260	VAL
1	A	278	CYS
1	A	293	GLN
1	A	295	ASN
1	A	311	LEU
1	A	314	LYS
1	A	315	GLU
1	A	317	GLU
1	A	318	MET
1	A	335	LEU
1	A	341	SER
1	A	350	LEU
1	A	353	VAL
1	A	356	ASP
1	A	358	HIS
1	A	361	GLN
1	A	365	PHE
1	A	373	ASP
1	A	387	ARG
1	A	394	TYR
1	A	413	ASN
1	A	415	MET
1	A	428	ARG
1	A	431	CYS
1	A	435	GLN
1	A	436	TRP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	458	PHE
1	A	461	LEU
1	A	465	SER
1	A	499	ILE
1	A	500	MET
1	A	506	VAL
1	A	510	THR
1	A	514	LEU
1	A	519	ASP
1	A	520	MET
1	A	523	HIS
1	A	524	PHE
1	A	541	LEU
1	A	555	SER
1	A	557	LYS
1	A	568	VAL
1	A	569	ASP
1	A	572	PHE
1	A	578	LEU
1	A	593	SER
1	A	610	ASP
1	A	637	GLN
1	A	650	ILE
1	A	673	MET
1	A	675	LEU
1	A	683	ILE
1	A	691	GLN
1	A	696	GLU
1	A	731	VAL
1	A	734	TYR
1	A	737	GLU
1	A	743	LEU
1	A	760	ASP
1	A	763	THR
1	A	778	LEU
1	A	782	SER
1	A	785	SER
1	A	796	LEU
1	A	797	THR
1	A	831	SER
1	A	835	LEU
1	A	843	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	846	HIS
1	A	847	CYS
1	A	848	ILE
1	A	854	GLN
1	A	857	SER
1	A	865	LEU
1	A	871	THR
1	A	877	LEU
1	A	878	GLU
1	A	879	SER
1	A	882	LEU
1	A	883	CYS
1	A	897	ASP
1	A	903	LEU
1	A	905	VAL
1	A	913	GLU
1	A	921	CYS
1	A	926	GLU
1	A	935	LEU
1	A	942	GLU
1	A	951	LEU
1	A	953	ASP
1	A	955	LEU
1	A	960	GLN
1	A	961	ASN
1	A	995	GLN
1	A	997	THR
1	A	1008	LEU
1	A	1017	ASN
1	A	1024	SER
1	A	1034	ARG
1	A	1036	GLN
1	A	1039	THR
1	A	1079	CYS
1	A	1086	LEU
1	A	1091	ILE
1	A	1096	GLU
1	A	1107	ILE
1	A	1109	LEU
1	A	1142	SER
1	A	1143	HIS
1	A	1170	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1172	GLU
1	A	1179	ASN
1	A	1187	GLN
1	A	1190	LYS
1	A	1197	TYR
1	A	1198	GLU
1	A	1207	GLU
1	A	1217	LEU
1	A	1224	THR
1	A	1233	ASN
1	A	1242	GLN
1	A	1263	LYS
1	A	1280	ILE
1	A	1289	LYS
1	A	1314	MET
1	A	1317	THR
1	A	1319	GLU
1	A	1325	GLN
1	A	1332	ILE
1	A	1336	LYS
1	A	1354	GLU
1	A	1389	PHE
1	A	1392	LEU
1	A	1425	GLN
1	A	1427	LEU
1	A	1434	LEU
1	A	1441	ASP
1	A	1442	LEU
1	B	30	GLN
1	B	31	TYR
1	B	41	THR
1	B	42	GLU
1	B	51	LEU
1	B	58	VAL
1	B	63	SER
1	B	76	ASP
1	B	77	LEU
1	B	84	LEU
1	B	114	PHE
1	B	117	ARG
1	B	118	THR
1	B	124	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	131	VAL
1	B	133	THR
1	B	149	VAL
1	B	151	MET
1	B	152	ASP
1	B	161	LEU
1	B	169	ASP
1	B	181	PHE
1	B	187	LEU
1	B	194	LEU
1	B	204	LYS
1	B	206	VAL
1	B	220	THR
1	B	224	PHE
1	B	233	VAL
1	B	238	ILE
1	B	246	MET
1	B	253	LEU
1	B	255	THR
1	B	260	VAL
1	B	270	ARG
1	B	272	TYR
1	B	273	SER
1	B	276	SER
1	B	295	ASN
1	B	305	LYS
1	B	311	LEU
1	B	313	ARG
1	B	318	MET
1	B	327	GLN
1	B	335	LEU
1	B	350	LEU
1	B	353	VAL
1	B	356	ASP
1	B	361	GLN
1	B	365	PHE
1	B	385	PHE
1	B	390	GLU
1	B	396	ASN
1	B	405	VAL
1	B	414	VAL
1	B	428	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	431	CYS
1	B	434	TYR
1	B	450	LEU
1	B	456	LYS
1	B	461	LEU
1	B	465	SER
1	B	480	TYR
1	B	486	THR
1	B	487	LEU
1	B	491	LYS
1	B	524	PHE
1	B	528	ILE
1	B	545	VAL
1	B	546	LEU
1	B	548	THR
1	B	555	SER
1	B	569	ASP
1	B	572	PHE
1	B	575	SER
1	B	578	LEU
1	B	610	ASP
1	B	636	ASP
1	B	637	GLN
1	B	645	ARG
1	B	650	ILE
1	B	673	MET
1	B	687	LYS
1	B	731	VAL
1	B	733	LYS
1	B	734	TYR
1	B	737	GLU
1	B	743	LEU
1	B	763	THR
1	B	778	LEU
1	B	782	SER
1	B	785	SER
1	B	796	LEU
1	B	797	THR
1	B	822	ILE
1	B	831	SER
1	B	835	LEU
1	B	842	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	856	VAL
1	B	857	SER
1	B	865	LEU
1	B	871	THR
1	B	878	GLU
1	B	882	LEU
1	B	883	CYS
1	B	897	ASP
1	B	903	LEU
1	B	905	VAL
1	B	908	GLU
1	B	921	CYS
1	B	926	GLU
1	B	935	LEU
1	B	940	VAL
1	B	955	LEU
1	B	965	LEU
1	B	966	LEU
1	B	993	THR
1	B	997	THR
1	B	1008	LEU
1	B	1017	ASN
1	B	1030	GLU
1	B	1056	ILE
1	B	1064	THR
1	B	1079	CYS
1	B	1086	LEU
1	B	1107	ILE
1	B	1177	LYS
1	B	1179	ASN
1	B	1180	SER
1	B	1209	THR
1	B	1224	THR
1	B	1242	GLN
1	B	1263	LYS
1	B	1298	LEU
1	B	1305	LEU
1	B	1314	MET
1	B	1317	THR
1	B	1331	ASN
1	B	1332	ILE
1	C	31	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	54	LEU
1	C	63	SER
1	C	76	ASP
1	C	80	GLU
1	C	111	THR
1	C	124	ASN
1	C	128	LEU
1	C	131	VAL
1	C	133	THR
1	C	149	VAL
1	C	164	LEU
1	C	169	ASP
1	C	187	LEU
1	C	188	LYS
1	C	194	LEU
1	C	204	LYS
1	C	220	THR
1	C	231	VAL
1	C	246	MET
1	C	253	LEU
1	C	255	THR
1	C	260	VAL
1	C	268	ILE
1	C	273	SER
1	C	276	SER
1	C	277	ASP
1	C	279	HIS
1	C	289	LYS
1	C	295	ASN
1	C	303	GLN
1	C	311	LEU
1	C	313	ARG
1	C	315	GLU
1	C	318	MET
1	C	319	LYS
1	C	341	SER
1	C	343	ILE
1	C	348	THR
1	C	353	VAL
1	C	356	ASP
1	C	361	GLN
1	C	365	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	373	ASP
1	C	375	LYS
1	C	417	THR
1	C	419	LEU
1	C	427	ASP
1	C	440	GLU
1	C	461	LEU
1	C	465	SER
1	C	486	THR
1	C	500	MET
1	C	510	THR
1	C	524	PHE
1	C	541	LEU
1	C	555	SER
1	C	557	LYS
1	C	568	VAL
1	C	569	ASP
1	C	575	SER
1	C	576	GLN
1	C	577	SER
1	C	578	LEU
1	C	593	SER
1	C	610	ASP
1	C	634	LEU
1	C	654	THR
1	C	673	MET
1	C	675	LEU
1	C	676	LYS
1	C	683	ILE
1	C	691	GLN
1	C	730	THR
1	C	731	VAL
1	C	737	GLU
1	C	743	LEU
1	C	763	THR
1	C	778	LEU
1	C	782	SER
1	C	785	SER
1	C	789	PHE
1	C	796	LEU
1	C	797	THR
1	C	822	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	823	ARG
1	C	831	SER
1	C	835	LEU
1	C	842	GLU
1	C	848	ILE
1	C	856	VAL
1	C	857	SER
1	C	865	LEU
1	C	871	THR
1	C	883	CYS
1	C	889	SER
1	C	893	HIS
1	C	897	ASP
1	C	903	LEU
1	C	904	LEU
1	C	921	CYS
1	C	926	GLU
1	C	935	LEU
1	C	938	ASN
1	C	942	GLU
1	C	945	ARG
1	C	953	ASP
1	C	965	LEU
1	C	993	THR
1	C	997	THR
1	C	1008	LEU
1	C	1017	ASN
1	C	1019	LYS
1	C	1021	TYR
1	C	1024	SER
1	C	1030	GLU
1	C	1032	TYR
1	C	1039	THR
1	C	1041	LEU
1	C	1056	ILE
1	C	1074	GLN
1	C	1079	CYS
1	C	1086	LEU
1	C	1107	ILE
1	C	1128	LEU
1	C	1142	SER
1	C	1170	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	1172	GLU
1	C	1179	ASN
1	C	1190	LYS
1	C	1206	VAL
1	C	1210	SER
1	C	1217	LEU
1	C	1224	THR
1	C	1242	GLN
1	C	1252	GLN
1	C	1263	LYS
1	C	1272	THR
1	C	1280	ILE
1	C	1291	GLN
1	C	1298	LEU
1	C	1314	MET
1	C	1317	THR
1	C	1333	LEU
1	C	1335	GLU
1	D	31	TYR
1	D	51	LEU
1	D	52	SER
1	D	54	LEU
1	D	63	SER
1	D	76	ASP
1	D	82	ASP
1	D	112	GLN
1	D	124	ASN
1	D	128	LEU
1	D	131	VAL
1	D	133	THR
1	D	142	GLN
1	D	149	VAL
1	D	156	HIS
1	D	169	ASP
1	D	187	LEU
1	D	194	LEU
1	D	204	LYS
1	D	220	THR
1	D	237	LYS
1	D	246	MET
1	D	253	LEU
1	D	255	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	260	VAL
1	D	277	ASP
1	D	295	ASN
1	D	311	LEU
1	D	313	ARG
1	D	316	TYR
1	D	319	LYS
1	D	335	LEU
1	D	339	GLN
1	D	341	SER
1	D	343	ILE
1	D	346	THR
1	D	347	ILE
1	D	350	LEU
1	D	353	VAL
1	D	356	ASP
1	D	361	GLN
1	D	365	PHE
1	D	371	LEU
1	D	372	VAL
1	D	373	ASP
1	D	413	ASN
1	D	428	ARG
1	D	432	TYR
1	D	438	SER
1	D	441	HIS
1	D	458	PHE
1	D	461	LEU
1	D	465	SER
1	D	486	THR
1	D	490	LEU
1	D	500	MET
1	D	510	THR
1	D	518	GLU
1	D	520	MET
1	D	524	PHE
1	D	533	ASP
1	D	541	LEU
1	D	545	VAL
1	D	555	SER
1	D	569	ASP
1	D	571	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	576	GLN
1	D	610	ASP
1	D	634	LEU
1	D	637	GLN
1	D	644	ASN
1	D	649	TYR
1	D	656	THR
1	D	661	THR
1	D	663	GLU
1	D	673	MET
1	D	675	LEU
1	D	676	LYS
1	D	688	MET
1	D	731	VAL
1	D	732	ARG
1	D	733	LYS
1	D	734	TYR
1	D	737	GLU
1	D	743	LEU
1	D	747	ASN
1	D	763	THR
1	D	774	GLU
1	D	778	LEU
1	D	782	SER
1	D	785	SER
1	D	796	LEU
1	D	797	THR
1	D	815	LEU
1	D	823	ARG
1	D	831	SER
1	D	835	LEU
1	D	843	GLN
1	D	846	HIS
1	D	848	ILE
1	D	853	ARG
1	D	857	SER
1	D	865	LEU
1	D	871	THR
1	D	877	LEU
1	D	879	SER
1	D	890	VAL
1	D	897	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	903	LEU
1	D	913	GLU
1	D	921	CYS
1	D	926	GLU
1	D	935	LEU
1	D	945	ARG
1	D	965	LEU
1	D	993	THR
1	D	997	THR
1	D	1008	LEU
1	D	1017	ASN
1	D	1024	SER
1	D	1036	GLN
1	D	1039	THR
1	D	1041	LEU
1	D	1056	ILE
1	D	1079	CYS
1	D	1082	SER
1	D	1086	LEU
1	D	1091	ILE
1	D	1092	LYS
1	D	1107	ILE
1	D	1139	ASP
1	D	1145	TYR
1	D	1170	LEU
1	D	1172	GLU
1	D	1179	ASN
1	D	1187	GLN
1	D	1188	LYS
1	D	1207	GLU
1	D	1217	LEU
1	D	1224	THR
1	D	1242	GLN
1	D	1252	GLN
1	D	1263	LYS
1	D	1272	THR
1	D	1280	ILE
1	D	1290	PHE
1	D	1298	LEU
1	D	1305	LEU
1	D	1308	LEU
1	D	1314	MET

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Mol	Chain	Res	Type
1	D	1331	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	584	HIS
1	A	693	GLN
1	B	584	HIS
1	B	827	GLN
1	B	843	GLN
1	B	960	GLN
1	C	1325	GLN
1	D	584	HIS
1	D	747	ASN
1	D	1252	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

50 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	1.24	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	E	2	2	14,14,15	0.46	0	17,19,21	1.49	2 (11%)
2	BMA	E	3	2	11,11,12	0.53	0	15,15,17	1.16	1 (6%)
2	MAN	E	4	2	11,11,12	0.58	0	15,15,17	1.06	2 (13%)
3	NAG	F	1	1,3	14,14,15	0.46	0	17,19,21	0.97	1 (5%)
3	NAG	F	2	3	14,14,15	0.41	0	17,19,21	0.91	1 (5%)
3	BMA	F	3	3	11,11,12	0.39	0	15,15,17	0.73	0
2	NAG	G	1	1,2	14,14,15	0.39	0	17,19,21	0.84	1 (5%)
2	NAG	G	2	2	14,14,15	0.48	0	17,19,21	0.95	2 (11%)
2	BMA	G	3	2	11,11,12	0.60	0	15,15,17	1.00	1 (6%)
2	MAN	G	4	2	11,11,12	0.71	0	15,15,17	1.51	2 (13%)
4	NAG	H	1	1,4	14,14,15	0.40	0	17,19,21	1.03	1 (5%)
4	NAG	H	2	4	14,14,15	0.37	0	17,19,21	0.55	0
3	NAG	I	1	1,3	14,14,15	0.33	0	17,19,21	0.66	0
3	NAG	I	2	3	14,14,15	0.40	0	17,19,21	0.89	2 (11%)
3	BMA	I	3	3	11,11,12	0.49	0	15,15,17	0.71	1 (6%)
2	NAG	J	1	1,2	14,14,15	0.54	0	17,19,21	1.20	1 (5%)
2	NAG	J	2	2	14,14,15	0.45	0	17,19,21	1.15	2 (11%)
2	BMA	J	3	2	11,11,12	0.48	0	15,15,17	0.77	0
2	MAN	J	4	2	11,11,12	0.54	0	15,15,17	1.14	2 (13%)
4	NAG	K	1	1,4	14,14,15	0.45	0	17,19,21	0.88	1 (5%)
4	NAG	K	2	4	14,14,15	0.41	0	17,19,21	0.63	0
4	NAG	L	1	1,4	14,14,15	0.44	0	17,19,21	1.16	2 (11%)
4	NAG	L	2	4	14,14,15	0.46	0	17,19,21	0.78	0
3	NAG	M	1	1,3	14,14,15	0.38	0	17,19,21	0.85	1 (5%)
3	NAG	M	2	3	14,14,15	0.45	0	17,19,21	1.06	2 (11%)
3	BMA	M	3	3	11,11,12	0.38	0	15,15,17	0.58	0
4	NAG	N	1	1,4	14,14,15	0.41	0	17,19,21	1.05	2 (11%)
4	NAG	N	2	4	14,14,15	0.46	0	17,19,21	1.58	3 (17%)
2	NAG	O	1	1,2	14,14,15	0.40	0	17,19,21	0.78	0
2	NAG	O	2	2	14,14,15	0.45	0	17,19,21	1.16	3 (17%)
2	BMA	O	3	2	11,11,12	0.58	0	15,15,17	0.76	0
2	MAN	O	4	2	11,11,12	0.43	0	15,15,17	0.86	0
4	NAG	P	1	1,4	14,14,15	0.41	0	17,19,21	0.59	0
4	NAG	P	2	4	14,14,15	0.51	0	17,19,21	0.99	1 (5%)
4	NAG	Q	1	1,4	14,14,15	0.40	0	17,19,21	1.03	2 (11%)
4	NAG	Q	2	4	14,14,15	0.42	0	17,19,21	0.57	0
3	NAG	R	1	1,3	14,14,15	0.29	0	17,19,21	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	R	2	3	14,14,15	0.46	0	17,19,21	1.52	3 (17%)
3	BMA	R	3	3	11,11,12	0.50	0	15,15,17	0.93	1 (6%)
4	NAG	S	1	1,4	14,14,15	0.40	0	17,19,21	0.79	1 (5%)
4	NAG	S	2	4	14,14,15	0.42	0	17,19,21	1.14	3 (17%)
4	NAG	T	1	1,4	14,14,15	0.39	0	17,19,21	0.79	0
4	NAG	T	2	4	14,14,15	0.42	0	17,19,21	1.16	2 (11%)
4	NAG	U	1	1,4	14,14,15	0.38	0	17,19,21	1.04	2 (11%)
4	NAG	U	2	4	14,14,15	0.37	0	17,19,21	0.68	0
2	NAG	V	1	1,2	14,14,15	0.40	0	17,19,21	1.38	4 (23%)
2	NAG	V	2	2	14,14,15	0.47	0	17,19,21	1.49	2 (11%)
2	BMA	V	3	2	11,11,12	0.49	0	15,15,17	0.91	0
2	MAN	V	4	2	11,11,12	0.46	0	15,15,17	1.03	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
2	BMA	E	3	2	-	1/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	BMA	G	3	2	-	2/2/19/22	0/1/1/1
2	MAN	G	4	2	-	1/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
2	NAG	J	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	BMA	J	3	2	-	1/2/19/22	0/1/1/1
2	MAN	J	4	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	1/6/23/26	0/1/1/1
4	NAG	L	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	1/6/23/26	0/1/1/1
3	BMA	M	3	3	-	0/2/19/22	0/1/1/1
4	NAG	N	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	O	2	2	-	3/6/23/26	0/1/1/1
2	BMA	O	3	2	-	2/2/19/22	0/1/1/1
2	MAN	O	4	2	-	0/2/19/22	0/1/1/1
4	NAG	P	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	1/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
3	BMA	R	3	3	-	0/2/19/22	0/1/1/1
4	NAG	S	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	S	2	4	-	1/6/23/26	0/1/1/1
4	NAG	T	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	1/6/23/26	0/1/1/1
4	NAG	U	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1
2	NAG	V	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	V	2	2	-	0/6/23/26	0/1/1/1
2	BMA	V	3	2	-	2/2/19/22	0/1/1/1
2	MAN	V	4	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	2	NAG	C1-C2-N2	4.91	118.87	110.49
2	G	4	MAN	C1-O5-C5	4.72	118.59	112.19
2	V	2	NAG	C1-C2-N2	4.06	117.42	110.49
2	E	2	NAG	C1-O5-C5	4.05	117.69	112.19
2	E	2	NAG	C1-C2-N2	3.73	116.86	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1	NAG	C1-O5-C5	3.73	117.24	112.19
3	R	2	NAG	C1-O5-C5	3.67	117.16	112.19
4	N	1	NAG	O5-C1-C2	-3.27	106.13	111.29
3	R	2	NAG	C1-C2-N2	3.24	116.02	110.49
3	M	1	NAG	C1-O5-C5	3.17	116.49	112.19
2	V	1	NAG	C1-O5-C5	3.16	116.47	112.19
4	P	2	NAG	C1-O5-C5	3.13	116.44	112.19
2	E	1	NAG	C1-O5-C5	3.03	116.29	112.19
3	R	3	BMA	C1-O5-C5	2.99	116.25	112.19
3	R	2	NAG	C2-N2-C7	2.96	127.12	122.90
4	H	1	NAG	O5-C1-C2	-2.96	106.62	111.29
4	T	2	NAG	C1-O5-C5	2.94	116.18	112.19
3	M	2	NAG	C2-N2-C7	2.92	127.05	122.90
4	N	2	NAG	C1-O5-C5	2.91	116.14	112.19
2	J	4	MAN	C1-C2-C3	2.90	113.23	109.67
4	Q	1	NAG	O5-C1-C2	-2.90	106.71	111.29
4	L	1	NAG	O5-C1-C2	-2.89	106.73	111.29
2	G	3	BMA	C1-O5-C5	2.86	116.07	112.19
4	S	2	NAG	C2-N2-C7	2.83	126.93	122.90
2	V	1	NAG	C2-N2-C7	2.78	126.86	122.90
4	U	1	NAG	C1-O5-C5	2.74	115.91	112.19
2	J	4	MAN	C1-O5-C5	2.74	115.90	112.19
4	U	1	NAG	O5-C1-C2	-2.73	106.98	111.29
2	E	3	BMA	C1-O5-C5	2.71	115.87	112.19
4	N	2	NAG	C2-N2-C7	2.71	126.76	122.90
2	G	2	NAG	C1-C2-N2	2.66	115.03	110.49
2	J	2	NAG	O5-C1-C2	2.64	115.46	111.29
2	O	2	NAG	O5-C1-C2	-2.63	107.14	111.29
4	L	1	NAG	C1-O5-C5	2.60	115.72	112.19
2	E	4	MAN	C1-O5-C5	2.60	115.71	112.19
2	G	4	MAN	C1-C2-C3	2.59	112.85	109.67
4	T	2	NAG	C2-N2-C7	2.58	126.58	122.90
4	S	2	NAG	C1-C2-N2	2.53	114.81	110.49
4	K	1	NAG	O4-C4-C3	2.52	116.18	110.35
4	S	2	NAG	C1-O5-C5	2.50	115.58	112.19
2	E	4	MAN	C1-C2-C3	2.46	112.69	109.67
2	O	2	NAG	C1-C2-N2	2.46	114.68	110.49
4	N	1	NAG	C1-O5-C5	2.45	115.50	112.19
2	V	1	NAG	O5-C1-C2	2.39	115.06	111.29
2	O	2	NAG	C2-N2-C7	2.37	126.28	122.90
2	V	2	NAG	C1-O5-C5	2.36	115.39	112.19
2	E	1	NAG	C3-C4-C5	2.36	114.44	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	C3-C4-C5	2.36	114.44	110.24
2	V	4	MAN	C1-C2-C3	2.27	112.46	109.67
4	S	1	NAG	C2-N2-C7	2.26	126.13	122.90
2	V	4	MAN	C1-O5-C5	2.26	115.25	112.19
4	Q	1	NAG	C1-O5-C5	2.24	115.22	112.19
2	V	1	NAG	C1-C2-N2	2.21	114.26	110.49
2	G	1	NAG	O5-C1-C2	-2.16	107.87	111.29
3	F	2	NAG	O5-C1-C2	-2.14	107.91	111.29
3	M	2	NAG	C1-O5-C5	2.14	115.09	112.19
3	I	2	NAG	C1-O5-C5	2.13	115.08	112.19
2	J	2	NAG	C1-C2-N2	-2.10	106.89	110.49
3	I	3	BMA	C1-O5-C5	2.10	115.04	112.19
3	I	2	NAG	O5-C1-C2	-2.00	108.12	111.29
2	G	2	NAG	C1-O5-C5	2.00	114.90	112.19

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	V	3	BMA	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
4	N	2	NAG	C1-C2-N2-C7
2	O	3	BMA	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
2	O	3	BMA	C4-C5-C6-O6
3	I	1	NAG	C1-C2-N2-C7
3	R	1	NAG	C1-C2-N2-C7
3	F	2	NAG	C4-C5-C6-O6
2	O	1	NAG	C1-C2-N2-C7
3	M	2	NAG	C1-C2-N2-C7
4	T	1	NAG	C4-C5-C6-O6
2	G	3	BMA	C4-C5-C6-O6
2	V	3	BMA	C4-C5-C6-O6
4	T	2	NAG	C1-C2-N2-C7
2	G	3	BMA	O5-C5-C6-O6
2	G	4	MAN	O5-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6

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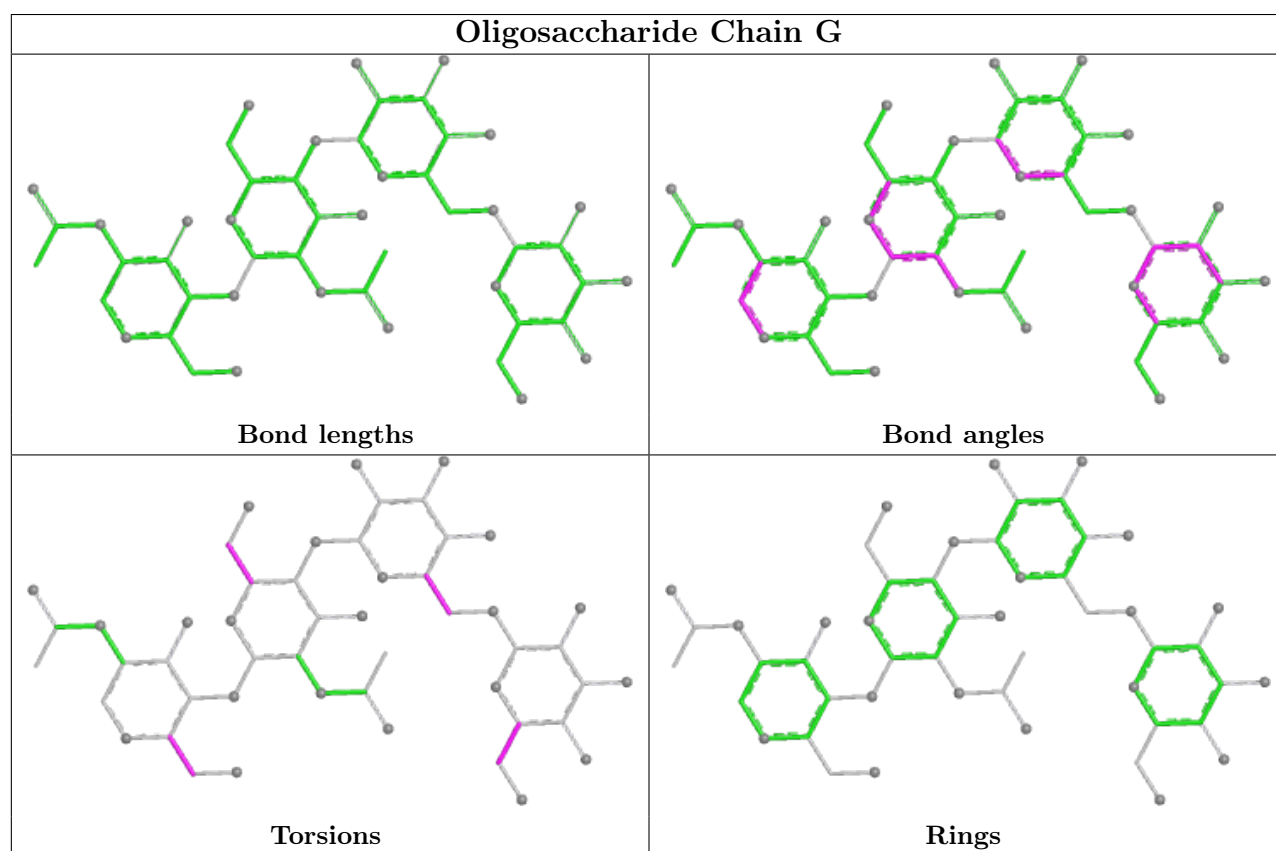
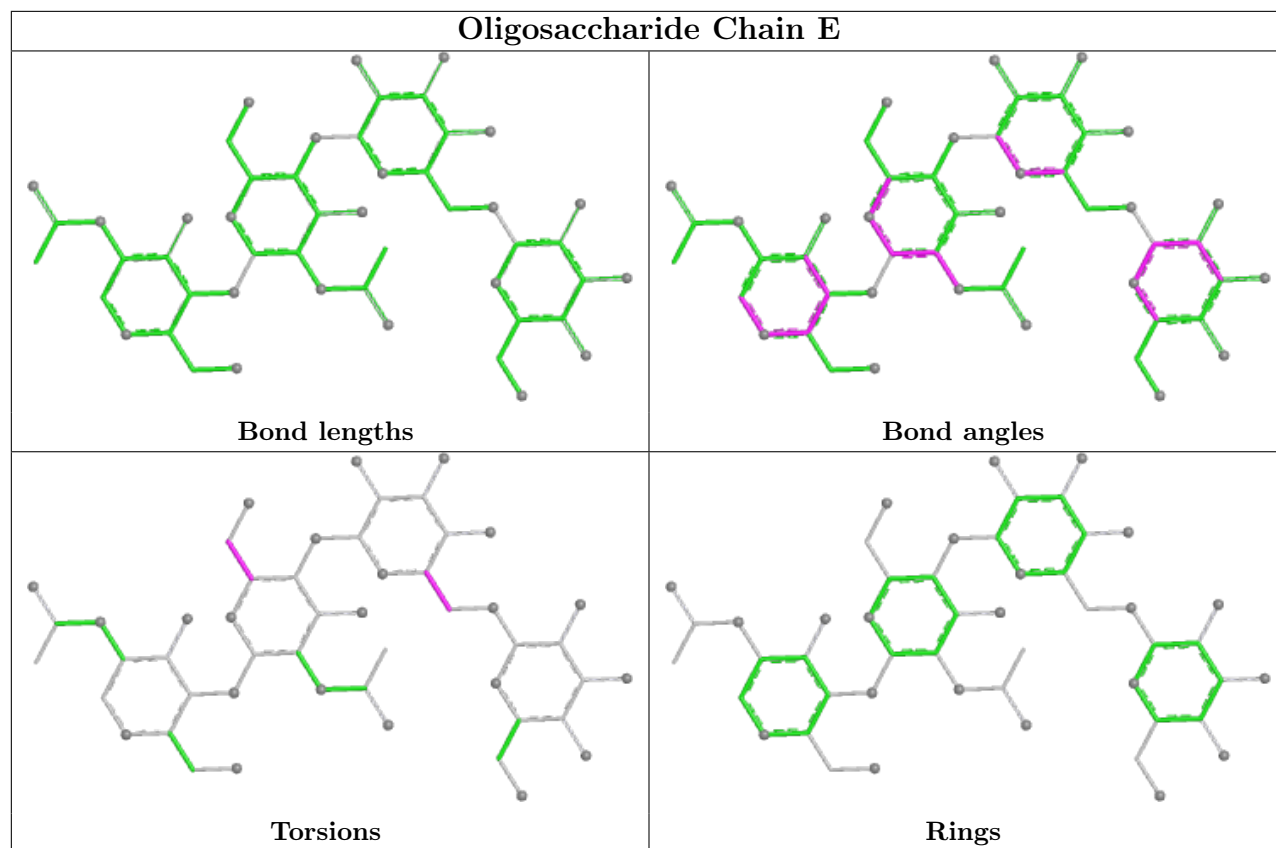
Mol	Chain	Res	Type	Atoms
4	N	2	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	V	1	NAG	C3-C2-N2-C7
2	G	2	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
3	R	2	NAG	C1-C2-N2-C7
4	S	2	NAG	C1-C2-N2-C7
2	G	2	NAG	O5-C5-C6-O6
4	L	2	NAG	C1-C2-N2-C7
2	O	2	NAG	C3-C2-N2-C7
4	H	2	NAG	C4-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	J	3	BMA	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
3	R	2	NAG	C3-C2-N2-C7
4	S	1	NAG	C3-C2-N2-C7

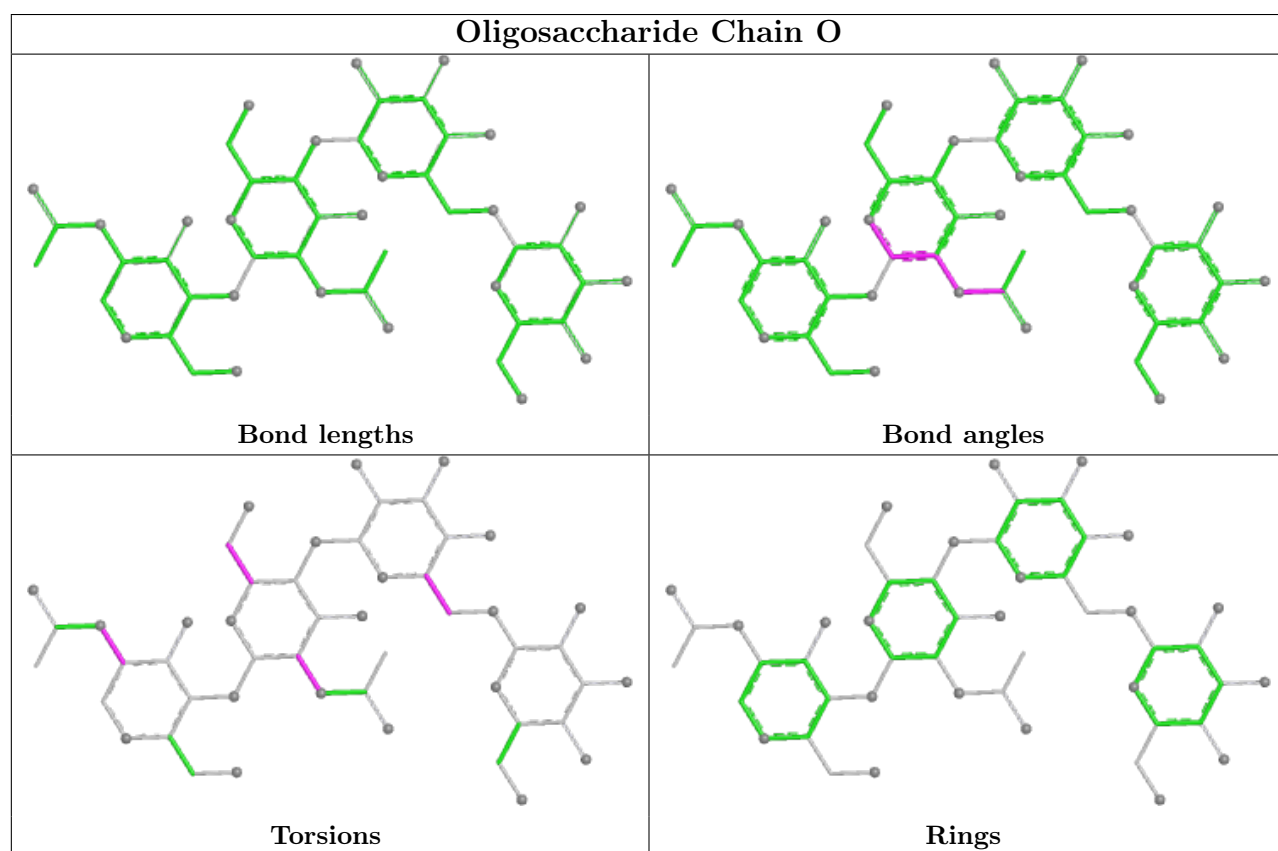
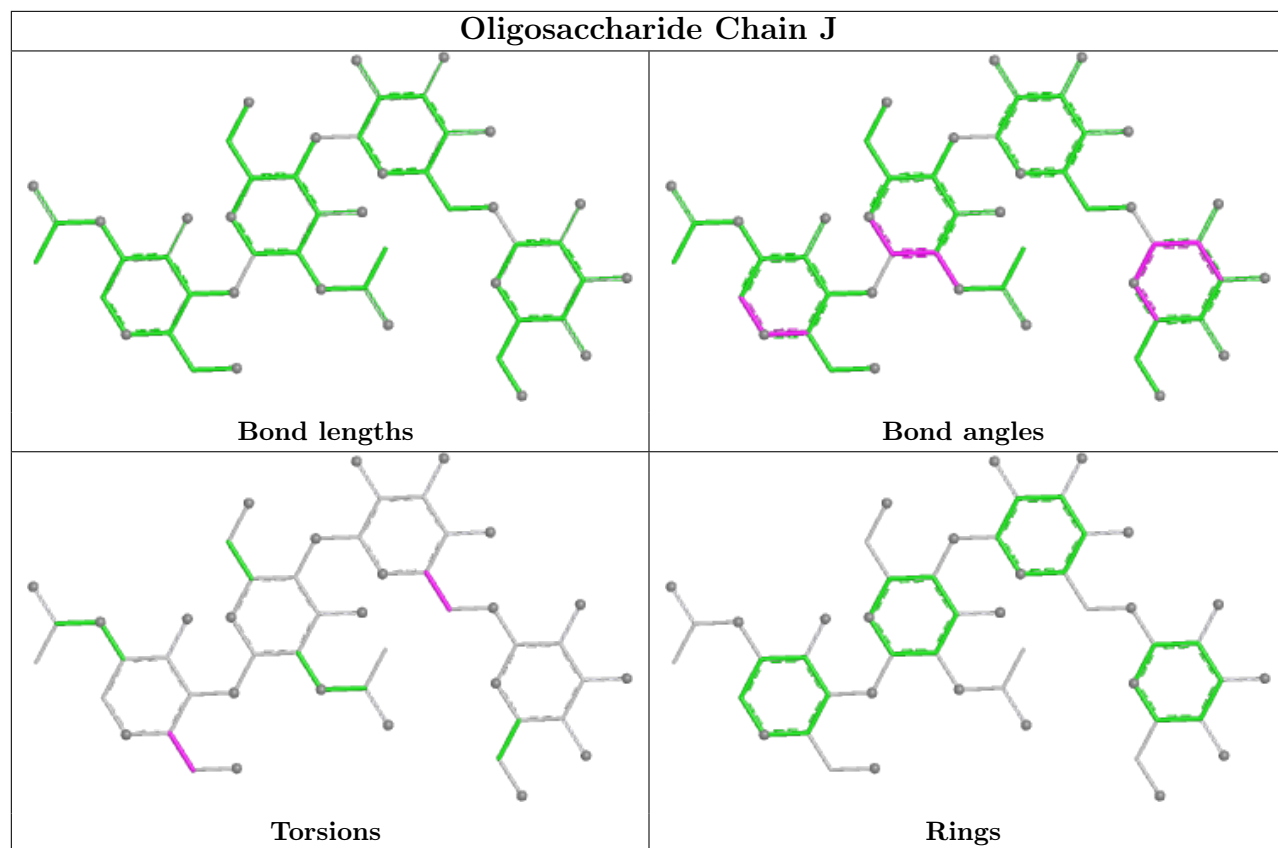
There are no ring outliers.

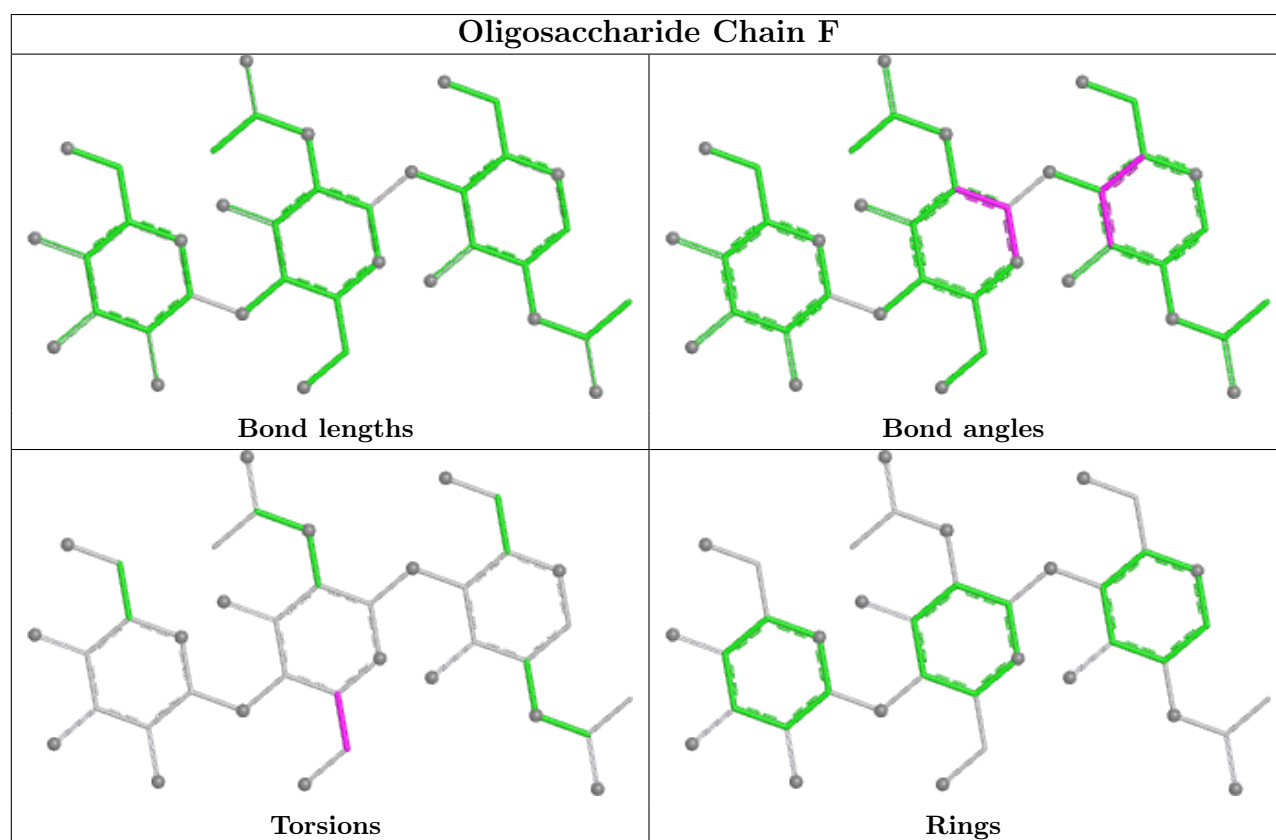
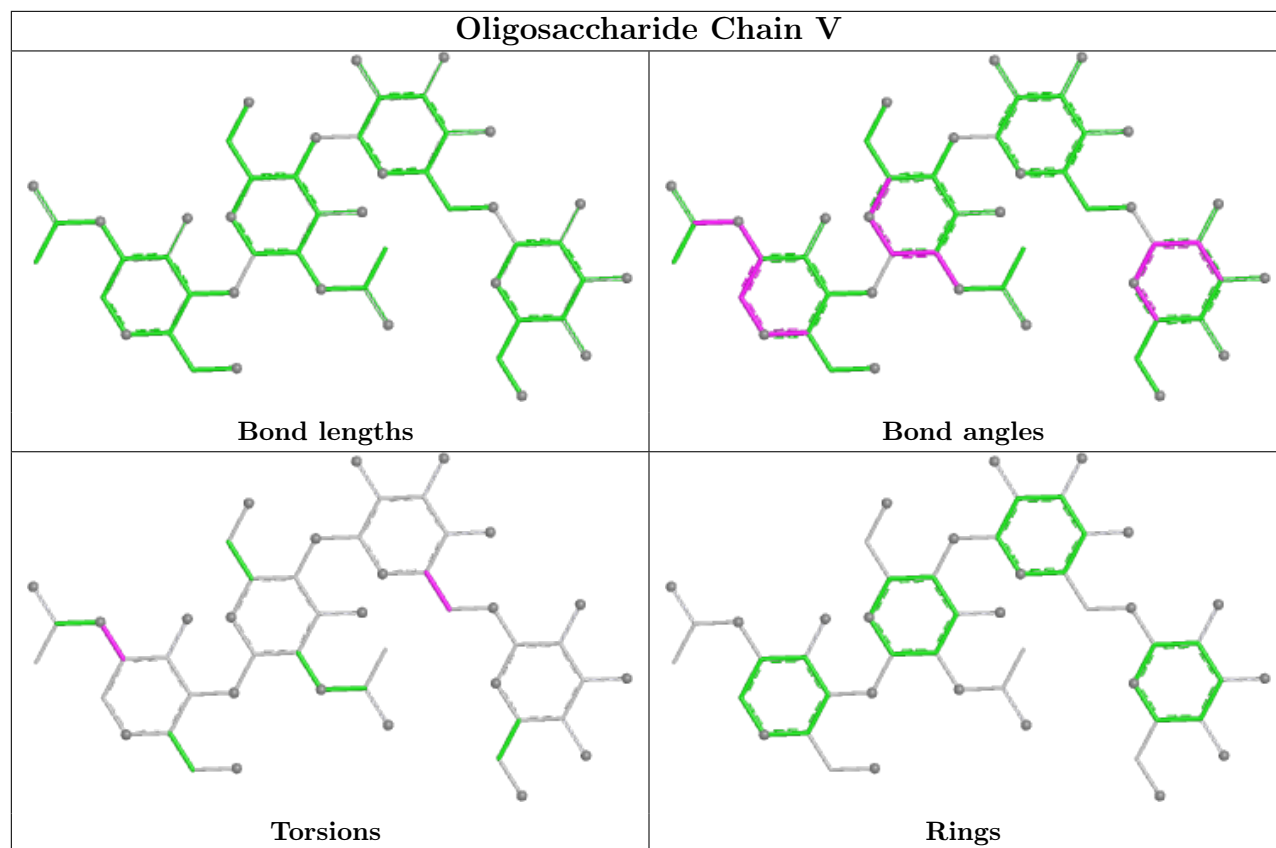
7 monomers are involved in 4 short contacts:

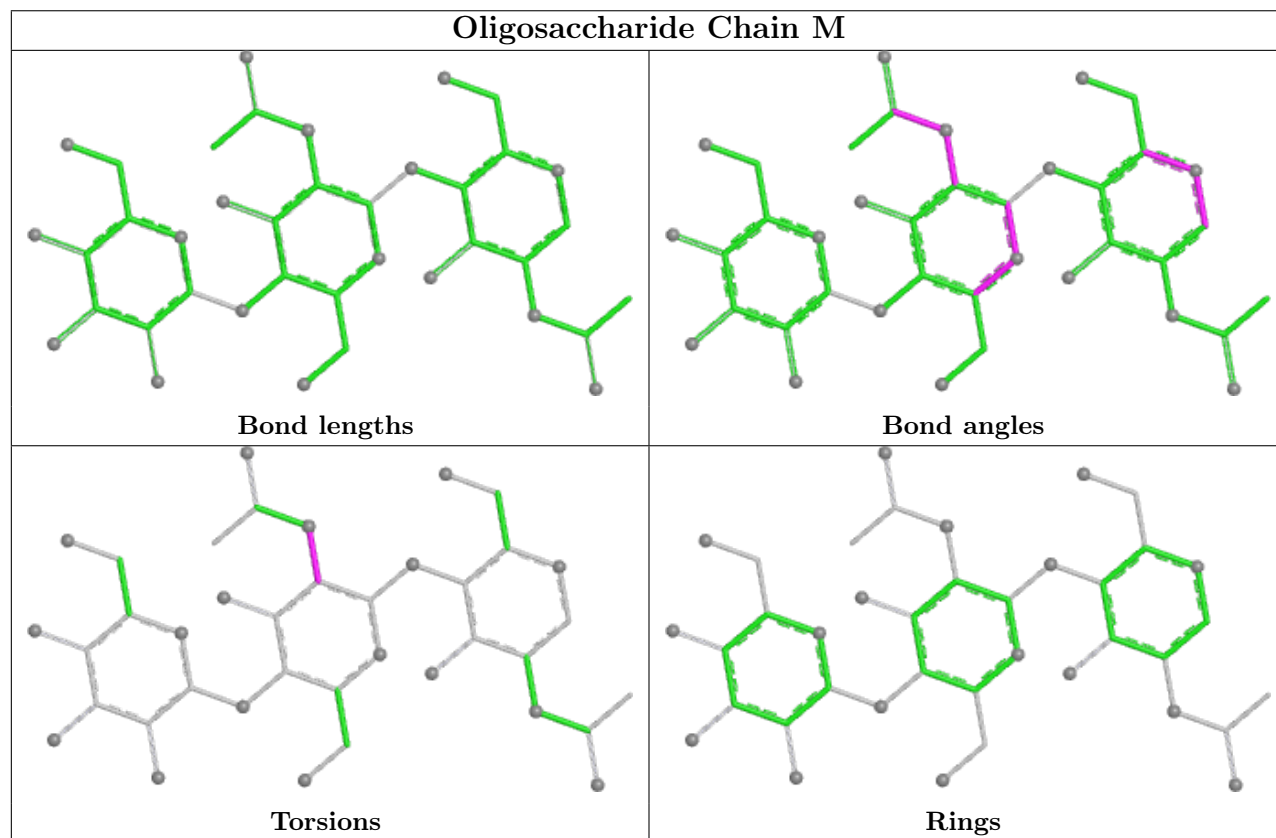
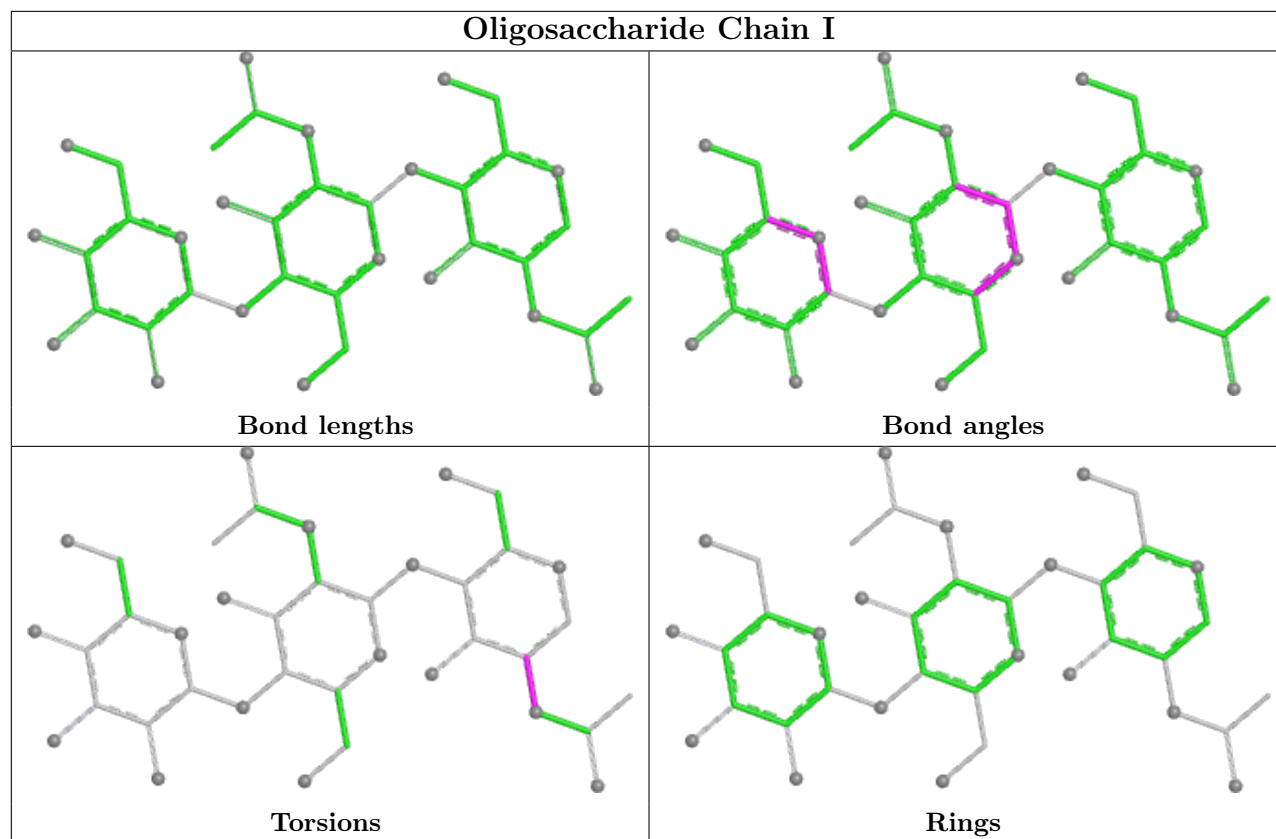
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	NAG	1	0
2	E	2	NAG	1	0
2	G	1	NAG	1	0
3	R	1	NAG	1	0
2	E	1	NAG	1	0
4	S	1	NAG	1	0
3	R	2	NAG	1	0

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

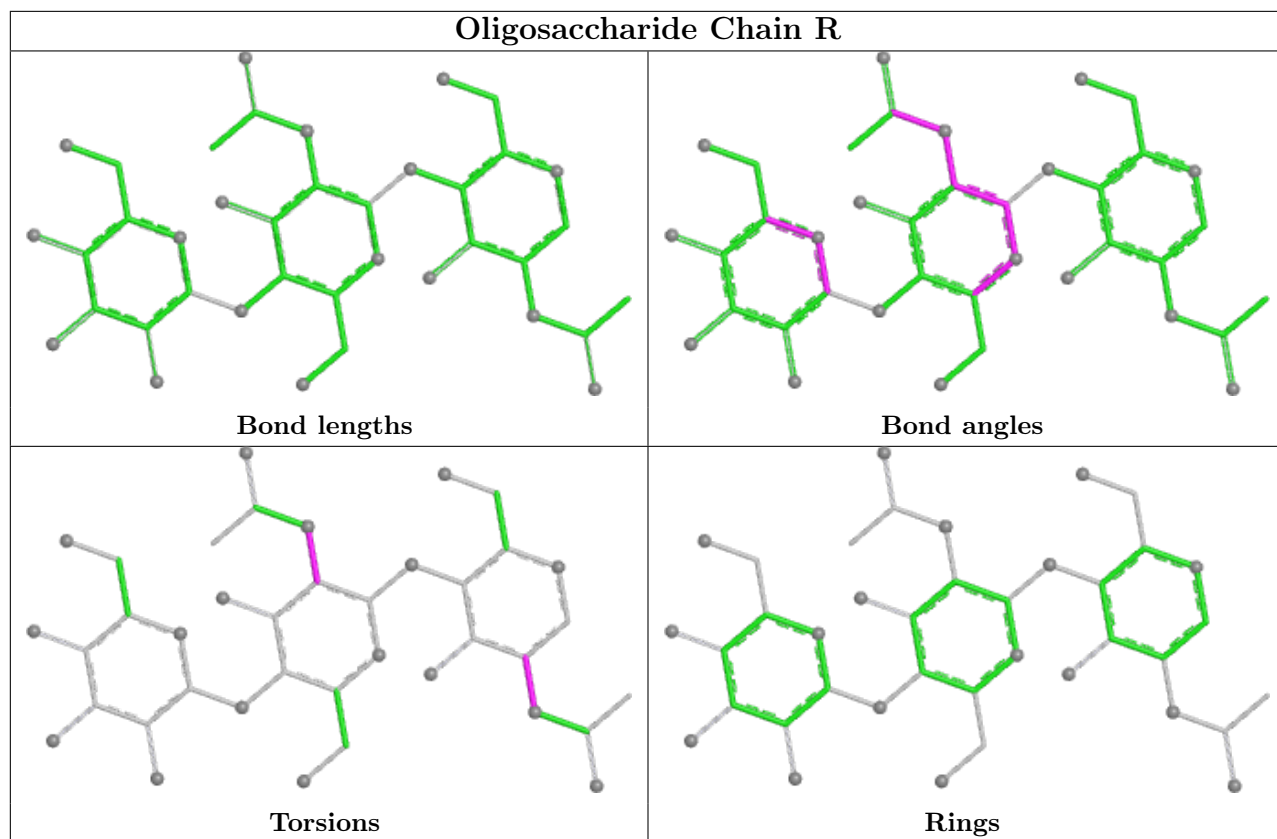


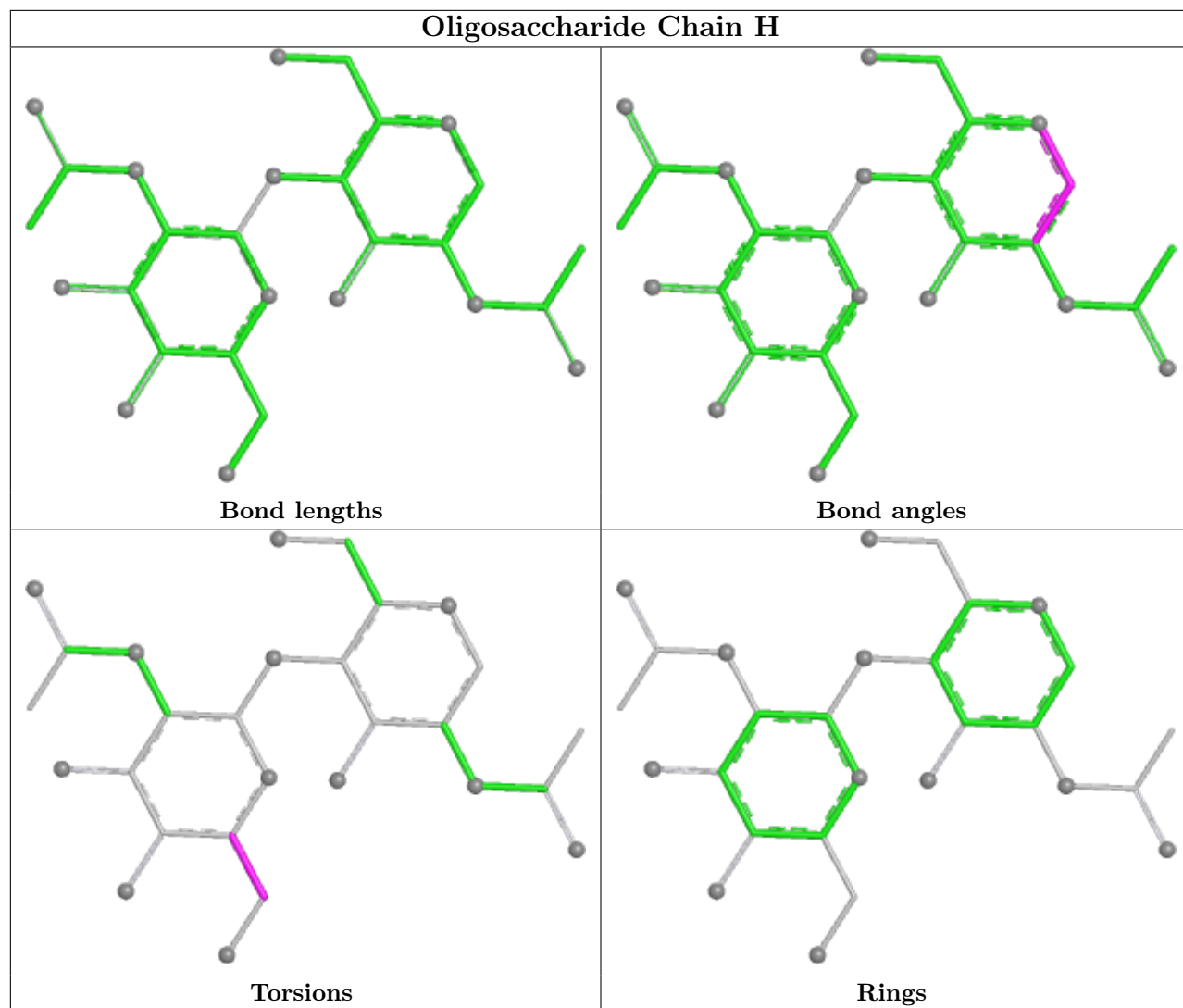


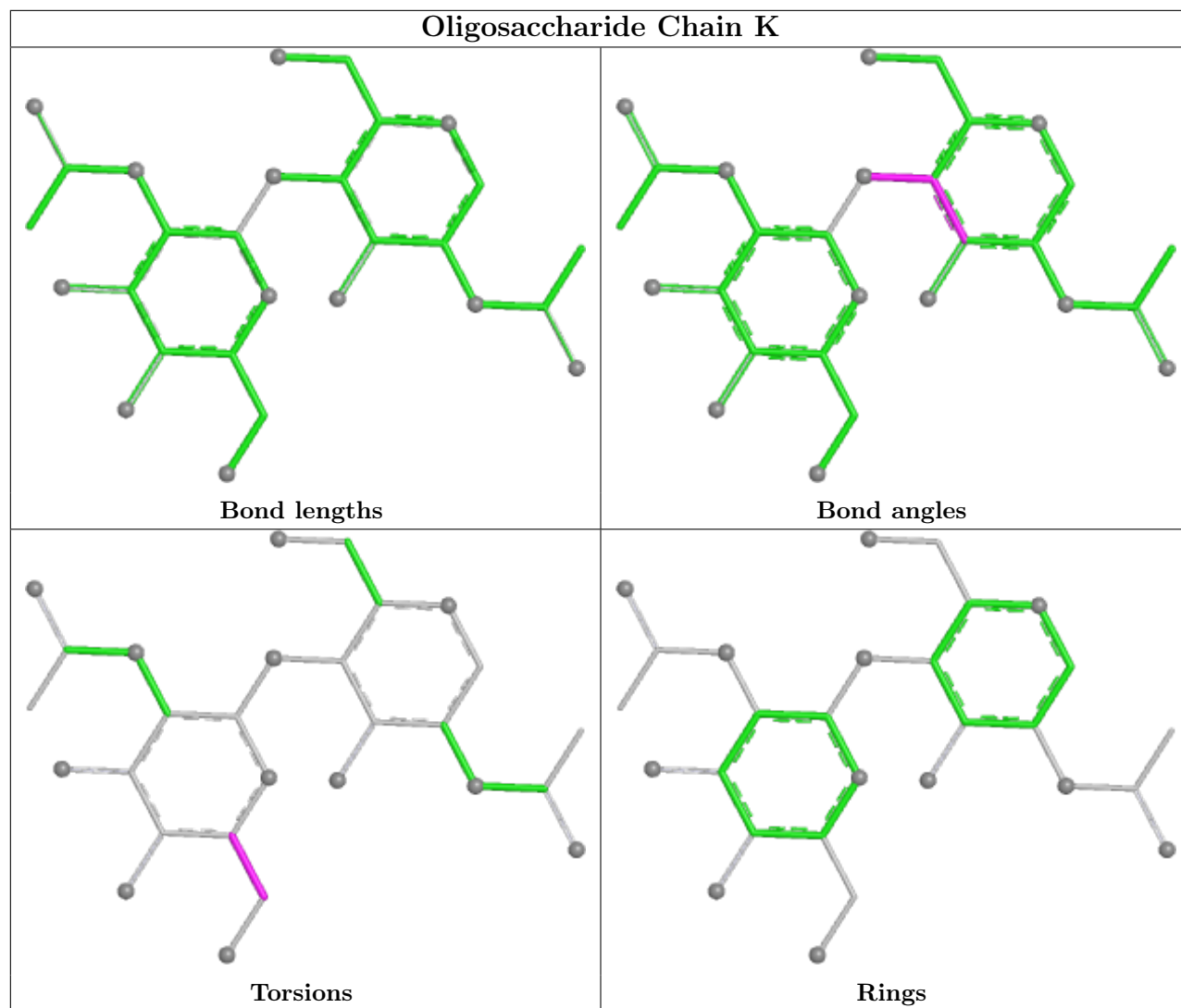


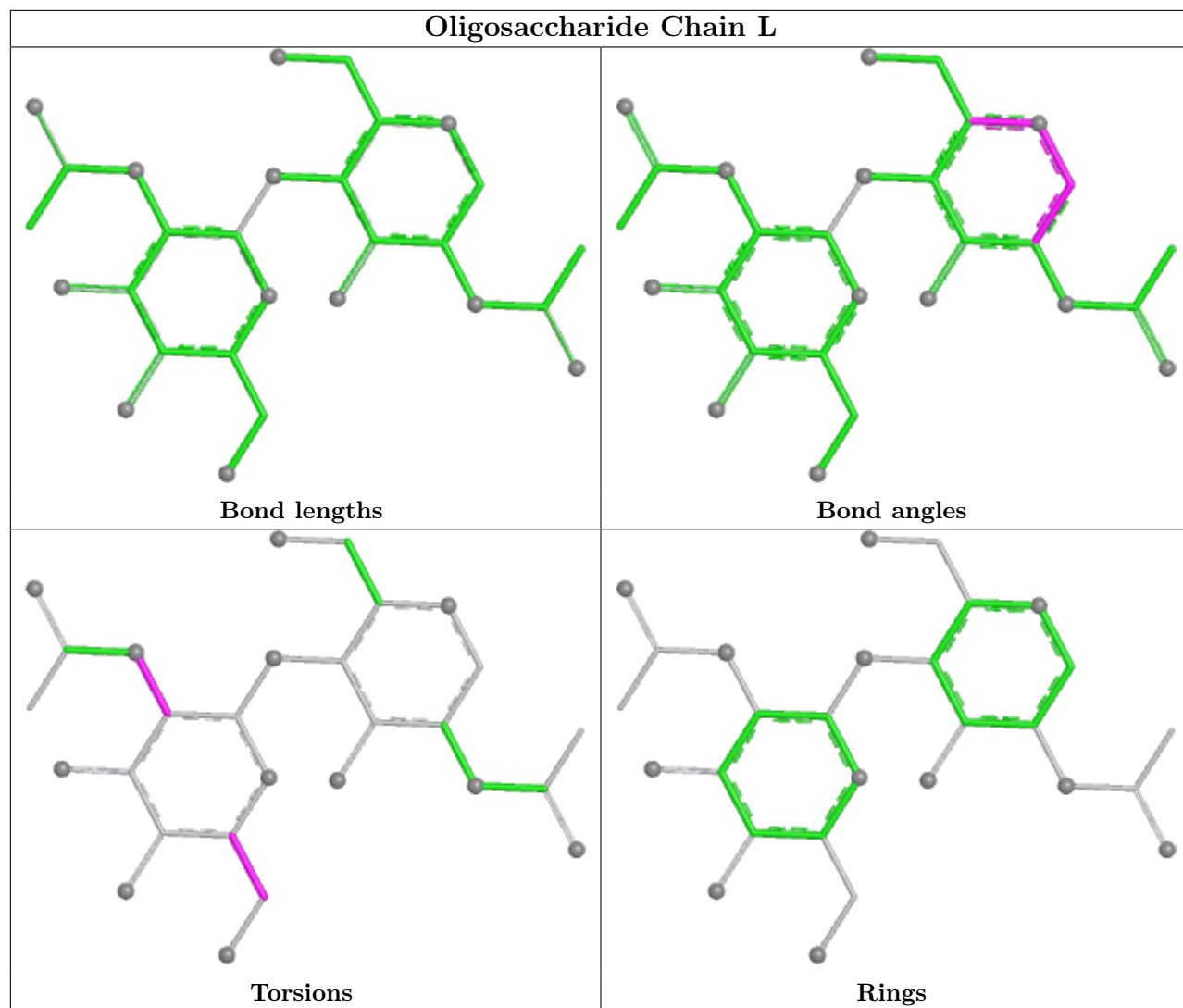


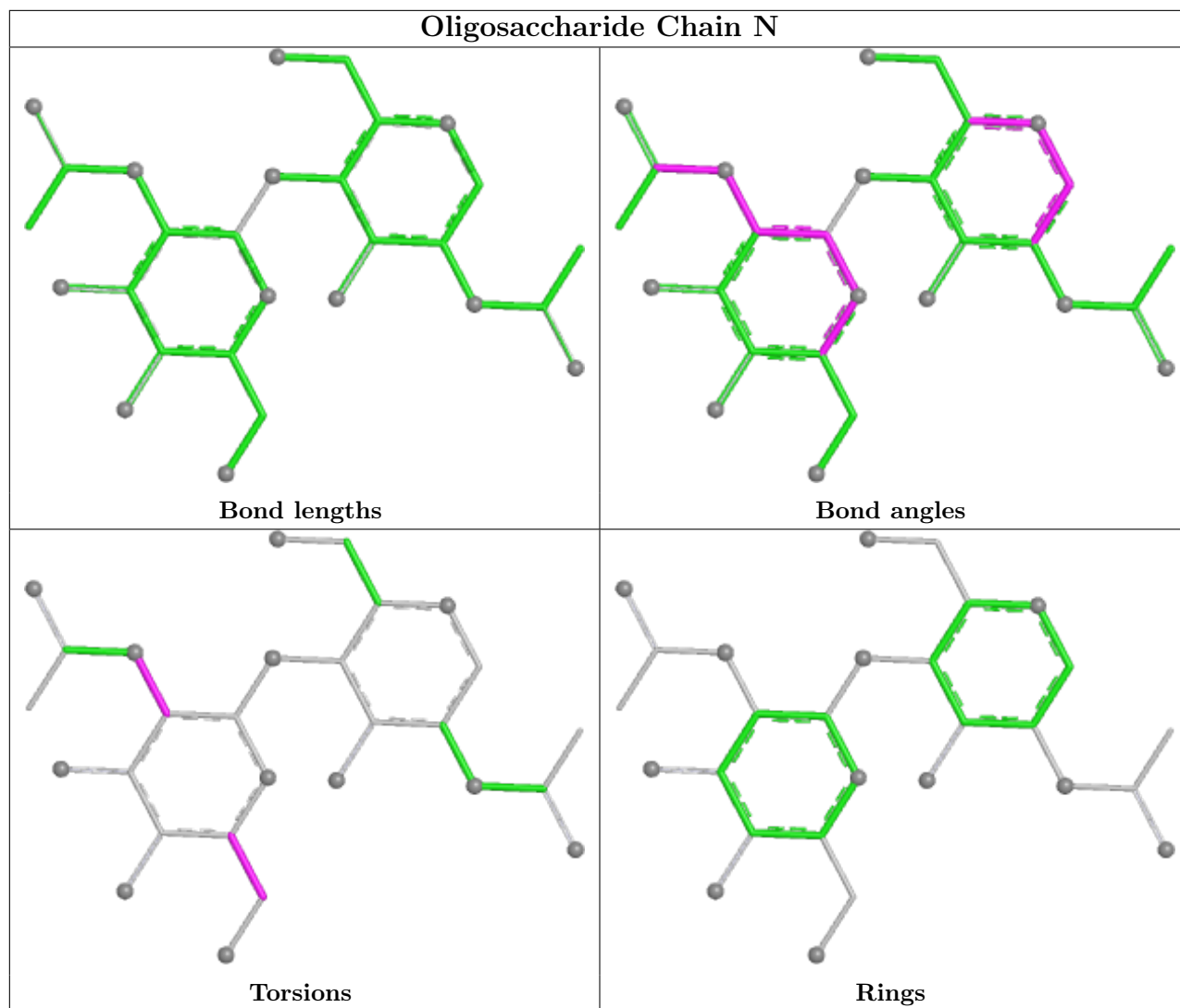


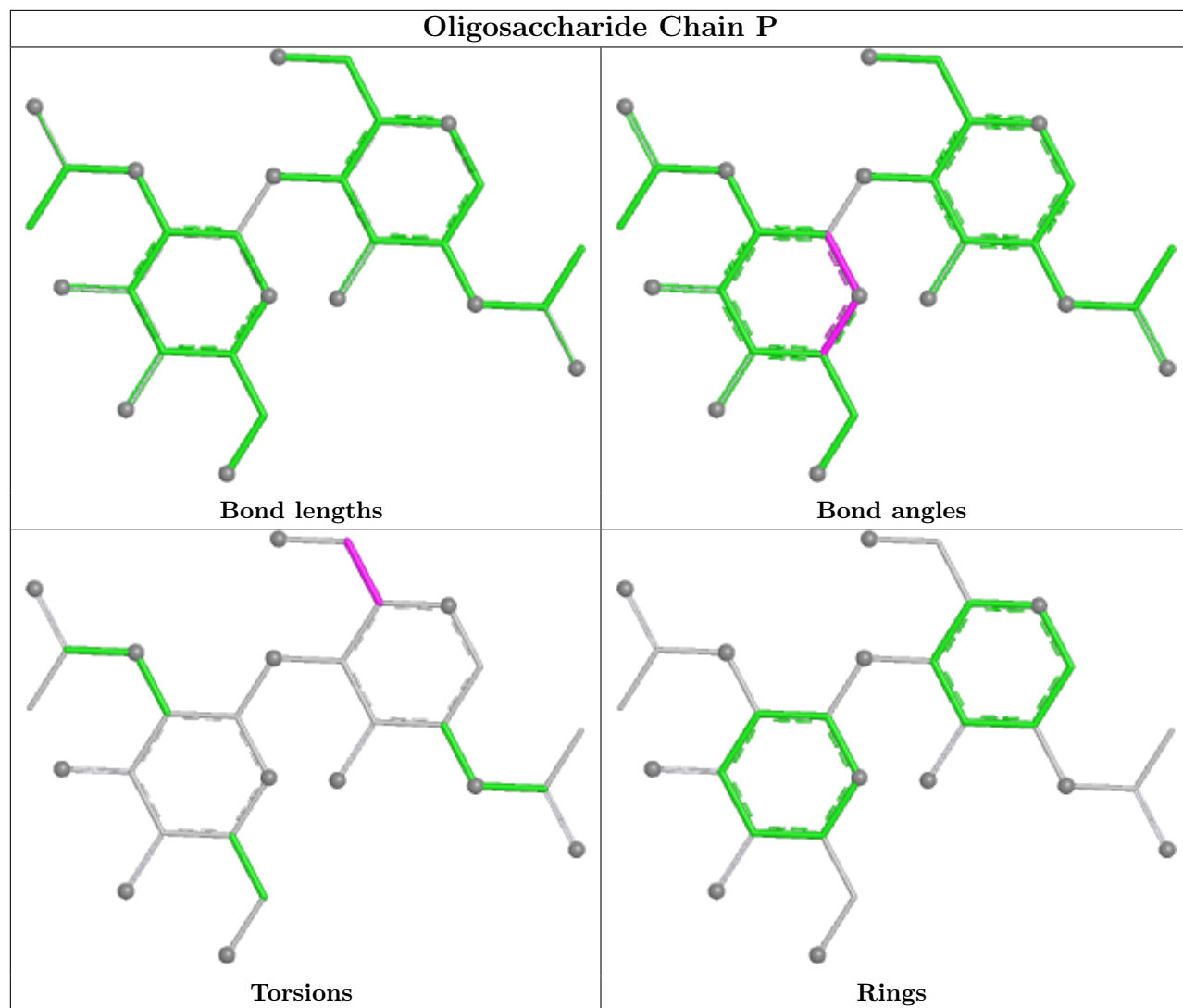


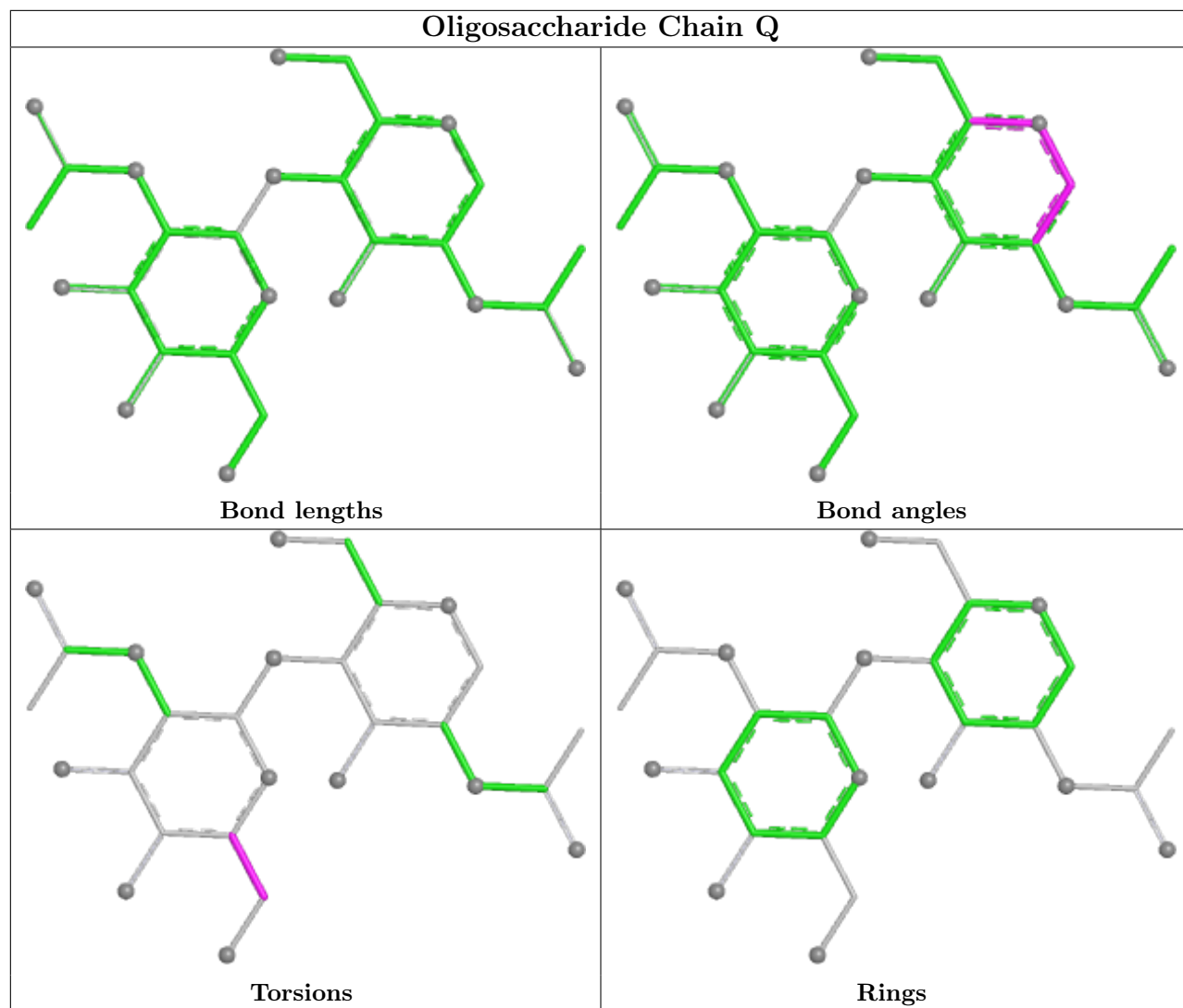


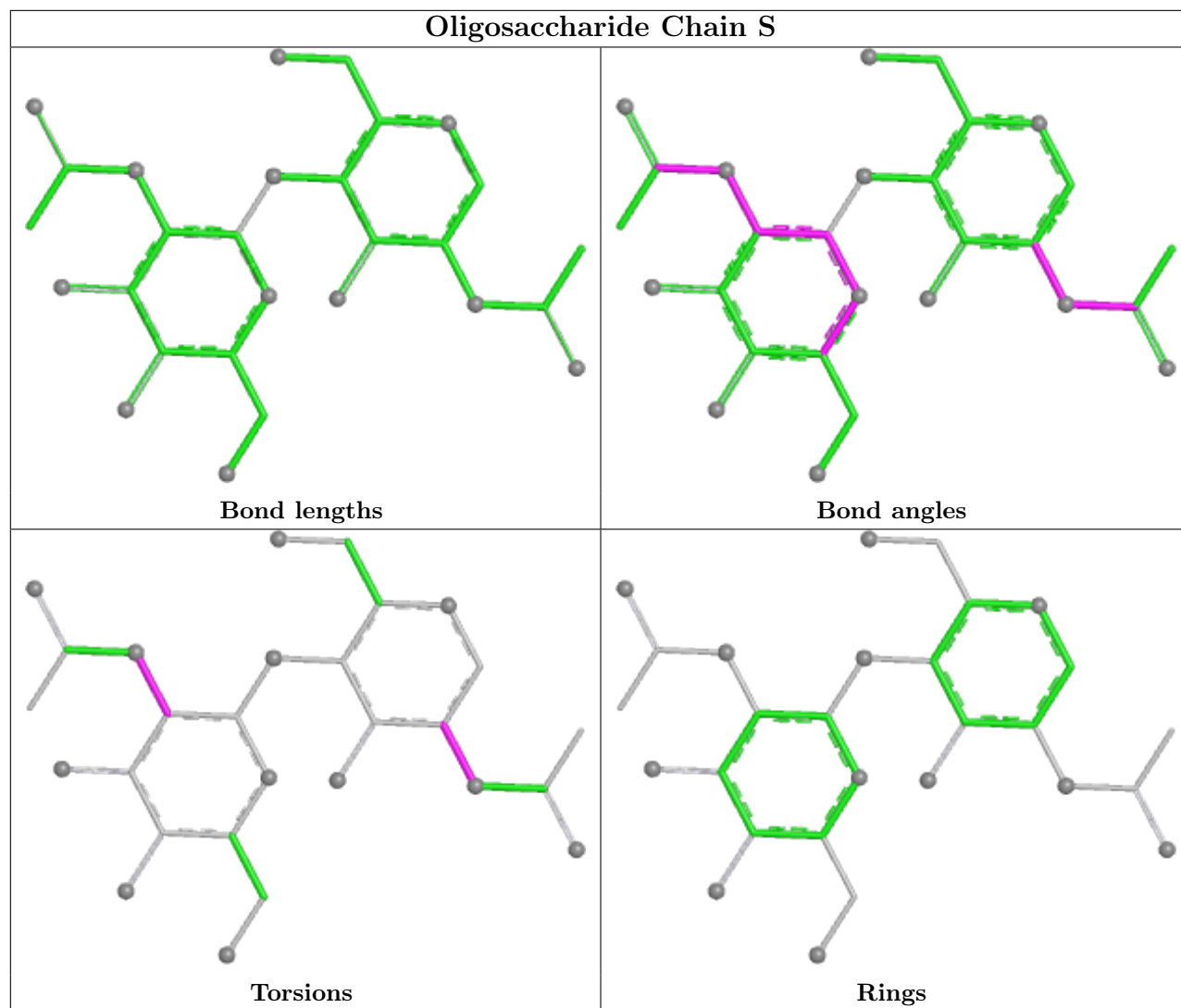




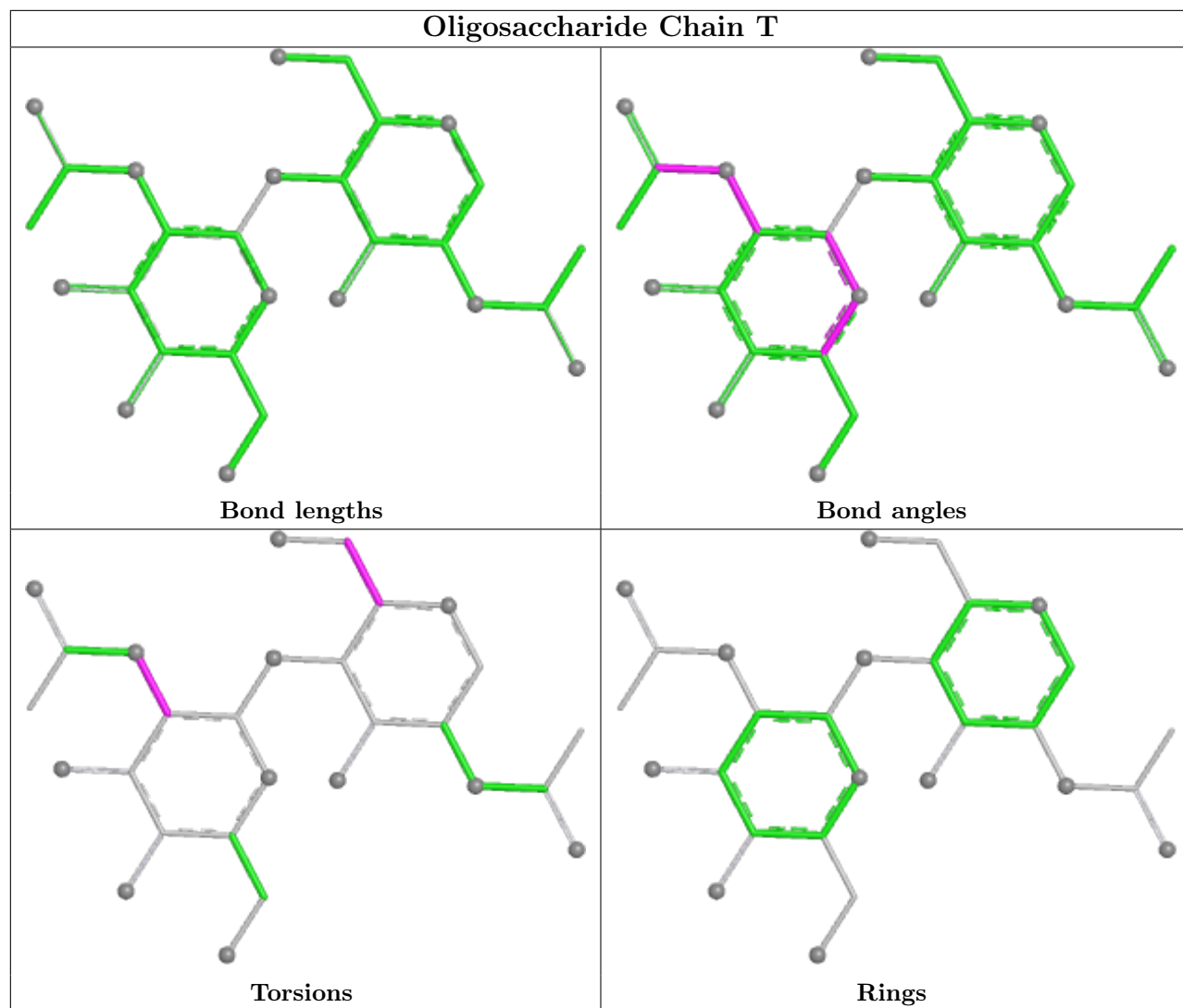


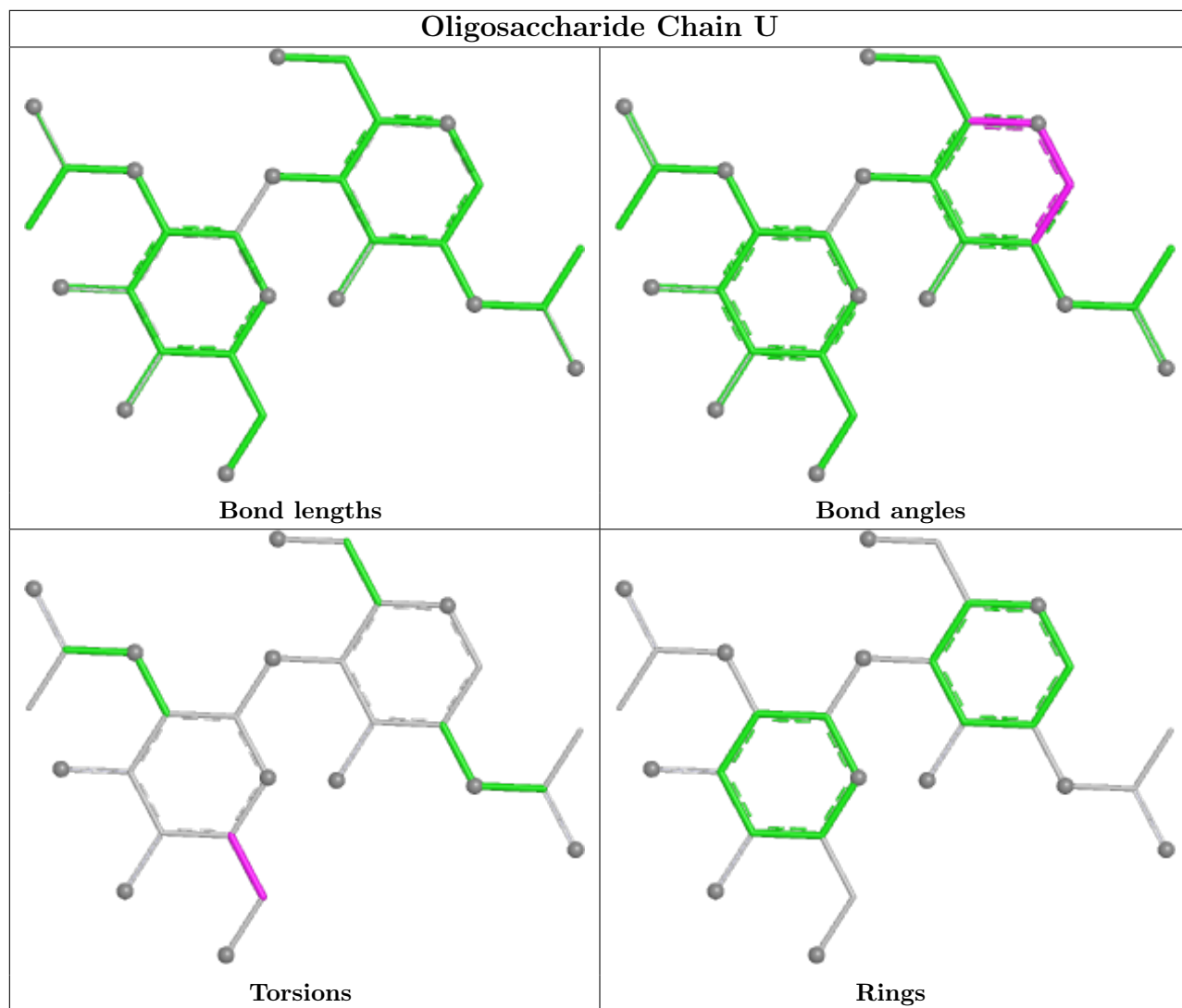












## 5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	D	2007	1	14,14,15	0.36	0	17,19,21	0.53	0
5	NAG	C	2004	1	14,14,15	0.41	0	17,19,21	0.75	0
5	NAG	D	2004	1	14,14,15	0.44	0	17,19,21	1.07	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	C	2001	1	14,14,15	0.43	0	17,19,21	1.50	3 (17%)
5	NAG	A	2019	1	14,14,15	0.49	0	17,19,21	1.43	2 (11%)
5	NAG	D	2003	1	14,14,15	0.45	0	17,19,21	0.82	0
5	NAG	A	2008	1	14,14,15	0.36	0	17,19,21	0.69	0
5	NAG	B	2012	1	14,14,15	0.48	0	17,19,21	1.24	3 (17%)
5	NAG	A	2013	1	14,14,15	0.40	0	17,19,21	0.48	0
5	NAG	C	2002	1	14,14,15	0.38	0	17,19,21	0.70	0
5	NAG	C	2003	1	14,14,15	0.34	0	17,19,21	0.57	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
5	NAG	D	2007	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2004	1	-	2/6/23/26	0/1/1/1
5	NAG	D	2004	1	-	1/6/23/26	0/1/1/1
5	NAG	C	2001	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2019	1	-	1/6/23/26	0/1/1/1
5	NAG	D	2003	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2008	1	-	0/6/23/26	0/1/1/1
5	NAG	B	2012	1	-	1/6/23/26	0/1/1/1
5	NAG	A	2013	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2002	1	-	0/6/23/26	0/1/1/1
5	NAG	C	2003	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2019	NAG	C1-O5-C5	4.69	118.55	112.19
5	C	2001	NAG	C1-C2-N2	3.65	116.73	110.49
5	C	2001	NAG	O5-C1-C2	-3.41	105.90	111.29
5	C	2001	NAG	C2-N2-C7	3.07	127.27	122.90
5	B	2012	NAG	C2-N2-C7	2.91	127.05	122.90
5	B	2012	NAG	C1-C2-N2	2.89	115.43	110.49
5	A	2019	NAG	C2-N2-C7	2.70	126.74	122.90
5	D	2004	NAG	O5-C1-C2	-2.59	107.20	111.29
5	D	2004	NAG	C1-O5-C5	2.52	115.61	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2012	NAG	O5-C1-C2	-2.24	107.74	111.29
5	D	2004	NAG	C1-C2-N2	2.03	113.95	110.49

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	2007	NAG	O5-C5-C6-O6
5	A	2013	NAG	O5-C5-C6-O6
5	D	2003	NAG	C4-C5-C6-O6
5	D	2007	NAG	C4-C5-C6-O6
5	D	2003	NAG	O5-C5-C6-O6
5	C	2004	NAG	C4-C5-C6-O6
5	D	2004	NAG	O5-C5-C6-O6
5	A	2019	NAG	C3-C2-N2-C7
5	A	2013	NAG	C4-C5-C6-O6
5	C	2004	NAG	O5-C5-C6-O6
5	C	2001	NAG	C3-C2-N2-C7
5	C	2001	NAG	C1-C2-N2-C7
5	B	2012	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.

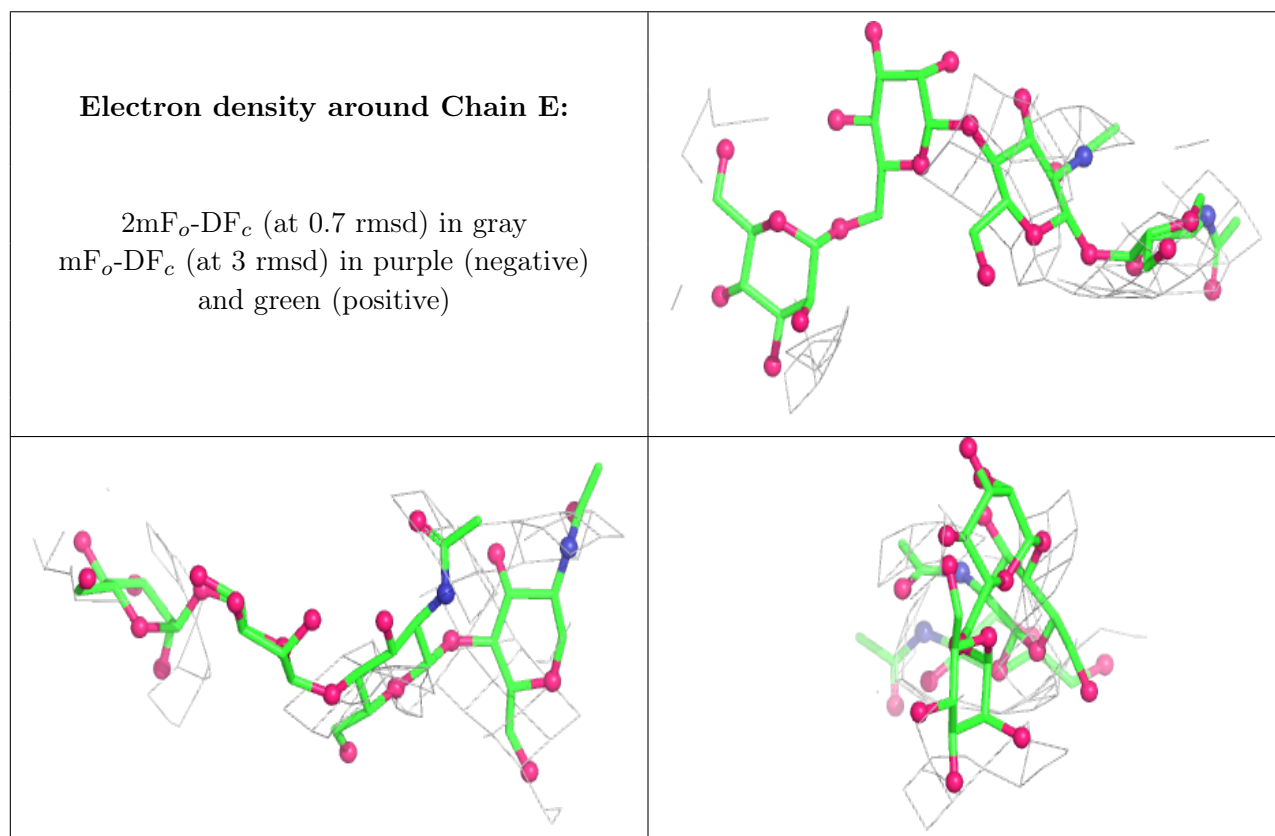
### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

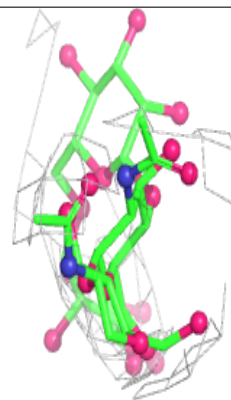
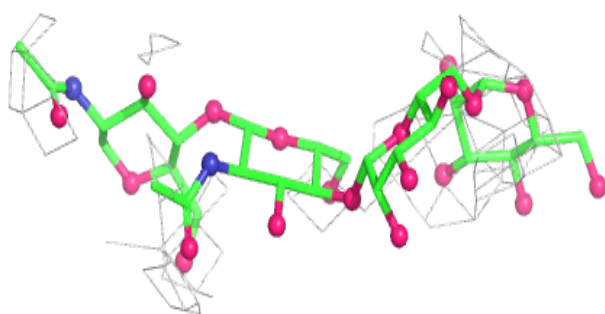
Unable to reproduce the depositor's R factor - this section is therefore empty.

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

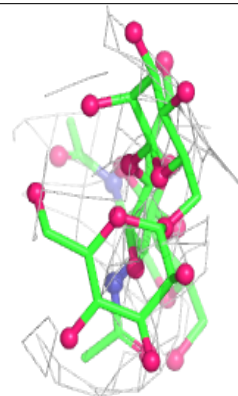
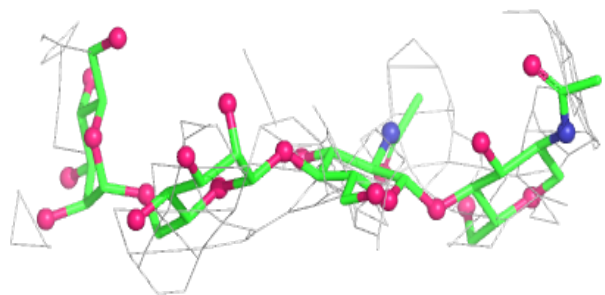
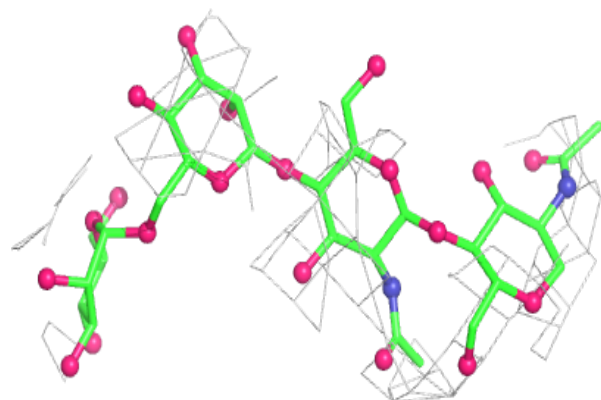


**Electron density around Chain G:**

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

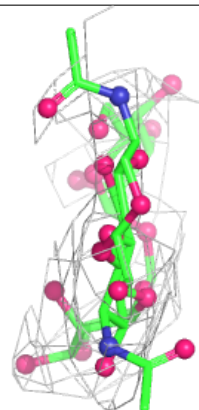
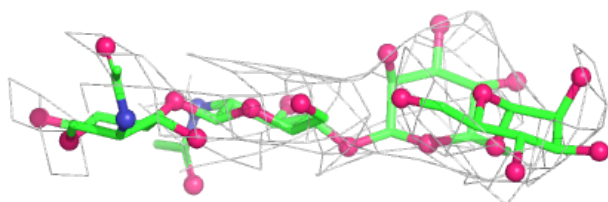
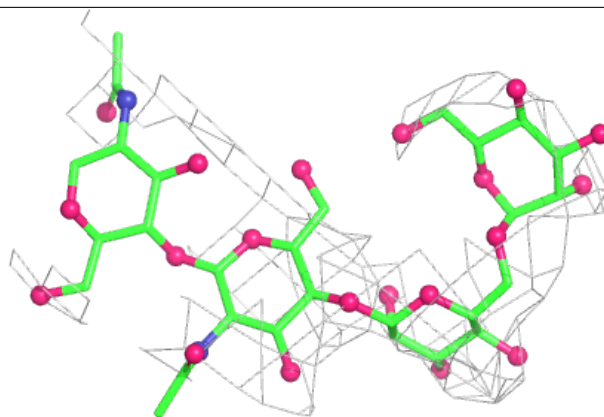
**Electron density around Chain J:**

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

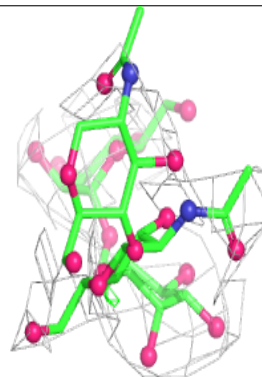
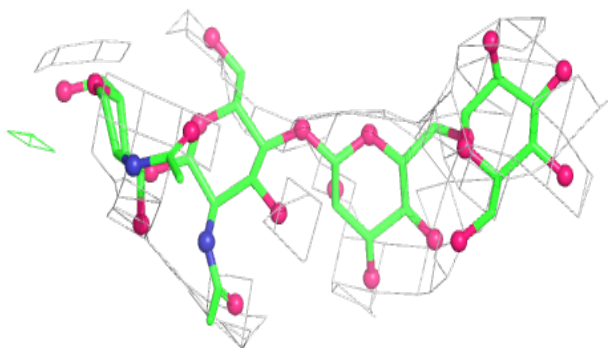
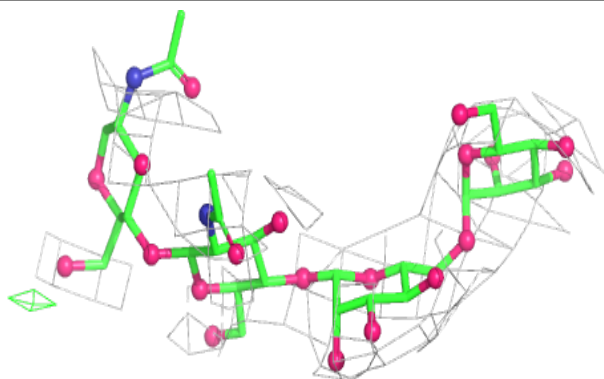


**Electron density around Chain O:**

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

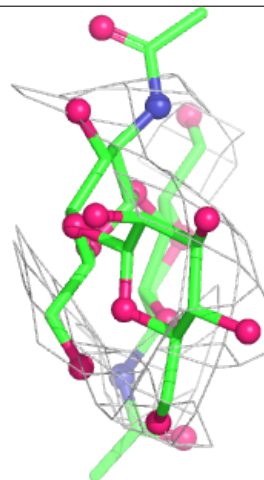
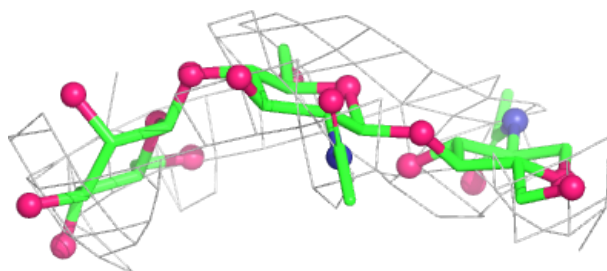
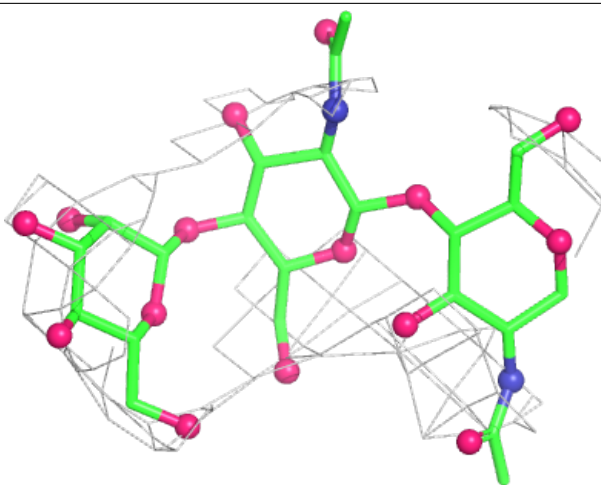
**Electron density around Chain V:**

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

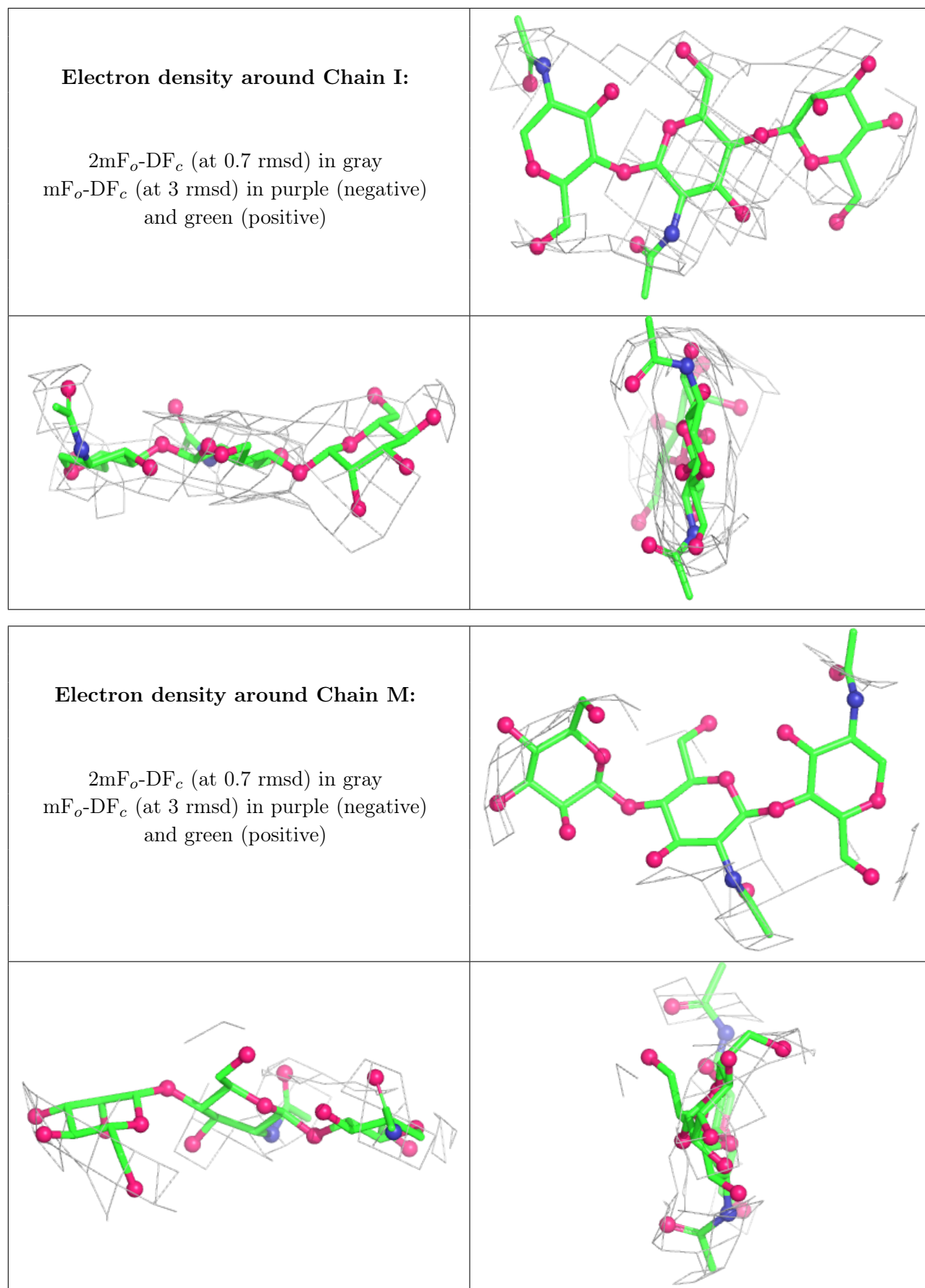


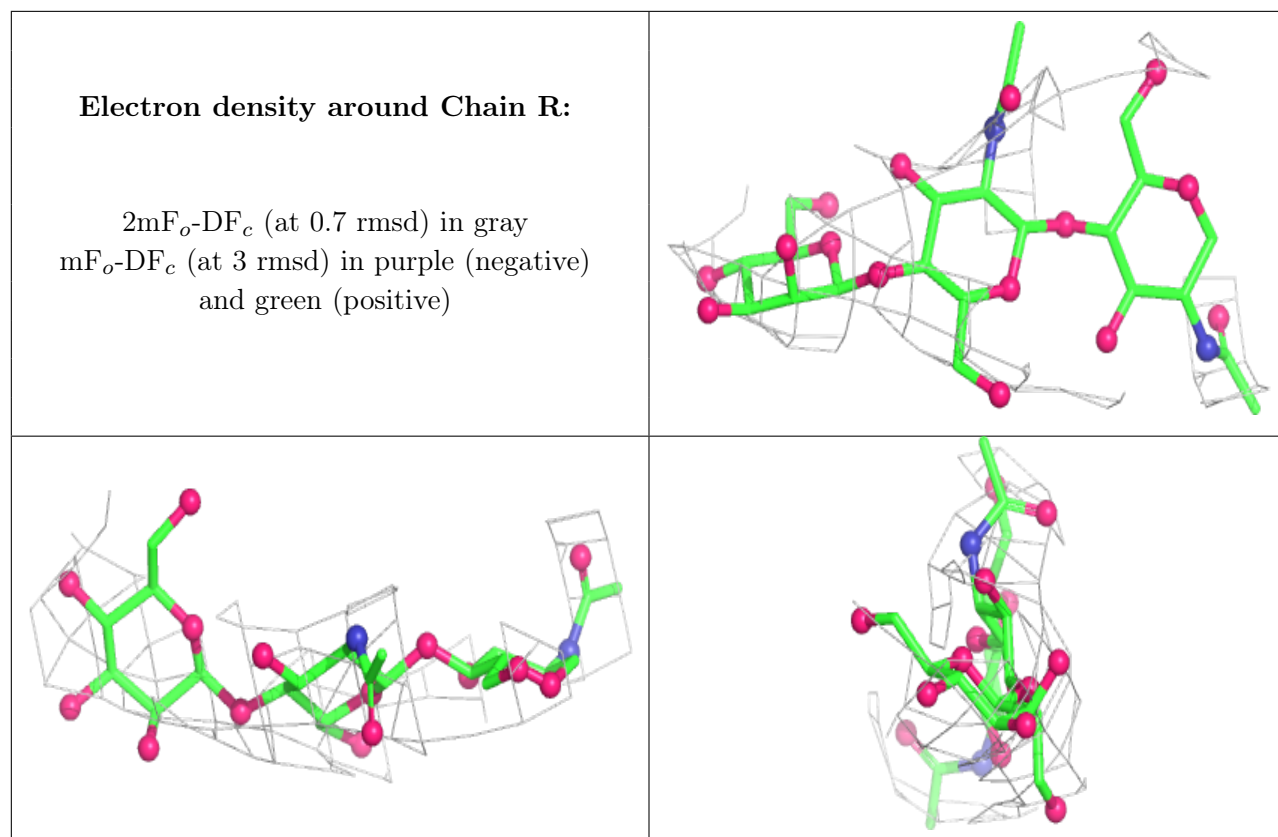
**Electron density around Chain F:**

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



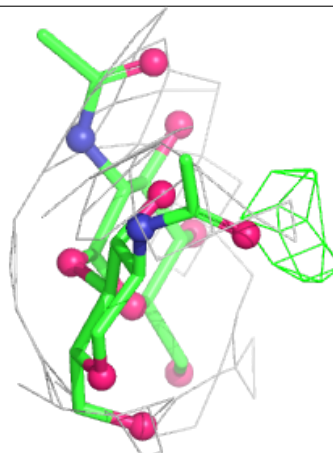
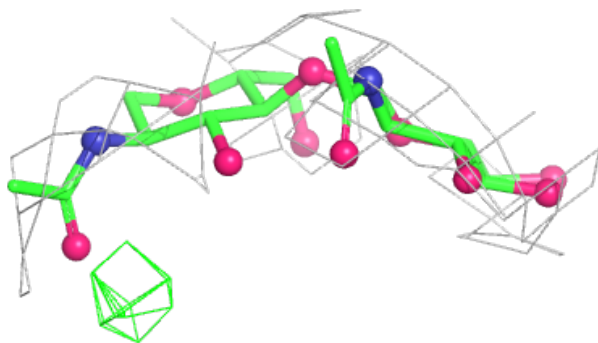
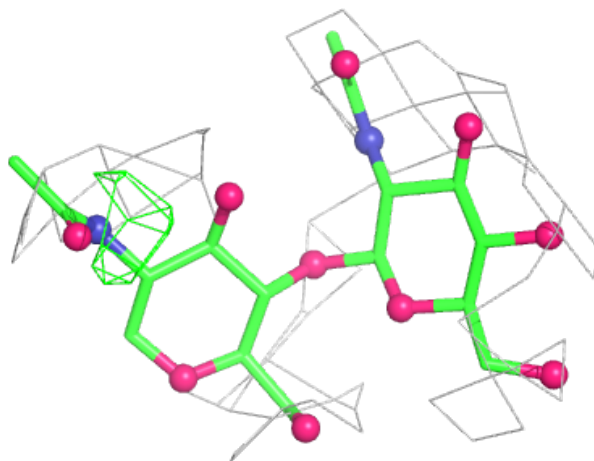






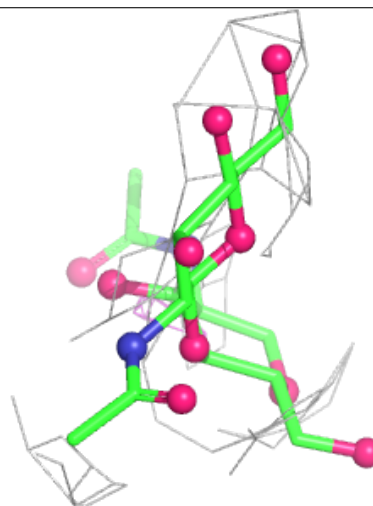
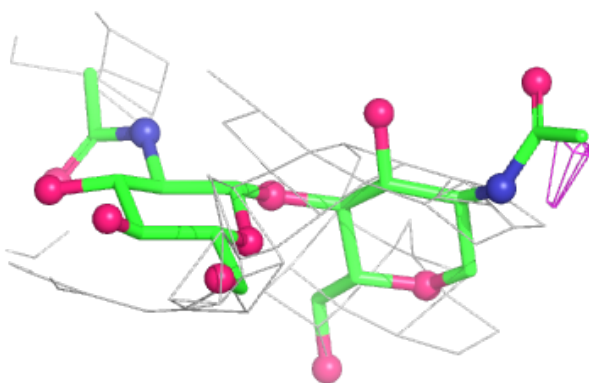
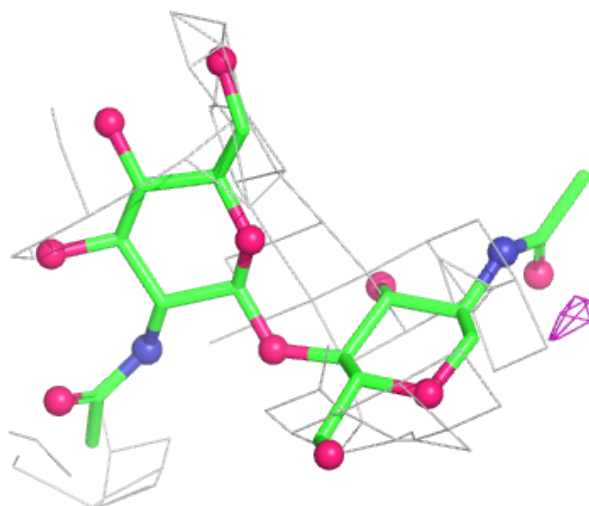
**Electron density around Chain H:**

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



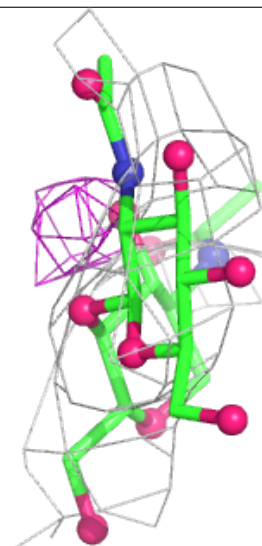
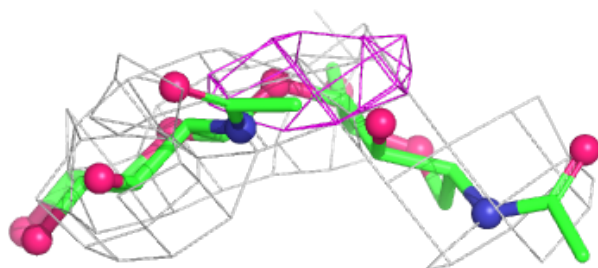
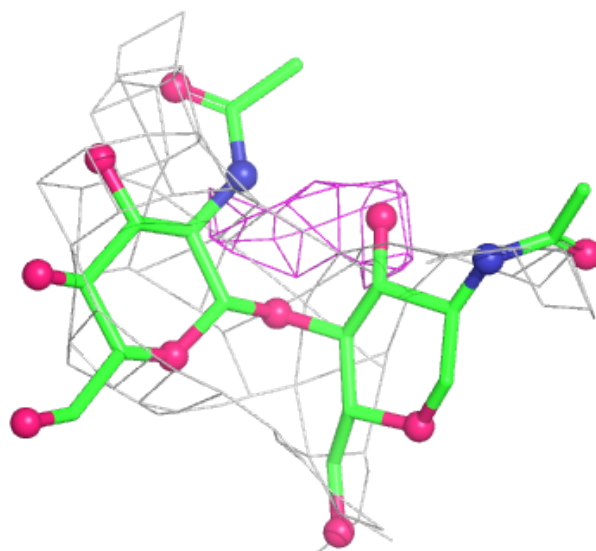
**Electron density around Chain K:**

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



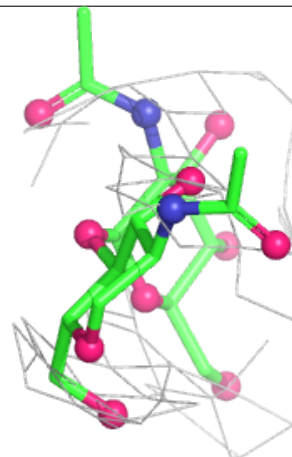
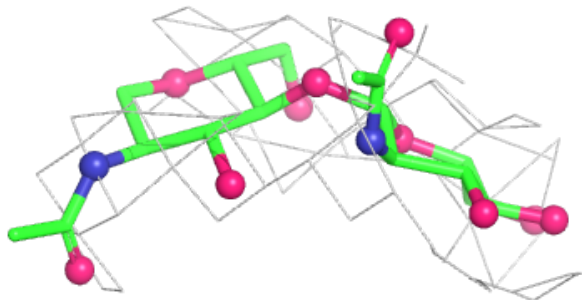
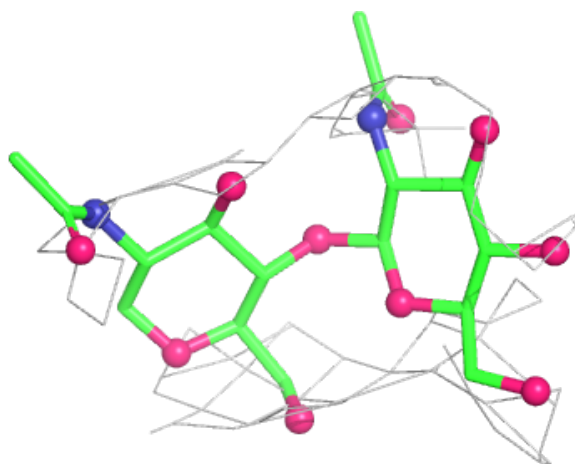
**Electron density around Chain L:**

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



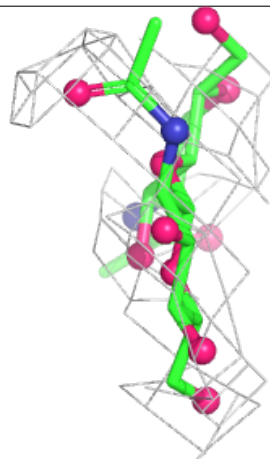
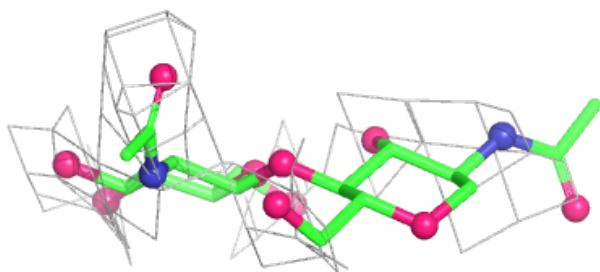
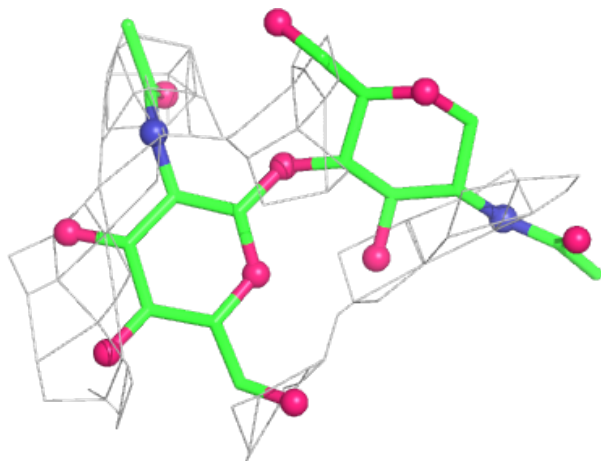
**Electron density around Chain N:**

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



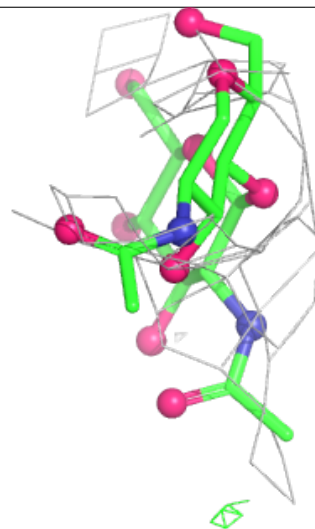
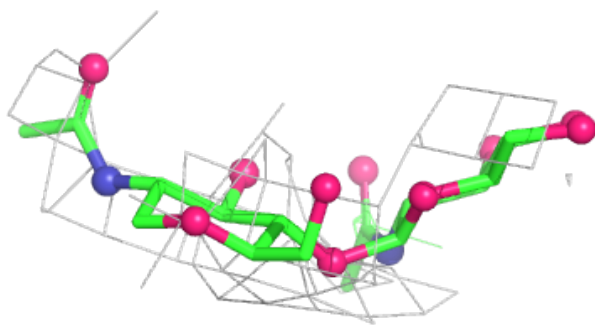
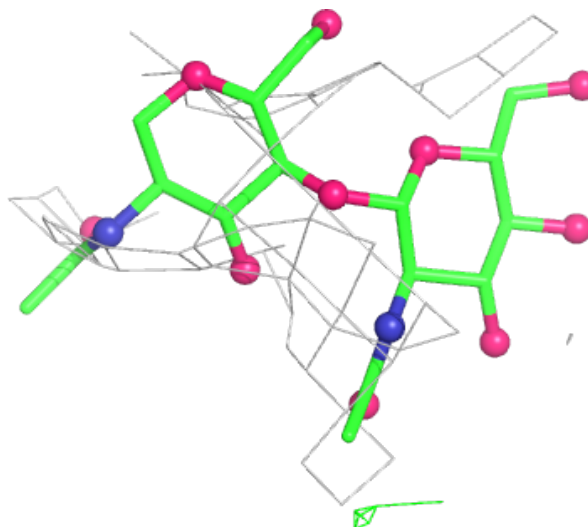
**Electron density around Chain P:**

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



**Electron density around Chain Q:**

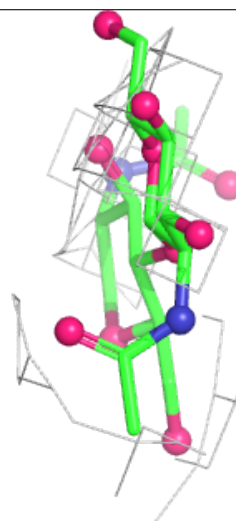
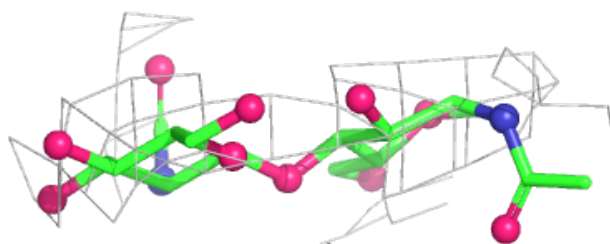
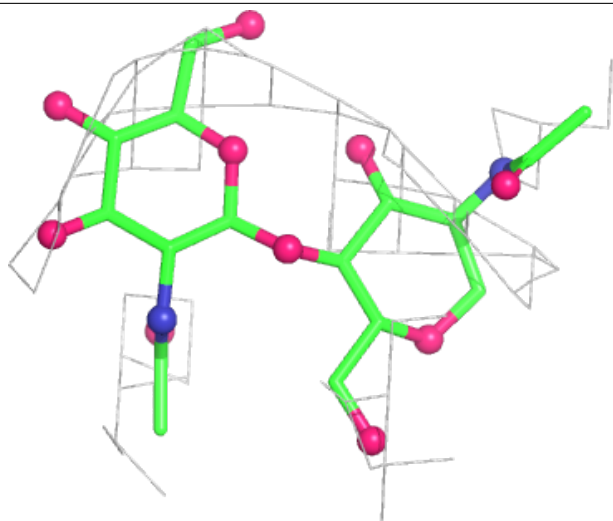
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





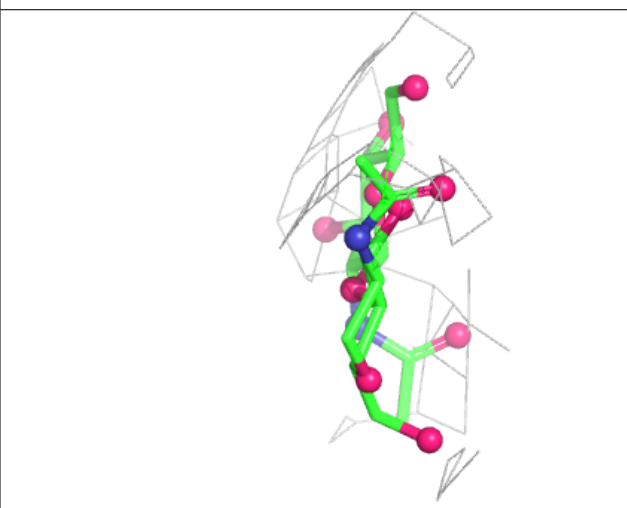
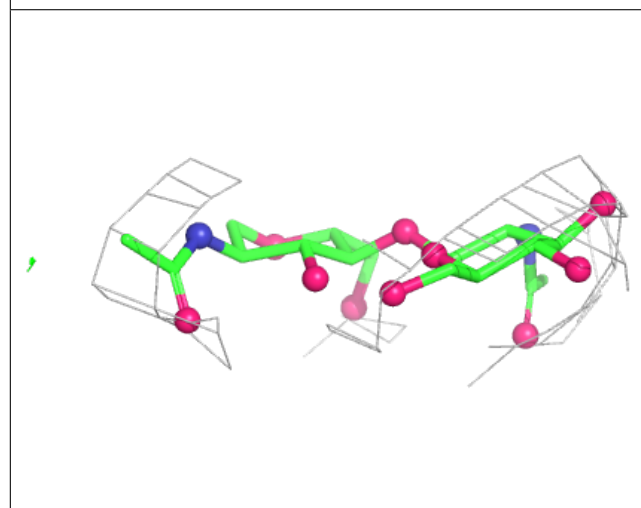
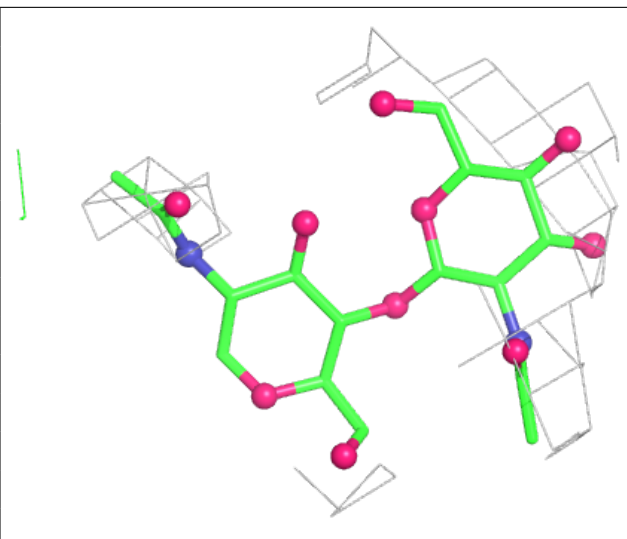
**Electron density around Chain S:**

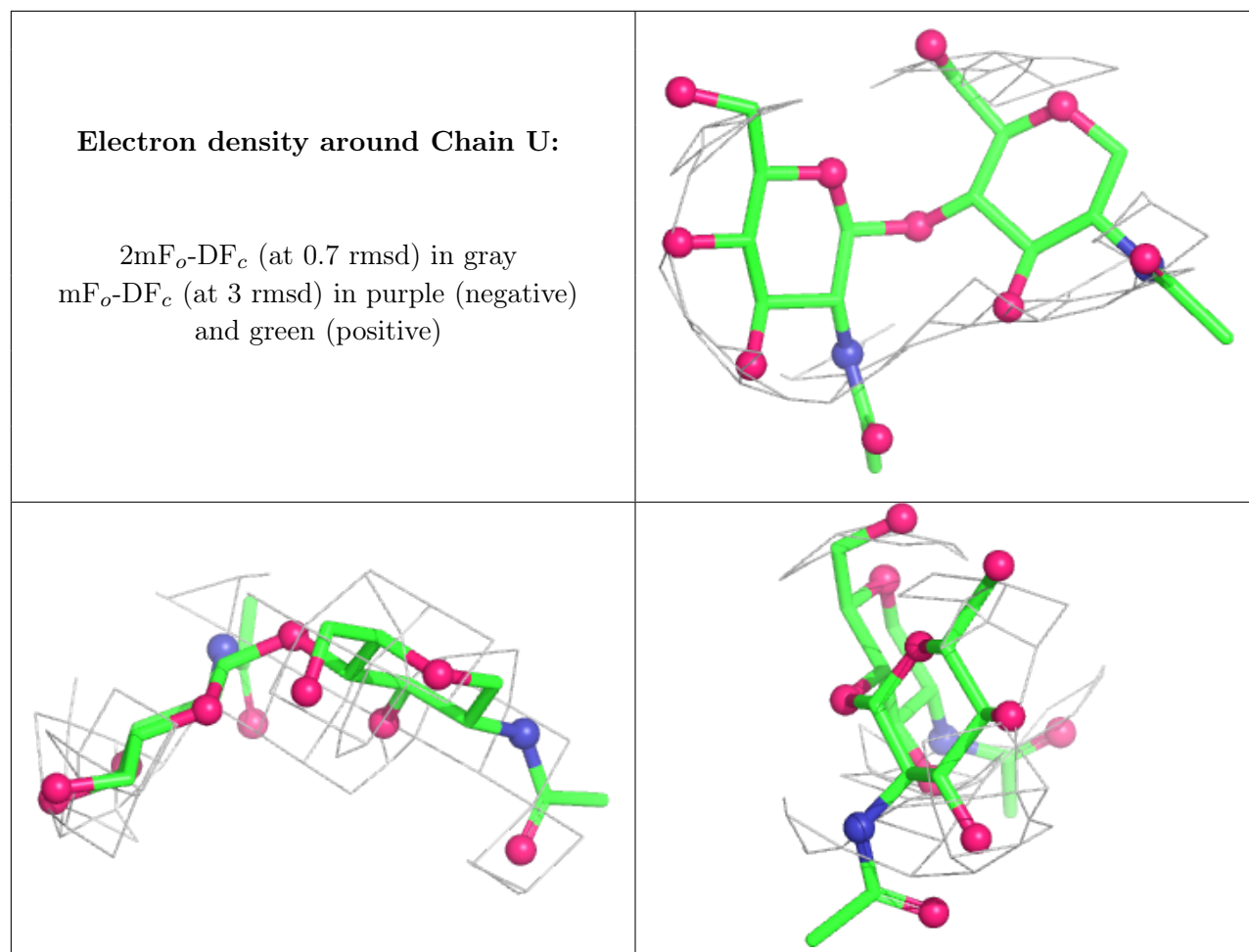
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain T:**

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





## 6.4 Ligands [i](#)

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

## 6.5 Other polymers [i](#)

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