



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 26, 2021 – 10:28 AM EST

PDB ID : 6WML  
Title : Human TLR8 bound to the potent agonist, GS-9688 (Selgantolimod)  
Authors : Appleby, T.C.; Perry, J.K.; Mish, M.; Villasenor, A.G.; Mackman, R.L.  
Deposited on : 2020-04-21  
Resolution : 2.50 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.

---

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 : 2.16  
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) : 2.16

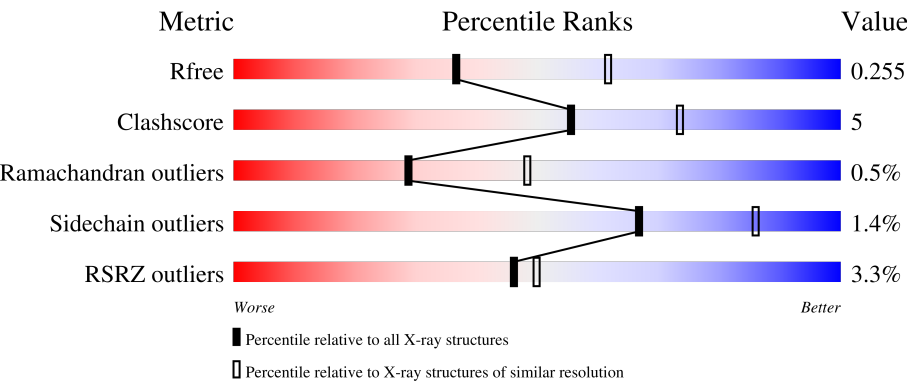
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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.



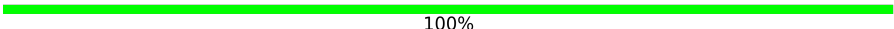
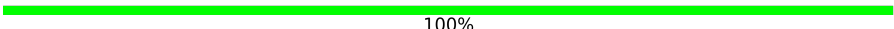
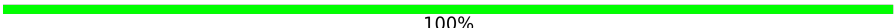


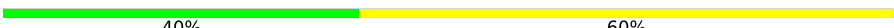
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	811	<div><div></div><div></div><div></div><div></div><div></div></div> <div>%83%8%8%</div>
1	B	811	<div><div></div><div></div><div></div><div></div><div></div></div> <div>2%79%12%7%</div>
1	C	811	<div><div></div><div></div><div></div><div></div><div></div></div> <div>4%71%13%16%</div>
1	D	811	<div><div></div><div></div><div></div><div></div><div></div></div> <div>4%75%12%13%</div>
2	E	4	<div><div></div><div></div></div> <div>50%50%</div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	F	2	 100%
4	G	3	 67% 33%
4	H	3	 33% 67%
4	I	3	 100%
4	J	3	 100%
4	L	3	 100%
4	M	3	 67% 33%
4	O	3	 67% 33%
5	K	4	 50% 50%
5	P	4	 75% 25%
6	N	5	 40% 60%

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
8	NAG	B	1016	-	-	-	X
8	NAG	C	916	X	-	-	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 23787 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 Toll-like receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	743	Total	C	N	O	S	0	3	0
			5716	3682	949	1067	18			
1	B	751	Total	C	N	O	S	0	0	0
			6015	3847	1021	1128	19			
1	C	681	Total	C	N	O	S	0	0	0
			5393	3449	919	1011	14			
1	D	708	Total	C	N	O	S	0	0	0
			5312	3394	913	988	17			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	expression tag	UNP Q9NR97
A	24	SER	-	expression tag	UNP Q9NR97
A	25	PRO	-	expression tag	UNP Q9NR97
A	26	TRP	-	expression tag	UNP Q9NR97
A	828	GLU	-	expression tag	UNP Q9NR97
A	829	PHE	-	expression tag	UNP Q9NR97
A	830	LEU	-	expression tag	UNP Q9NR97
A	831	VAL	-	expression tag	UNP Q9NR97
A	832	PRO	-	expression tag	UNP Q9NR97
A	833	ARG	-	expression tag	UNP Q9NR97
B	23	ARG	-	expression tag	UNP Q9NR97
B	24	SER	-	expression tag	UNP Q9NR97
B	25	PRO	-	expression tag	UNP Q9NR97
B	26	TRP	-	expression tag	UNP Q9NR97
B	828	GLU	-	expression tag	UNP Q9NR97
B	829	PHE	-	expression tag	UNP Q9NR97
B	830	LEU	-	expression tag	UNP Q9NR97
B	831	VAL	-	expression tag	UNP Q9NR97
B	832	PRO	-	expression tag	UNP Q9NR97
B	833	ARG	-	expression tag	UNP Q9NR97
C	23	ARG	-	expression tag	UNP Q9NR97

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	24	SER	-	expression tag	UNP Q9NR97
C	25	PRO	-	expression tag	UNP Q9NR97
C	26	TRP	-	expression tag	UNP Q9NR97
C	828	GLU	-	expression tag	UNP Q9NR97
C	829	PHE	-	expression tag	UNP Q9NR97
C	830	LEU	-	expression tag	UNP Q9NR97
C	831	VAL	-	expression tag	UNP Q9NR97
C	832	PRO	-	expression tag	UNP Q9NR97
C	833	ARG	-	expression tag	UNP Q9NR97
D	23	ARG	-	expression tag	UNP Q9NR97
D	24	SER	-	expression tag	UNP Q9NR97
D	25	PRO	-	expression tag	UNP Q9NR97
D	26	TRP	-	expression tag	UNP Q9NR97
D	828	GLU	-	expression tag	UNP Q9NR97
D	829	PHE	-	expression tag	UNP Q9NR97
D	830	LEU	-	expression tag	UNP Q9NR97
D	831	VAL	-	expression tag	UNP Q9NR97
D	832	PRO	-	expression tag	UNP Q9NR97
D	833	ARG	-	expression tag	UNP Q9NR97

- 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.



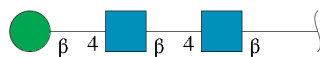
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			25	14	1	10			

- 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.



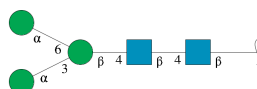
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	L	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	M	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	O	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



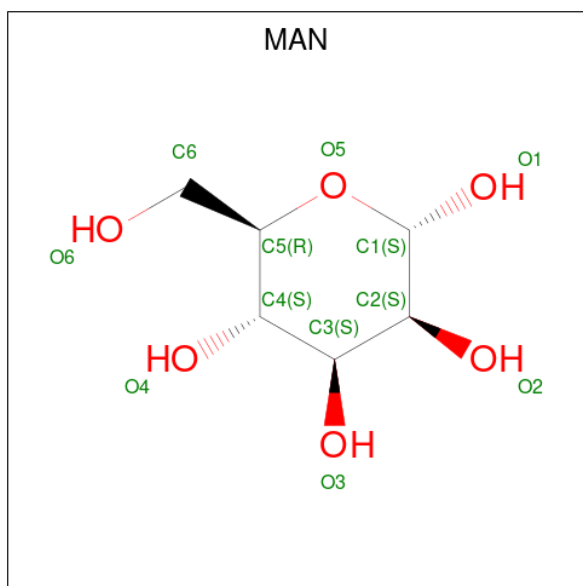
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	K	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	P	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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
6	N	5	Total	C	N	O	0	0	0
			61	34	2	25			

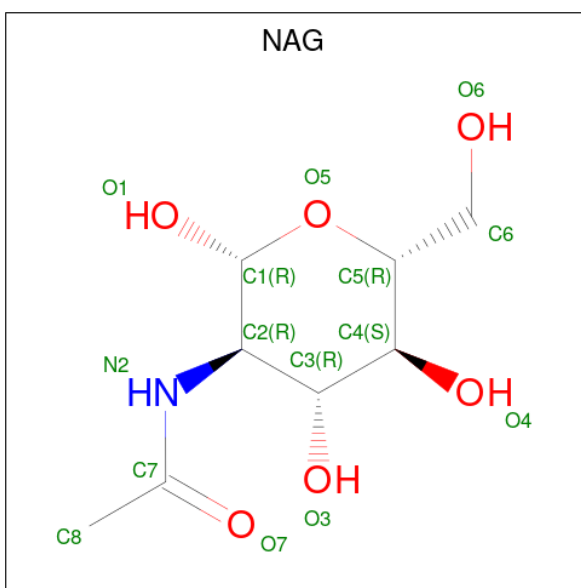
- Molecule 7 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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

- Molecule 8 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>).



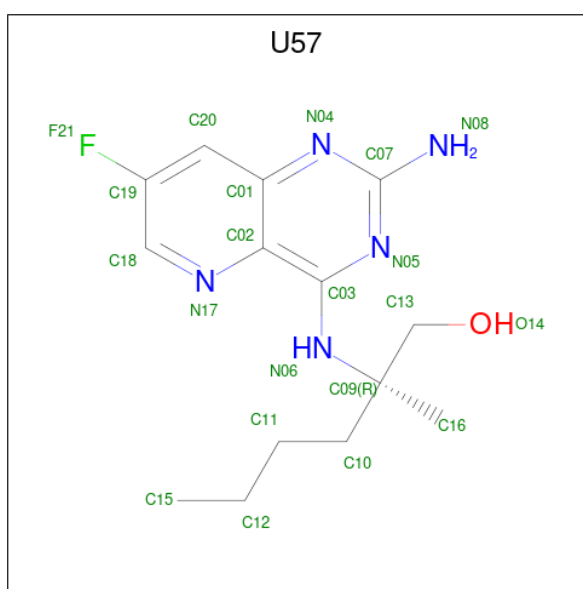
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1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

*Continued on next page...*

Continued from previous page...

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

- Molecule 9 is (2R)-2-[(2-amino-7-fluoropyrido[3,2-d]pyrimidin-4-yl)amino]-2-methylhexan-1-ol (three-letter code: U57) (formula: C<sub>14</sub>H<sub>20</sub>FN<sub>5</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total 21	C 14	F 1	N 5	O 1	0	0
9	B	1	Total 21	C 14	F 1	N 5	O 1	0	0
9	C	1	Total 21	C 14	F 1	N 5	O 1	0	0
9	D	1	Total 21	C 14	F 1	N 5	O 1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	155	Total	O	0	0
			155	155		

Continued on next page...

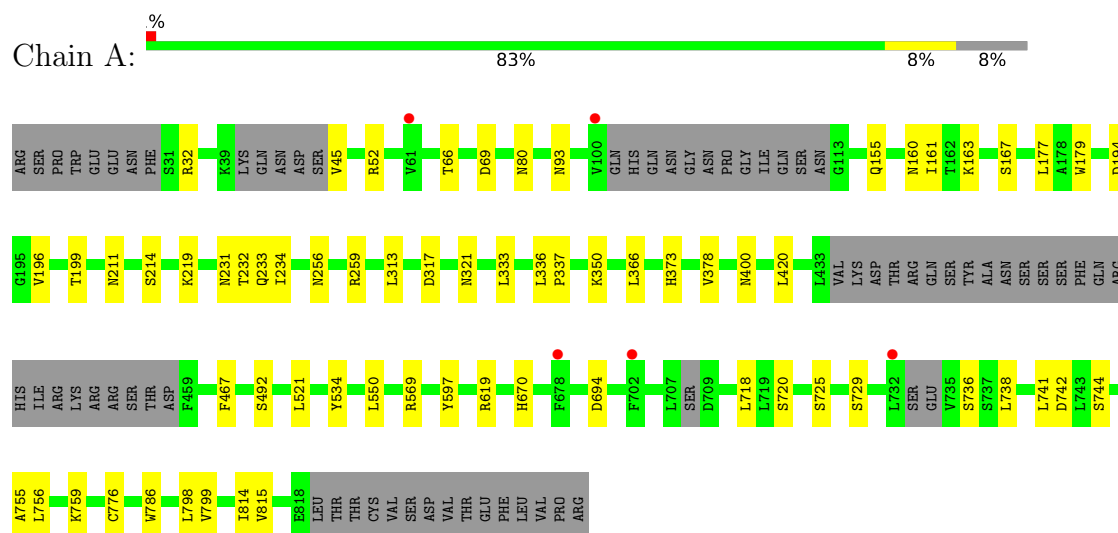
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	110	Total 110	O 110	0	0
10	C	87	Total 87	O 87	0	0
10	D	72	Total 72	O 72	0	0

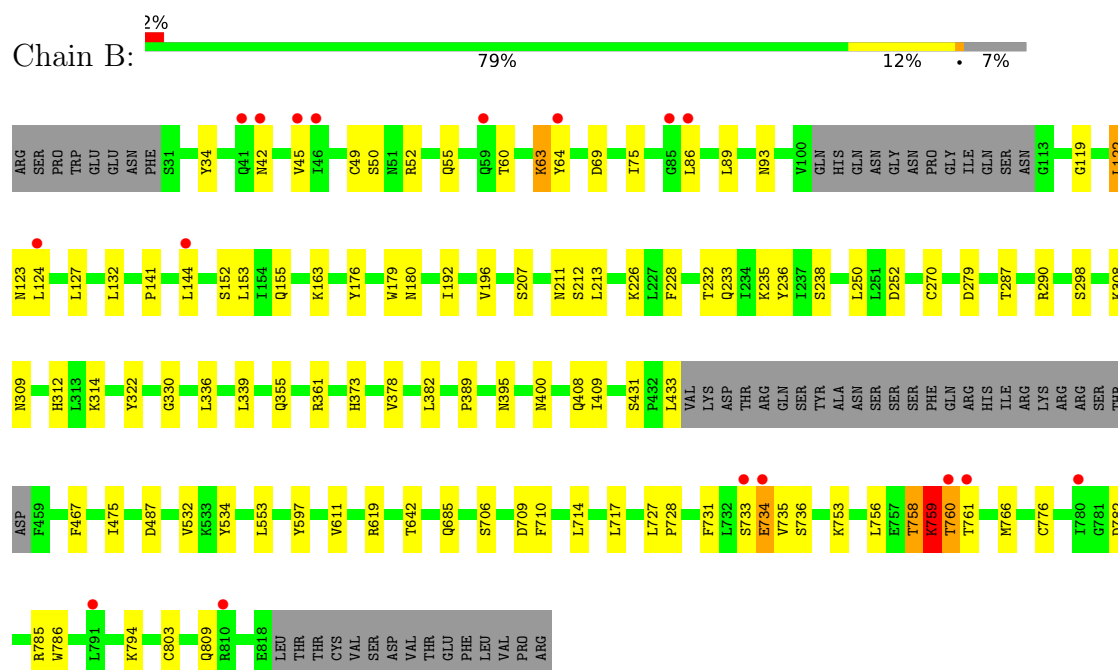
### 3 Residue-property plots [i](#)

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.

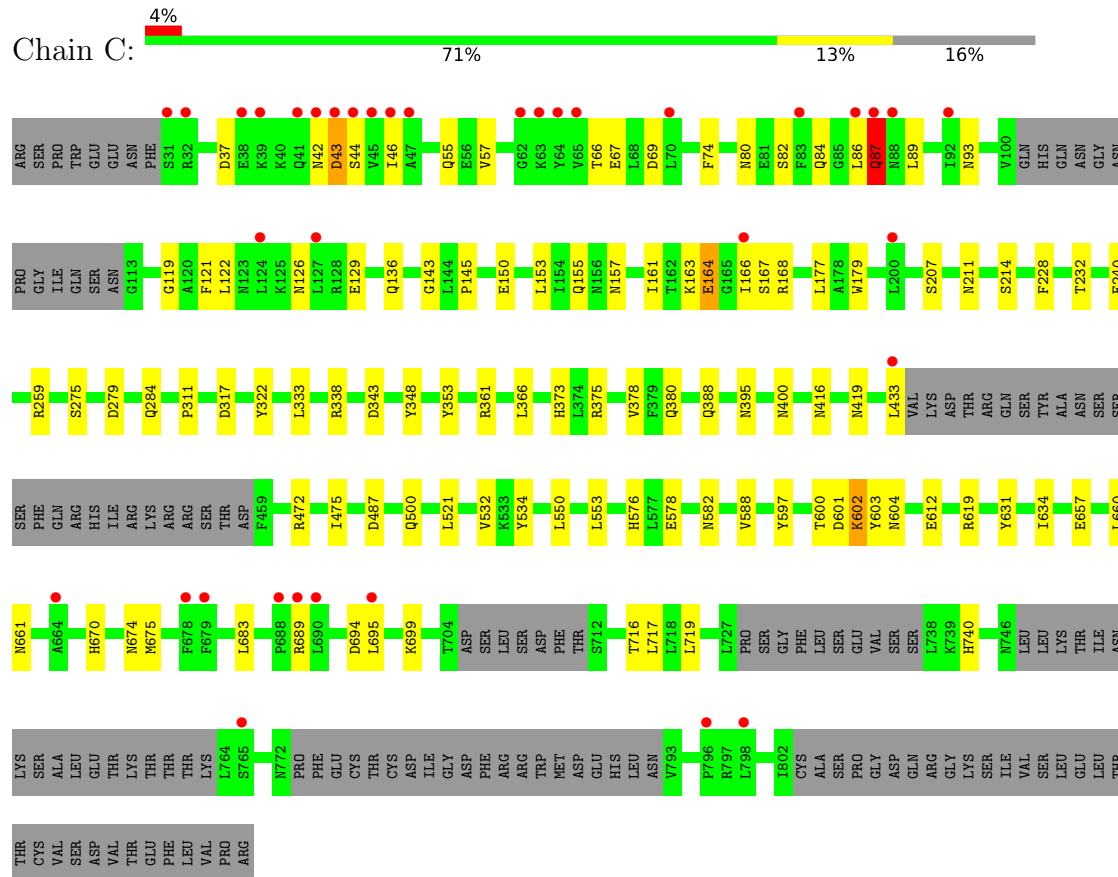
#### • Molecule 1: Toll-like receptor 8



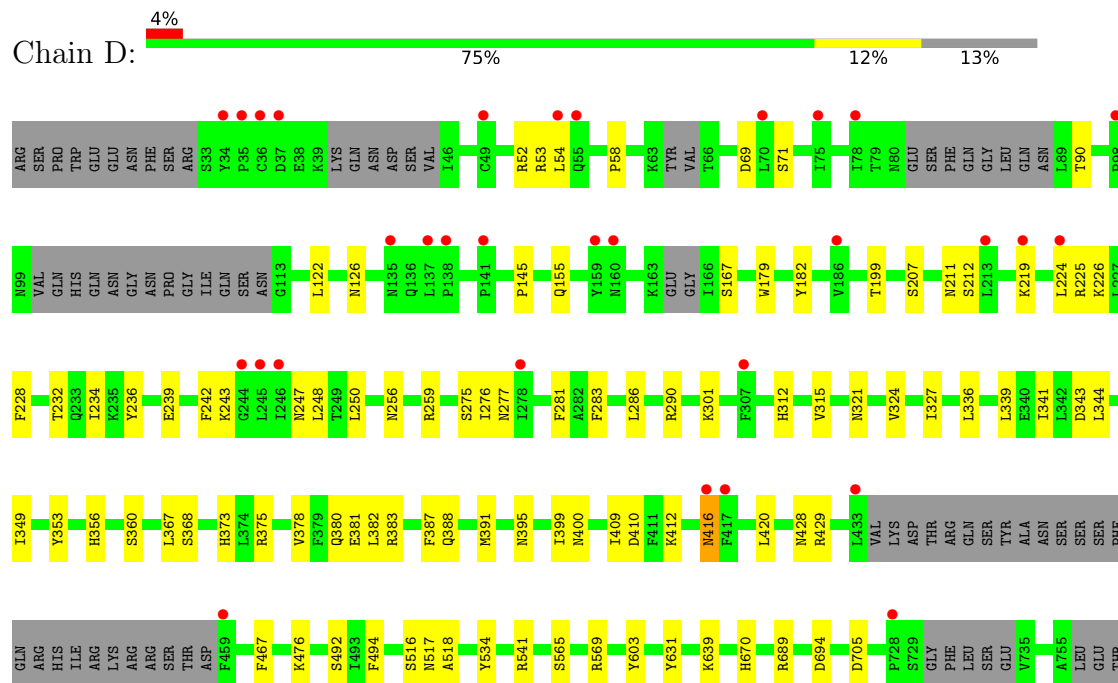
#### • Molecule 1: Toll-like receptor 8

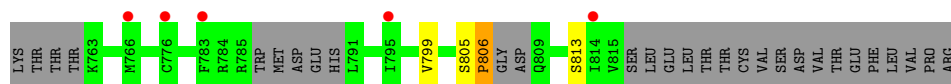


• Molecule 1: Toll-like receptor 8



• Molecule 1: Toll-like receptor 8





- 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%



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

Chain F: 100%



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

Chain G: 67%



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

Chain H: 33%



- 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: 100%



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

Chain J: 100%



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

Chain L:  100%

MAG1  
MAG2  
BMA3

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

Chain M:  67% 33%

MAG1  
MAG2  
BMA3

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

Chain O:  67% 33%

MAG1  
MAG2  
BMA3

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%

MAG1  
MAG2  
BMA3  
MAN4

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  75% 25%

MAG1  
MAG2  
BMA3  
MAN4

- Molecule 6: alpha-D-mannopyranose-(1-3)-[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 N:  40% 60%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.82Å 141.57Å 171.26Å 90.00° 90.41° 90.00°	Depositor
Resolution (Å)	47.86 – 2.50 47.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.8 (47.86-2.50) 88.6 (47.86-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.211 , 0.255 0.211 , 0.255	Depositor DCC
$R_{free}$ test set	1932 reflections (1.42%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.6	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	23787	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: U57, BMA, NAG, 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	0.24	0/5844	0.43	0/7973
1	B	0.25	0/6140	0.45	2/8332 (0.0%)
1	C	0.25	0/5501	0.43	0/7470
1	D	0.26	0/5417	0.45	0/7375
All	All	0.25	0/22902	0.44	2/31150 (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	B	0	3
1	C	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	308	LYS	CD-CE-NZ	-8.72	91.64	111.70
1	B	86	LEU	CA-CB-CG	5.43	127.80	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	758	THR	Peptide
1	B	759	LYS	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	B	760	THR	Peptide
1	C	87	GLN	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	5716	0	5411	33	0
1	B	6015	0	5956	59	0
1	C	5393	0	5236	68	1
1	D	5312	0	4887	65	0
2	E	50	0	42	1	0
3	F	25	0	22	0	0
4	G	39	0	33	2	0
4	H	39	0	32	3	0
4	I	39	0	34	0	0
4	J	39	0	32	0	0
4	L	39	0	34	0	0
4	M	39	0	32	3	0
4	O	39	0	34	1	0
5	K	50	0	42	3	0
5	P	50	0	42	0	0
6	N	61	0	52	1	0
7	A	22	0	20	2	0
7	B	44	0	40	2	0
7	C	33	0	30	6	0
7	D	11	0	10	0	0
8	A	70	0	64	0	0
8	B	56	0	52	3	0
8	C	42	0	39	0	0
8	D	56	0	52	5	1
9	A	21	0	0	0	0
9	B	21	0	0	0	0
9	C	21	0	0	0	0
9	D	21	0	0	0	0
10	A	155	0	0	5	0
10	B	110	0	0	1	0
10	C	87	0	0	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	72	0	0	1	0
All	All	23787	0	22228	234	1

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 5.

All (234) 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)
7:B:1004:MAN:C1	4:H:3:BMA:O3	1.64	1.42
7:C:913:MAN:C1	4:M:3:BMA:O6	1.64	1.41
7:A:1013:MAN:C1	4:G:3:BMA:O6	1.66	1.41
7:C:905:MAN:C1	5:K:3:BMA:O6	1.65	1.40
1:D:395:ASN:HD21	8:D:916:NAG:C1	1.35	1.36
1:D:395:ASN:ND2	8:D:916:NAG:C1	2.03	1.19
1:B:395:ASN:HD21	8:B:1016:NAG:C1	1.68	1.05
1:B:395:ASN:ND2	8:B:1016:NAG:C1	2.20	1.05
1:C:87:GLN:OE1	1:C:87:GLN:O	1.76	1.04
1:C:87:GLN:NE2	1:C:126:ASN:H	1.62	0.96
1:B:395:ASN:HD21	8:B:1016:NAG:C2	1.86	0.88
1:B:124:LEU:HD23	1:B:127:LEU:HB2	1.60	0.83
1:C:87:GLN:HE22	1:C:126:ASN:H	1.26	0.83
1:B:733:SER:HB3	1:B:758:THR:HA	1.64	0.80
1:D:399:ILE:HG13	1:D:420:LEU:HD21	1.65	0.78
1:B:736:SER:OG	1:B:761:THR:O	2.02	0.76
1:B:733:SER:O	1:B:735:VAL:N	2.19	0.74
1:D:242:PHE:H	1:D:243:LYS:HE2	1.51	0.74
7:B:1004:MAN:C1	4:H:3:BMA:C3	2.66	0.74
1:B:279:ASP:OD2	10:B:1101:HOH:O	2.06	0.73
1:D:239:GLU:HG3	1:D:281:PHE:HB2	1.70	0.73
1:B:141:PRO:HB2	1:B:144:LEU:HD21	1.69	0.72
1:D:167:SER:HA	1:D:199:THR:HG21	1.75	0.69
1:C:119:GLY:HA2	1:C:122:LEU:HD13	1.75	0.67
1:C:87:GLN:HE22	1:C:126:ASN:N	1.92	0.67
1:C:582:ASN:ND2	10:C:1002:HOH:O	2.28	0.66
1:C:475:ILE:HD11	1:C:487:ASP:HB2	1.77	0.66
1:C:388:GLN:NE2	10:C:1003:HOH:O	2.28	0.66
1:C:87:GLN:HE22	1:C:126:ASN:HB2	1.61	0.65
1:C:87:GLN:O	1:C:87:GLN:CD	2.35	0.65
1:D:395:ASN:CG	8:D:916:NAG:C1	2.65	0.65
1:B:34:TYR:O	1:B:60:THR:OG1	2.14	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:ARG:NH2	1:C:348:TYR:O	2.30	0.64
1:C:46:ILE:HB	1:C:67:GLU:HB2	1.78	0.64
7:C:905:MAN:C1	5:K:3:BMA:C6	2.74	0.64
1:B:163:LYS:HA	1:B:196:VAL:HG23	1.80	0.64
1:A:52:ARG:HG2	1:A:799:VAL:HG11	1.80	0.63
1:B:759:LYS:HB3	1:B:760:THR:OG1	1.98	0.63
1:C:416:ASN:ND2	10:C:1006:HOH:O	2.33	0.62
1:D:122:LEU:HA	1:D:145:PRO:HG3	1.82	0.60
1:C:240:GLU:N	1:C:240:GLU:OE1	2.33	0.60
1:D:375:ARG:HD2	1:D:400:ASN:HD21	1.67	0.59
1:C:716:THR:HG23	1:C:740:HIS:HB3	1.84	0.58
1:D:242:PHE:N	1:D:243:LYS:HE2	2.17	0.58
1:B:475:ILE:HD11	1:B:487:ASP:HB2	1.86	0.58
1:D:368:SER:HA	1:D:395:ASN:HD22	1.69	0.58
1:C:395:ASN:ND2	10:C:1008:HOH:O	2.35	0.58
1:D:52:ARG:HG2	1:D:799:VAL:HG21	1.86	0.57
1:D:395:ASN:ND2	8:D:916:NAG:O5	2.37	0.57
1:D:167:SER:CA	1:D:199:THR:HG21	2.34	0.57
1:C:602:LYS:HD3	1:C:603:TYR:H	1.69	0.57
1:B:119:GLY:CA	1:B:122:LEU:HD22	2.35	0.57
1:C:211:ASN:O	1:C:232:THR:HA	2.05	0.56
1:B:228:PHE:HA	1:B:252:ASP:HB3	1.87	0.56
1:A:350:LYS:NZ	10:A:1109:HOH:O	2.39	0.56
1:D:639:LYS:HA	1:D:639:LYS:HE2	1.87	0.56
1:B:753:LYS:HA	1:B:756:LEU:HD12	1.88	0.55
1:B:63:LYS:H	1:B:63:LYS:HE2	1.70	0.55
1:C:80:ASN:O	1:C:84:GLN:NE2	2.39	0.55
1:B:756:LEU:HB3	1:B:786:TRP:CD1	2.41	0.55
1:C:660:LEU:HD21	1:C:683:LEU:HD22	1.89	0.54
1:D:518:ALA:HB2	1:D:541:ARG:HG3	1.90	0.54
1:C:57:VAL:HG11	1:C:82:SER:HB3	1.90	0.54
1:A:231:ASN:ND2	10:A:1111:HOH:O	2.41	0.54
1:C:69:ASP:HA	1:C:93:ASN:HB3	1.89	0.54
7:C:913:MAN:C1	4:M:3:BMA:C6	2.78	0.54
1:D:388:GLN:HA	1:D:391:MET:HE3	1.90	0.54
1:D:356:HIS:CE1	1:D:383:ARG:HH11	2.26	0.54
1:B:192:ILE:HD11	1:B:213:LEU:HD22	1.91	0.53
1:C:42:ASN:O	1:C:43:ASP:HB2	2.08	0.53
1:C:87:GLN:NE2	1:C:126:ASN:N	2.42	0.53
7:C:913:MAN:C2	4:M:3:BMA:O6	2.51	0.53
1:A:161:ILE:HD12	1:A:177:LEU:HD13	1.91	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:521:LEU:HD13	1:C:550:LEU:HD21	1.90	0.53
1:D:476:LYS:HD2	4:O:1:NAG:H83	1.91	0.53
1:A:194:ASP:OD2	1:A:219:LYS:NZ	2.35	0.53
1:A:521:LEU:HD13	1:A:550:LEU:HD21	1.91	0.53
1:A:211:ASN:O	1:A:232:THR:HA	2.08	0.52
1:B:611:VAL:HG13	1:B:642:THR:HG22	1.91	0.52
1:D:259:ARG:NH1	1:D:321:ASN:O	2.42	0.52
1:C:129:GLU:HG3	1:C:150:GLU:HB3	1.91	0.52
1:C:419:ASN:O	1:C:419:ASN:ND2	2.43	0.52
1:B:45:VAL:HG11	1:B:64:TYR:HD1	1.74	0.52
1:B:706:SER:HB3	1:B:709:ASP:OD1	2.09	0.52
1:C:375:ARG:NH1	10:C:1016:HOH:O	2.43	0.52
1:D:670:HIS:HA	1:D:694:ASP:HB3	1.92	0.51
1:D:242:PHE:H	1:D:243:LYS:CE	2.21	0.51
1:D:234:ILE:O	1:D:256:ASN:HB3	2.11	0.51
1:C:284:GLN:NE2	10:C:1011:HOH:O	2.40	0.50
1:D:399:ILE:HD12	1:D:420:LEU:HD11	1.92	0.50
1:C:717:LEU:CD2	1:C:719:LEU:HG	2.41	0.50
1:D:207:SER:HA	1:D:228:PHE:HB2	1.92	0.50
1:B:212:SER:OG	1:B:233:GLN:OE1	2.24	0.50
1:D:367:LEU:O	1:D:395:ASN:ND2	2.45	0.50
1:D:467:PHE:HB3	6:N:1:NAG:H81	1.93	0.50
1:B:782:ASP:OD1	1:B:785:ARG:NH2	2.43	0.50
1:B:532:VAL:HB	1:B:553:LEU:HD22	1.94	0.50
1:D:387:PHE:O	1:D:391:MET:HG3	2.11	0.49
1:B:336:LEU:HB3	1:B:339:LEU:HB2	1.95	0.49
1:B:373:HIS:HA	1:B:400:ASN:HB3	1.94	0.49
1:B:597:TYR:HB3	1:B:619:ARG:HB2	1.94	0.49
1:C:136:GLN:HG2	1:C:157:ASN:HD21	1.77	0.49
1:B:207:SER:HA	1:B:228:PHE:HB2	1.94	0.49
1:B:236:TYR:CE2	1:B:238:SER:HB3	2.47	0.49
1:A:569:ARG:NH2	10:A:1121:HOH:O	2.45	0.49
1:C:86:LEU:HB3	1:C:89:LEU:HG	1.95	0.48
1:C:333:LEU:HD22	1:C:366:LEU:HD11	1.96	0.48
1:D:225:ARG:HA	1:D:248:LEU:HA	1.95	0.48
1:D:226:LYS:HG2	1:D:250:LEU:HB3	1.94	0.48
1:B:298:SER:HB3	1:B:322:TYR:HE2	1.78	0.48
1:B:734:GLU:HG2	1:B:735:VAL:H	1.77	0.48
1:D:391:MET:SD	1:D:416:ASN:HB3	2.54	0.48
1:A:729:SER:HA	1:A:755:ALA:HA	1.95	0.48
1:B:180:ASN:HB2	1:B:211:ASN:OD1	2.14	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:GLN:HA	1:D:179:TRP:O	2.13	0.48
1:B:211:ASN:O	1:B:232:THR:HA	2.14	0.48
1:C:657:GLU:O	1:C:661:ASN:ND2	2.47	0.48
1:A:718:LEU:HA	1:A:742:ASP:HB3	1.96	0.47
1:B:287:THR:HA	1:B:309:ASN:O	2.14	0.47
1:C:87:GLN:NE2	1:C:126:ASN:HB2	2.27	0.47
1:D:290:ARG:HD2	1:D:312:HIS:O	2.14	0.47
1:D:54:LEU:HD13	1:D:58:PRO:HD3	1.97	0.47
1:C:161:ILE:HD12	1:C:177:LEU:HD13	1.96	0.47
1:D:327:ILE:HG12	1:D:344:LEU:HD13	1.96	0.47
1:A:756:LEU:HD13	1:A:786:TRP:HB2	1.96	0.47
1:C:87:GLN:HE22	1:C:126:ASN:CB	2.28	0.47
1:D:382:LEU:HB3	1:D:409:ILE:HD13	1.96	0.47
1:A:798:LEU:HD22	1:A:815:VAL:HG11	1.97	0.47
1:B:290:ARG:HD2	1:B:312:HIS:O	2.15	0.47
1:D:283:PHE:HA	1:D:286:LEU:HD12	1.96	0.47
1:D:705:ASP:N	1:D:705:ASP:OD1	2.45	0.47
1:D:375:ARG:HD2	1:D:400:ASN:ND2	2.30	0.46
1:C:207:SER:HA	1:C:228:PHE:HB2	1.96	0.46
1:C:532:VAL:HB	1:C:553:LEU:HD22	1.97	0.46
1:D:343:ASP:HA	1:D:373:HIS:HB2	1.96	0.46
1:D:410:ASP:OD1	1:D:412:LYS:HE3	2.16	0.46
1:C:689:ARG:HG2	1:C:689:ARG:HH11	1.80	0.46
1:A:597:TYR:HB3	1:A:619:ARG:HB2	1.98	0.46
1:B:760:THR:HG22	1:B:761:THR:N	2.30	0.46
1:D:53:ARG:HB2	1:D:53:ARG:HE	1.53	0.46
1:A:333:LEU:HD22	1:A:366:LEU:HD11	1.98	0.46
1:A:467:PHE:HB3	2:E:1:NAG:H81	1.97	0.46
1:B:119:GLY:O	1:B:122:LEU:CD2	2.64	0.46
1:A:670:HIS:HA	1:A:694:ASP:HB3	1.98	0.46
1:C:597:TYR:HB3	1:C:619:ARG:HB2	1.99	0.45
1:A:163:LYS:HA	1:A:196:VAL:HG23	1.98	0.45
1:D:420:LEU:HA	1:D:420:LEU:HD23	1.72	0.45
7:C:905:MAN:C2	5:K:3:BMA:O6	2.56	0.45
1:D:211:ASN:O	1:D:232:THR:HA	2.17	0.45
1:B:803:CYS:HB2	1:B:809:GLN:O	2.17	0.45
1:D:90:THR:HA	1:D:126:ASN:O	2.16	0.45
1:D:336:LEU:HD13	1:D:339:LEU:HD22	1.98	0.45
1:D:689:ARG:NH1	10:D:1012:HOH:O	2.50	0.45
1:B:55:GLN:O	1:B:75:ILE:HA	2.17	0.45
1:B:685:GLN:HG3	1:B:710:PHE:HA	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:600:THR:O	1:C:602:LYS:N	2.51	0.45
1:A:45:VAL:N	1:A:66:THR:HG1	2.15	0.44
7:A:1013:MAN:C5	4:G:3:BMA:O6	2.65	0.44
1:A:373:HIS:HA	1:A:400:ASN:HB3	1.98	0.44
1:C:603:TYR:HB3	1:C:631:TYR:CD1	2.53	0.44
1:D:324:VAL:HG11	1:D:349:ILE:HD11	2.00	0.44
1:B:382:LEU:HB3	1:B:409:ILE:HG12	2.00	0.44
1:B:467:PHE:HB3	4:H:1:NAG:H81	2.00	0.44
1:C:259:ARG:HG3	1:C:322:TYR:CZ	2.53	0.44
1:D:429:ARG:NH1	1:D:492:SER:OG	2.49	0.44
1:C:670:HIS:HA	1:C:694:ASP:HB3	2.00	0.44
1:D:315:VAL:HG22	1:D:341:ILE:HB	2.00	0.44
1:D:494:PHE:HA	1:D:517:ASN:HA	2.00	0.43
1:A:80:ASN:ND2	10:A:1126:HOH:O	2.49	0.43
1:B:132:LEU:HB2	1:B:153:LEU:HD23	2.00	0.43
1:B:69:ASP:HA	1:B:93:ASN:HB3	1.99	0.43
1:C:153:LEU:HB2	1:C:177:LEU:HD23	2.00	0.43
1:A:492:SER:OG	10:A:1101:HOH:O	2.21	0.43
1:A:214:SER:HA	1:A:233:GLN:O	2.19	0.43
1:B:290:ARG:NH2	1:B:314:LYS:HD3	2.34	0.43
1:C:674:ASN:HB3	1:C:675:MET:H	1.63	0.43
1:B:714:LEU:HD21	1:B:717:LEU:HD13	1.99	0.43
1:C:121:PHE:O	1:C:145:PRO:HG3	2.19	0.43
1:B:152:SER:HA	1:B:176:TYR:HB2	1.99	0.43
1:B:727:LEU:HD23	1:B:727:LEU:HA	1.87	0.43
1:C:604:ASN:HA	1:C:634:ILE:HA	2.00	0.43
1:C:163:LYS:HG2	1:C:167:SER:OG	2.18	0.43
1:A:69:ASP:HA	1:A:93:ASN:HB3	2.01	0.43
1:C:375:ARG:HD3	1:C:400:ASN:HD21	1.83	0.43
1:B:119:GLY:C	1:B:122:LEU:HD22	2.39	0.42
1:B:235:LYS:HG2	1:B:270:CYS:SG	2.59	0.42
1:B:728:PRO:HG2	1:B:731:PHE:CD1	2.54	0.42
1:C:343:ASP:HA	1:C:373:HIS:HB2	2.01	0.42
1:C:576:HIS:ND1	1:C:578:GLU:OE2	2.46	0.42
1:A:720:SER:HA	1:A:744:SER:O	2.20	0.42
1:C:55:GLN:HA	1:C:74:PHE:HB2	2.02	0.42
1:D:69:ASP:OD1	1:D:71:SER:OG	2.27	0.42
1:A:155:GLN:HA	1:A:179:TRP:O	2.19	0.42
1:A:167:SER:O	1:A:199:THR:HG21	2.19	0.42
1:D:805:SER:HA	1:D:806:PRO:HA	1.82	0.42
1:C:166:ILE:HA	1:C:166:ILE:HD13	1.87	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:603:TYR:HB3	1:D:631:TYR:CD1	2.55	0.42
1:A:738:LEU:HD21	1:A:741:LEU:HD13	2.01	0.42
1:C:602:LYS:CE	1:C:602:LYS:HA	2.50	0.42
1:C:588:VAL:HG13	1:C:612:GLU:HB3	2.01	0.42
1:D:373:HIS:HA	1:D:400:ASN:HB3	2.01	0.42
1:D:395:ASN:OD1	8:D:916:NAG:C1	2.68	0.42
1:C:164:GLU:HA	1:C:168:ARG:HH12	1.85	0.41
1:B:155:GLN:HA	1:B:179:TRP:O	2.20	0.41
1:D:353:TYR:CZ	1:D:380:GLN:HG2	2.55	0.41
1:D:356:HIS:HE1	1:D:381:GLU:OE1	2.04	0.41
1:A:313:LEU:HD23	1:A:336:LEU:HD22	2.03	0.41
1:A:420:LEU:HA	1:A:420:LEU:HD23	1.90	0.41
1:C:603:TYR:HB3	1:C:631:TYR:CE1	2.54	0.41
1:C:311:PRO:O	1:C:338:ARG:NE	2.48	0.41
1:C:602:LYS:HE2	1:C:602:LYS:HA	2.01	0.41
1:D:428:ASN:O	1:D:429:ARG:HD2	2.20	0.41
1:A:776:CYS:SG	1:A:814:ILE:HG22	2.60	0.41
1:C:155:GLN:HA	1:C:179:TRP:O	2.19	0.41
1:A:259:ARG:NH1	1:A:321:ASN:O	2.52	0.41
1:D:224:LEU:HA	1:D:224:LEU:HD23	1.86	0.41
1:D:242:PHE:HB3	1:D:286:LEU:HD21	2.02	0.41
1:B:226:LYS:HG2	1:B:250:LEU:HB3	2.03	0.41
1:A:337:PRO:HB2	1:C:311:PRO:HB3	2.01	0.41
1:C:353:TYR:CZ	1:C:380:GLN:HG2	2.56	0.41
1:C:87:GLN:HE22	1:C:126:ASN:CA	2.33	0.41
1:B:361:ARG:HA	1:B:389:PRO:HB3	2.03	0.41
1:D:155:GLN:NE2	1:D:182:TYR:OH	2.26	0.41
1:B:776:CYS:HB2	1:B:803:CYS:HB3	1.99	0.41
1:C:695:LEU:HB2	1:C:719:LEU:HD23	2.02	0.41
1:D:275:SER:OG	1:D:276:ILE:N	2.53	0.41
1:D:236:TYR:HD1	1:D:277:ASN:HB3	1.85	0.41
1:D:565:SER:O	1:D:569:ARG:HG3	2.21	0.41
1:A:234:ILE:O	1:A:256:ASN:HB3	2.20	0.40
1:B:766:MET:HB2	1:B:794:LYS:HZ2	1.87	0.40
1:B:50:SER:O	1:B:52:ARG:NH1	2.55	0.40
1:B:89:LEU:HD23	1:B:89:LEU:HA	1.85	0.40
1:C:433:LEU:H	1:C:500:GLN:HE22	1.69	0.40
1:C:44:SER:HB3	1:C:66:THR:OG1	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:ASP:OD1	8:D:916:NAG:O4[2_756]	2.17	0.03

## 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	734/811 (90%)	690 (94%)	41 (6%)	3 (0%)	34	54
1	B	745/811 (92%)	695 (93%)	45 (6%)	5 (1%)	22	39
1	C	667/811 (82%)	626 (94%)	37 (6%)	4 (1%)	25	43
1	D	688/811 (85%)	642 (93%)	44 (6%)	2 (0%)	41	61
All	All	2834/3244 (87%)	2653 (94%)	167 (6%)	14 (0%)	29	48

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	734	GLU
1	A	759	LYS
1	B	759	LYS
1	A	736	SER
1	C	43	ASP
1	A	378	VAL
1	B	42	ASN
1	C	601	ASP
1	B	330	GLY
1	B	378	VAL
1	C	143	GLY
1	C	378	VAL
1	D	378	VAL
1	D	806	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	609/755 (81%)	604 (99%)	5 (1%)	81	93
1	B	687/755 (91%)	678 (99%)	9 (1%)	69	87
1	C	597/755 (79%)	586 (98%)	11 (2%)	59	81
1	D	536/755 (71%)	527 (98%)	9 (2%)	60	82
All	All	2429/3020 (80%)	2395 (99%)	34 (1%)	67	86

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	160	ASN
1	A	317	ASP
1	A	534	TYR
1	A	725	SER
1	B	49	CYS
1	B	63	LYS
1	B	122	LEU
1	B	123	ASN
1	B	355	GLN
1	B	408	GLN
1	B	431	SER
1	B	433	LEU
1	B	534	TYR
1	C	37	ASP
1	C	87	GLN
1	C	164	GLU
1	C	214	SER
1	C	275	SER
1	C	317	ASP
1	C	361	ARG
1	C	472	ARG
1	C	534	TYR
1	C	602	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	699	LYS
1	D	212	SER
1	D	219	LYS
1	D	247	ASN
1	D	301	LYS
1	D	360	SER
1	D	416	ASN
1	D	516	SER
1	D	534	TYR
1	D	813	SER

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

Mol	Chain	Res	Type
1	B	42	ASN
1	B	231	ASN
1	B	388	GLN
1	B	395	ASN
1	C	41	GLN
1	C	87	GLN
1	C	595	ASN
1	D	356	HIS
1	D	395	ASN
1	D	416	ASN

### 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 ⓘ

40 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	0.28	0	17,19,21	0.35	0
2	NAG	E	2	2	14,14,15	0.21	0	17,19,21	0.39	0
2	BMA	E	3	2	11,11,12	0.58	0	15,15,17	0.78	0
2	MAN	E	4	2	11,11,12	0.70	0	15,15,17	1.05	2 (13%)
3	NAG	F	1	3	14,14,15	0.24	0	17,19,21	0.38	0
3	BMA	F	2	3	11,11,12	0.71	0	15,15,17	0.83	0
4	NAG	G	1	1,4	14,14,15	0.27	0	17,19,21	0.35	0
4	NAG	G	2	4	14,14,15	0.30	0	17,19,21	0.39	0
4	BMA	G	3	4	11,11,12	0.65	0	15,15,17	0.78	0
4	NAG	H	1	4	14,14,15	0.24	0	17,19,21	0.36	0
4	NAG	H	2	4	14,14,15	0.19	0	17,19,21	0.42	0
4	BMA	H	3	4	11,11,12	0.64	0	15,15,17	0.77	0
4	NAG	I	1	1,4	14,14,15	0.26	0	17,19,21	0.43	0
4	NAG	I	2	4	14,14,15	0.23	0	17,19,21	0.42	0
4	BMA	I	3	4	11,11,12	0.73	0	15,15,17	0.81	0
4	NAG	J	1	1,4	14,14,15	0.28	0	17,19,21	0.35	0
4	NAG	J	2	4	14,14,15	0.28	0	17,19,21	0.37	0
4	BMA	J	3	4	11,11,12	0.60	0	15,15,17	0.78	0
5	NAG	K	1	1,5	14,14,15	0.28	0	17,19,21	0.35	0
5	NAG	K	2	5	14,14,15	0.20	0	17,19,21	0.42	0
5	BMA	K	3	5	11,11,12	0.64	0	15,15,17	0.80	0
5	MAN	K	4	5	11,11,12	0.78	1 (9%)	15,15,17	1.00	2 (13%)
4	NAG	L	1	1,4	14,14,15	0.24	0	17,19,21	0.39	0
4	NAG	L	2	4	14,14,15	0.28	0	17,19,21	0.36	0
4	BMA	L	3	4	11,11,12	0.71	0	15,15,17	0.84	0
4	NAG	M	1	4	14,14,15	0.25	0	17,19,21	0.37	0
4	NAG	M	2	4	14,14,15	0.22	0	17,19,21	0.40	0
4	BMA	M	3	4	11,11,12	0.64	0	15,15,17	0.87	0
6	NAG	N	1	1,6	14,14,15	0.23	0	17,19,21	0.37	0
6	NAG	N	2	6	14,14,15	0.18	0	17,19,21	0.45	0
6	BMA	N	3	6	11,11,12	0.59	0	15,15,17	0.83	0
6	MAN	N	4	6	11,11,12	0.68	0	15,15,17	1.12	2 (13%)
6	MAN	N	5	6	11,11,12	0.69	0	15,15,17	1.11	2 (13%)
4	NAG	O	1	1,4	14,14,15	0.25	0	17,19,21	0.40	0
4	NAG	O	2	4	14,14,15	0.25	0	17,19,21	0.37	0
4	BMA	O	3	4	11,11,12	0.62	0	15,15,17	0.80	0
5	NAG	P	1	1,5	14,14,15	0.23	0	17,19,21	0.39	0
5	NAG	P	2	5	14,14,15	0.26	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BMA	P	3	5	11,11,12	0.63	0	15,15,17	0.76	0
5	MAN	P	4	5	11,11,12	0.68	0	15,15,17	1.09	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	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	2/2/19/22	0/1/1/1
3	NAG	F	1	3	-	0/6/23/26	0/1/1/1
3	BMA	F	2	3	-	0/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	NAG	H	1	4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1
4	NAG	I	1	1,4	-	0/6/23/26	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
4	NAG	J	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
5	NAG	K	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
5	MAN	K	4	5	-	0/2/19/22	0/1/1/1
4	NAG	L	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1
4	BMA	L	3	4	-	0/2/19/22	0/1/1/1
4	NAG	M	1	4	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	BMA	M	3	4	-	0/2/19/22	0/1/1/1
6	NAG	N	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	2/6/23/26	0/1/1/1
6	BMA	N	3	6	-	0/2/19/22	0/1/1/1
6	MAN	N	4	6	-	0/2/19/22	0/1/1/1

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	N	5	6	-	2/2/19/22	0/1/1/1
4	NAG	O	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	BMA	O	3	4	-	2/2/19/22	0/1/1/1
5	NAG	P	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
5	BMA	P	3	5	-	0/2/19/22	0/1/1/1
5	MAN	P	4	5	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	4	MAN	O5-C1	-2.01	1.40	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	4	MAN	C1-O5-C5	2.47	115.54	112.19
5	K	4	MAN	C1-O5-C5	2.39	115.43	112.19
5	P	4	MAN	C1-O5-C5	2.37	115.41	112.19
6	N	5	MAN	C1-O5-C5	2.35	115.38	112.19
2	E	4	MAN	C1-O5-C5	2.32	115.34	112.19
2	E	4	MAN	O2-C2-C3	-2.25	105.63	110.14
5	P	4	MAN	O2-C2-C3	-2.23	105.68	110.14
6	N	5	MAN	O2-C2-C3	-2.21	105.70	110.14
6	N	4	MAN	O2-C2-C3	-2.20	105.74	110.14
5	K	4	MAN	O2-C2-C3	-2.18	105.76	110.14

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	O	3	BMA	O5-C5-C6-O6
6	N	5	MAN	O5-C5-C6-O6
2	E	4	MAN	O5-C5-C6-O6
2	E	4	MAN	C4-C5-C6-O6
6	N	5	MAN	C4-C5-C6-O6
4	O	3	BMA	C4-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
4	I	3	BMA	O5-C5-C6-O6
6	N	2	NAG	C4-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

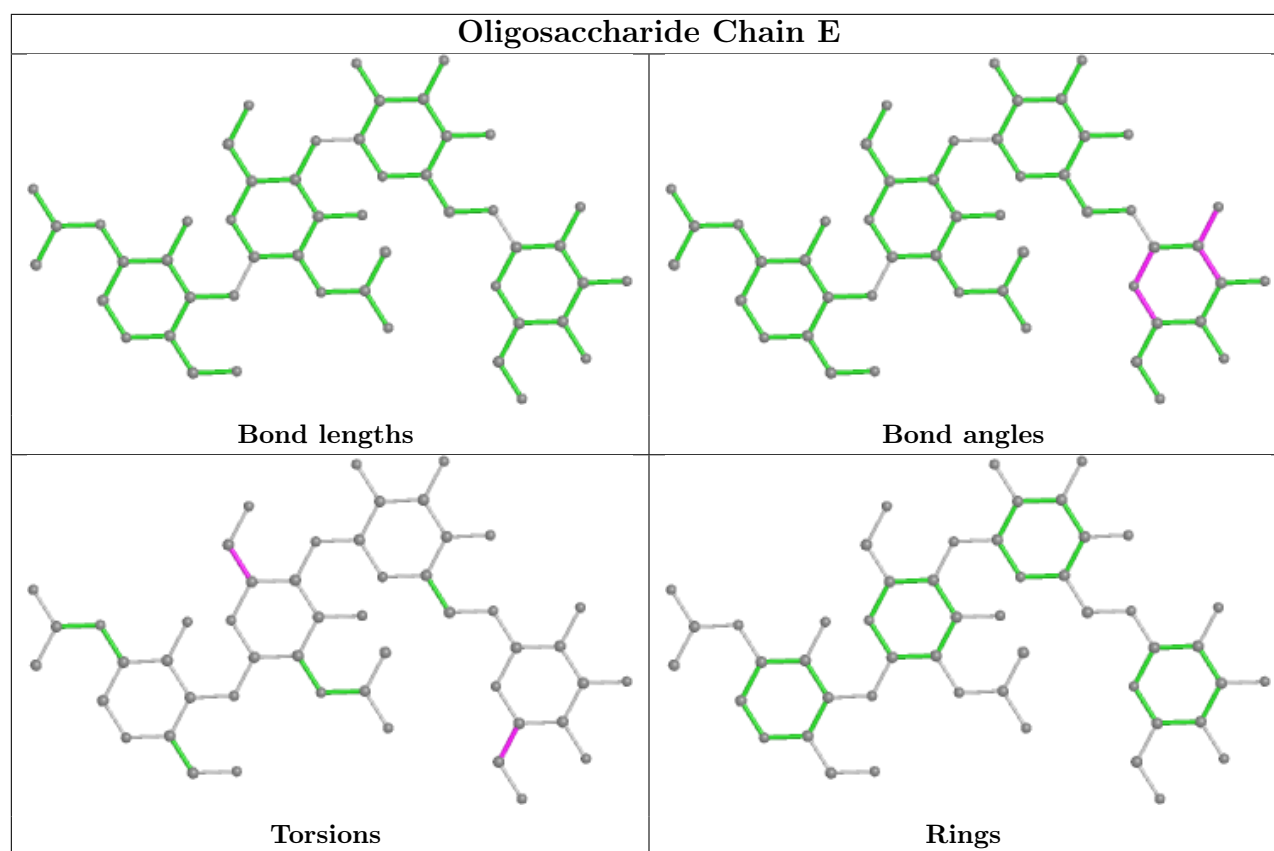
Mol	Chain	Res	Type	Atoms
4	I	3	BMA	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6

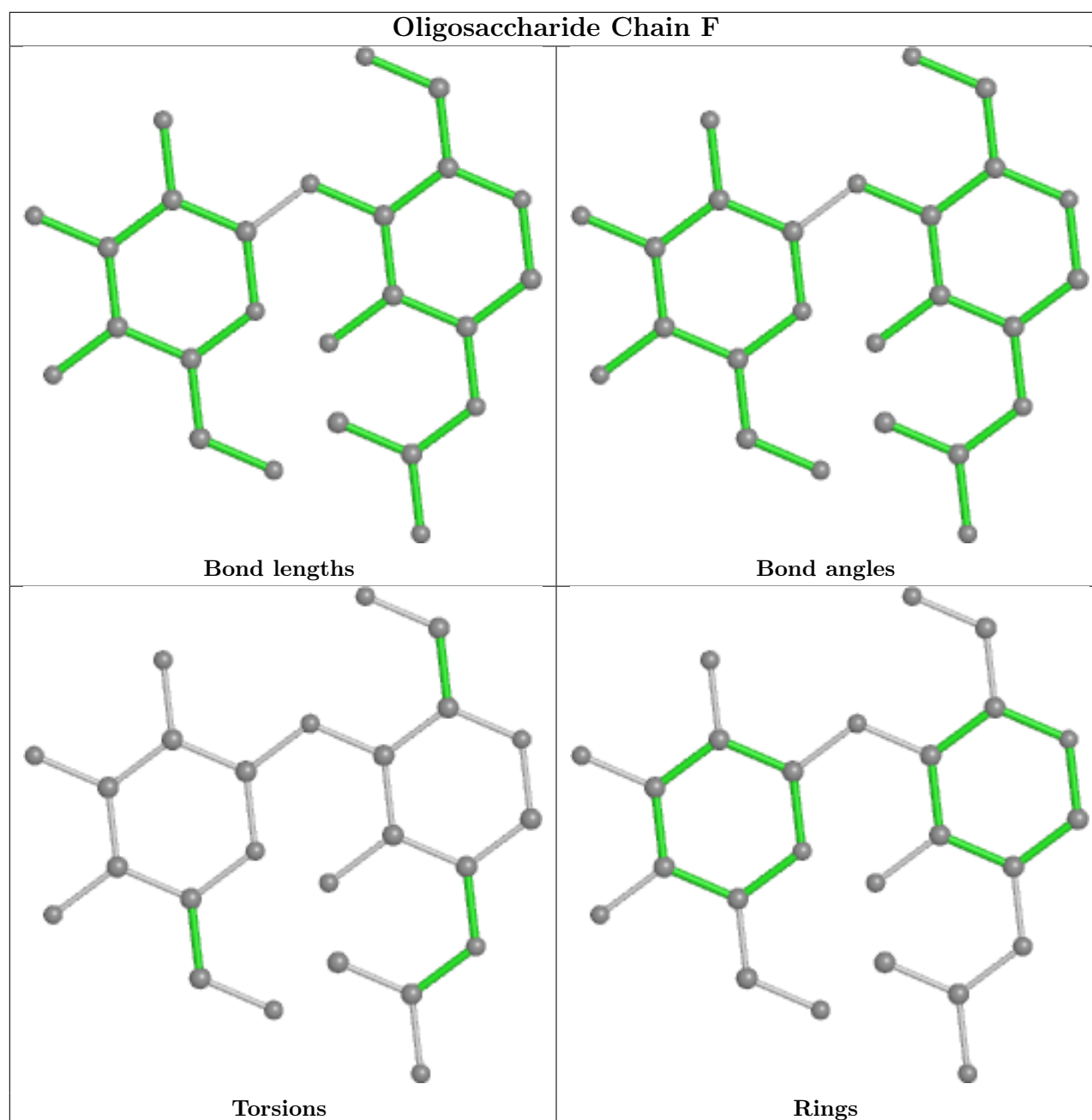
There are no ring outliers.

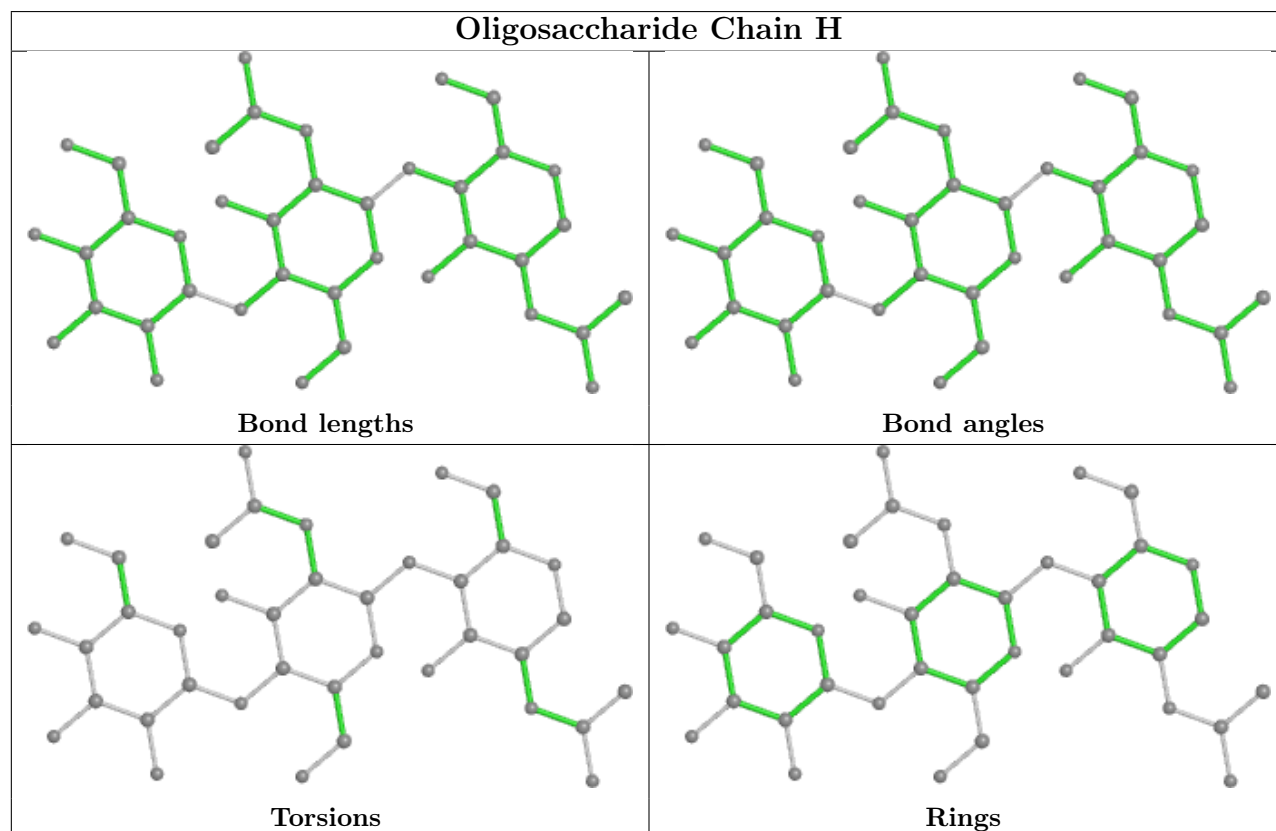
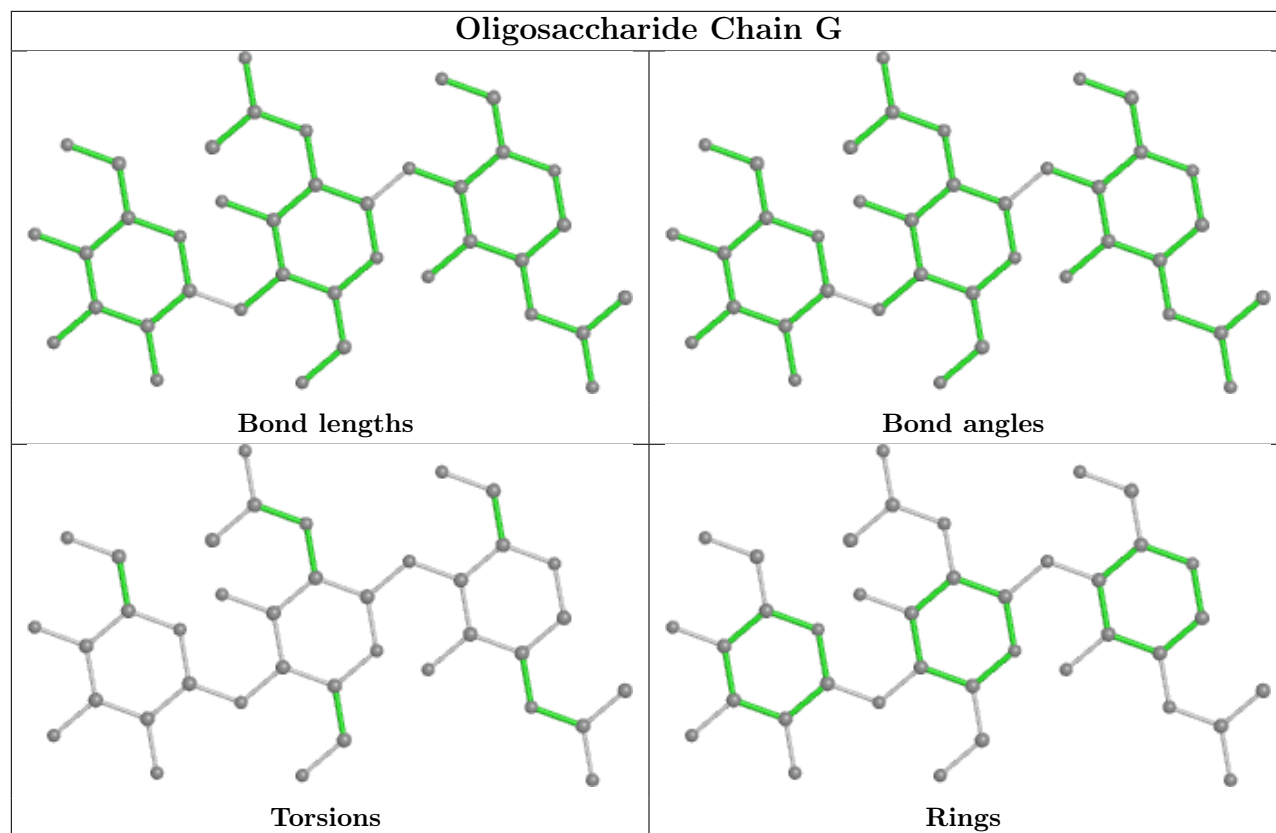
8 monomers are involved in 14 short contacts:

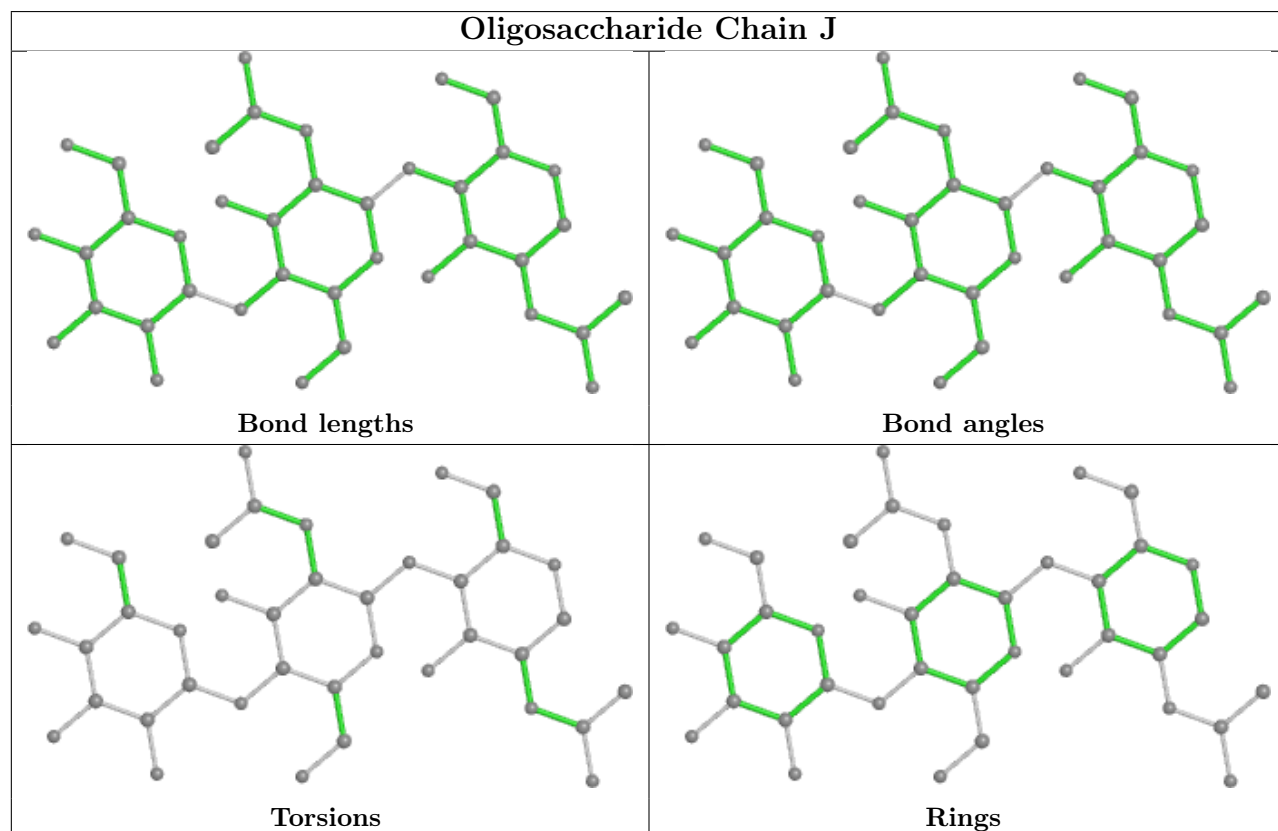
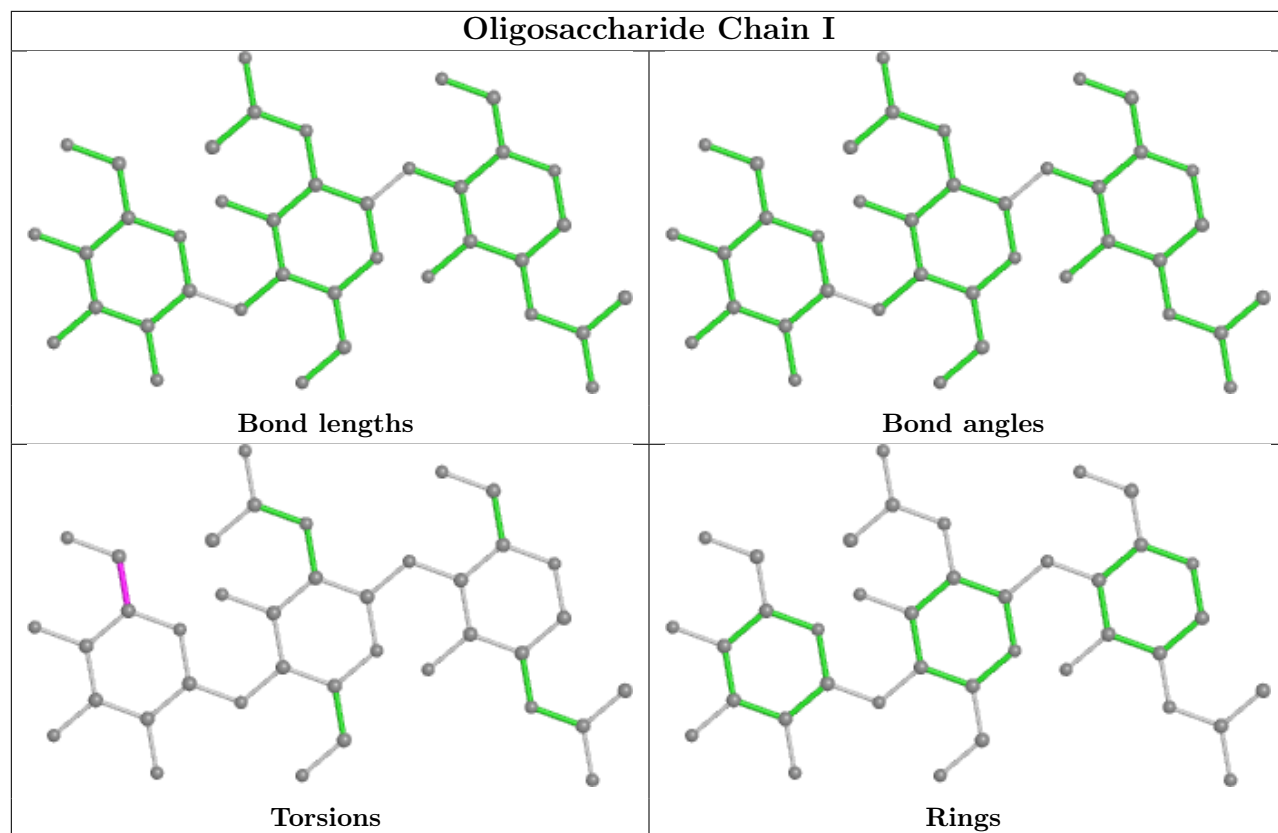
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	3	BMA	3	0
6	N	1	NAG	1	0
4	O	1	NAG	1	0
5	K	3	BMA	3	0
4	H	3	BMA	2	0
2	E	1	NAG	1	0
4	H	1	NAG	1	0
4	G	3	BMA	2	0

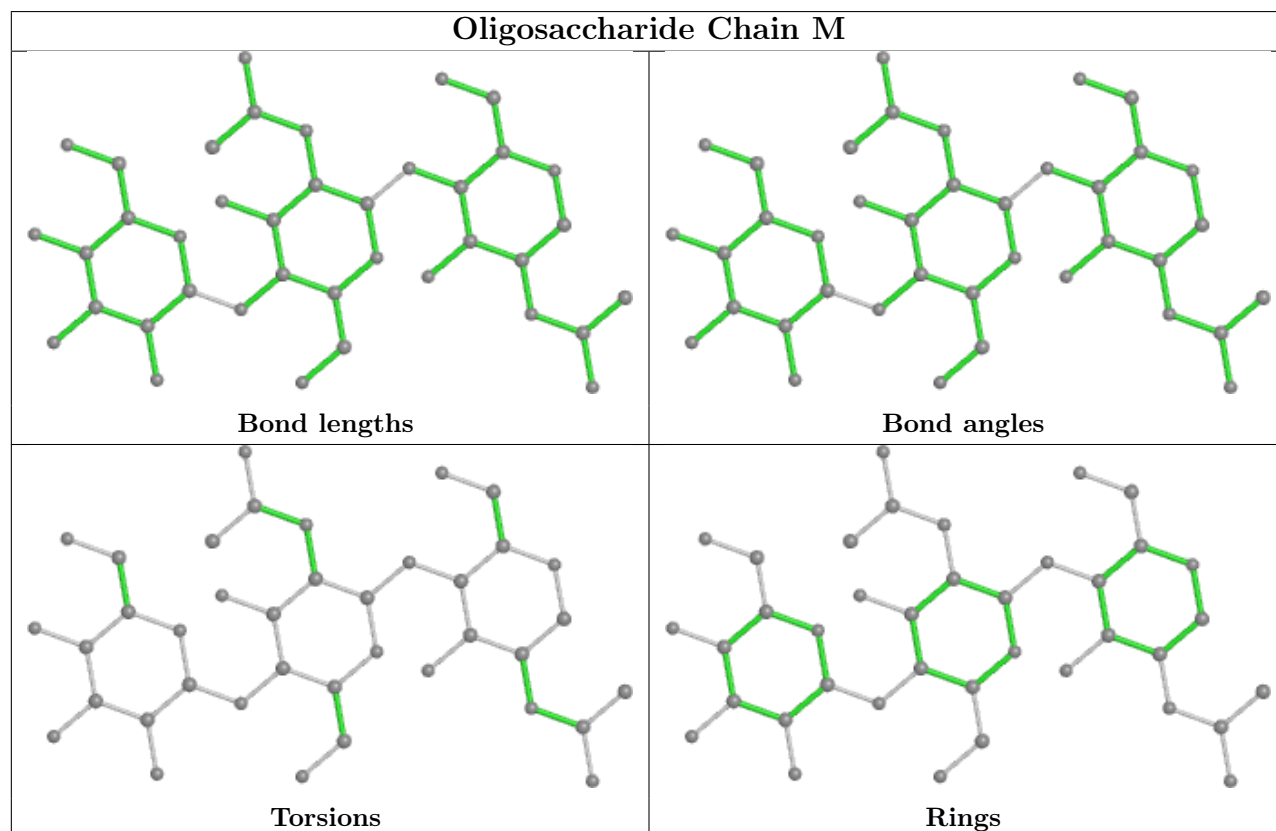
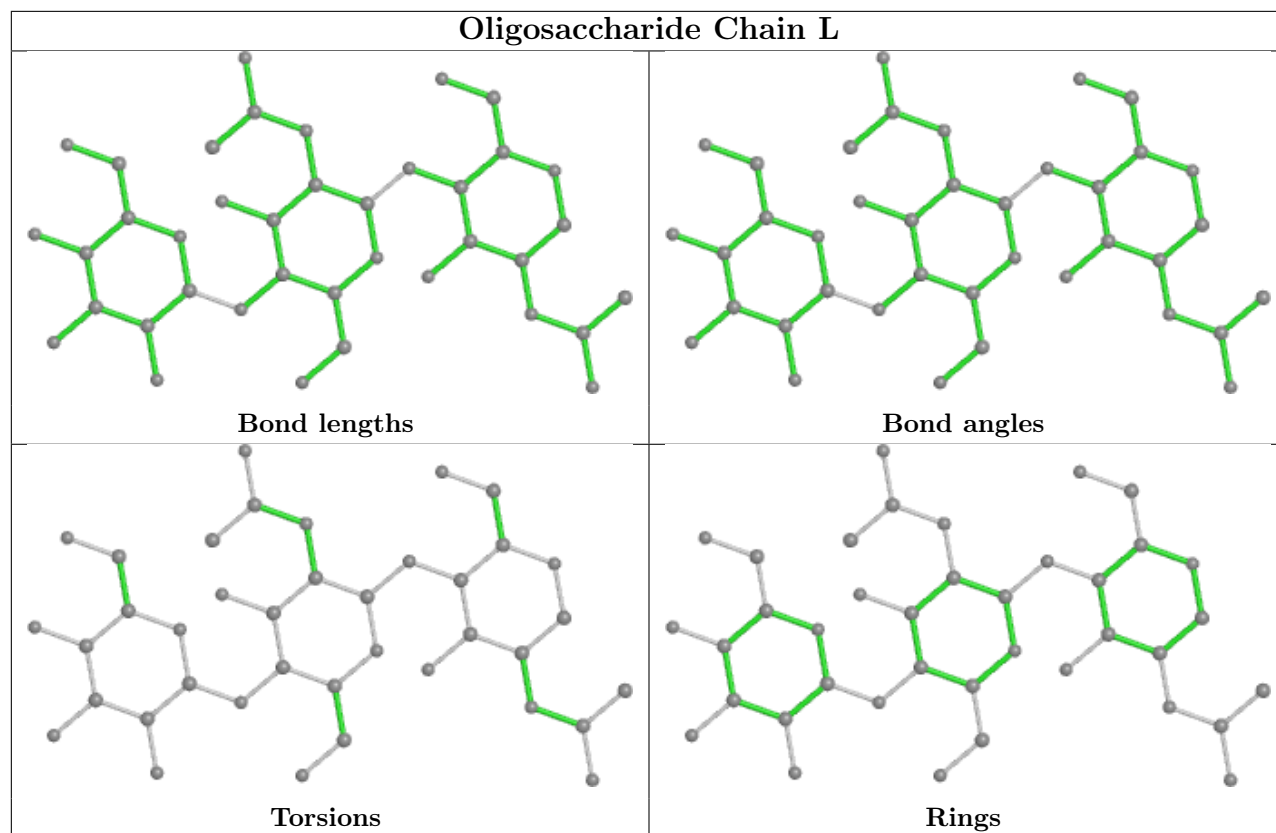
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

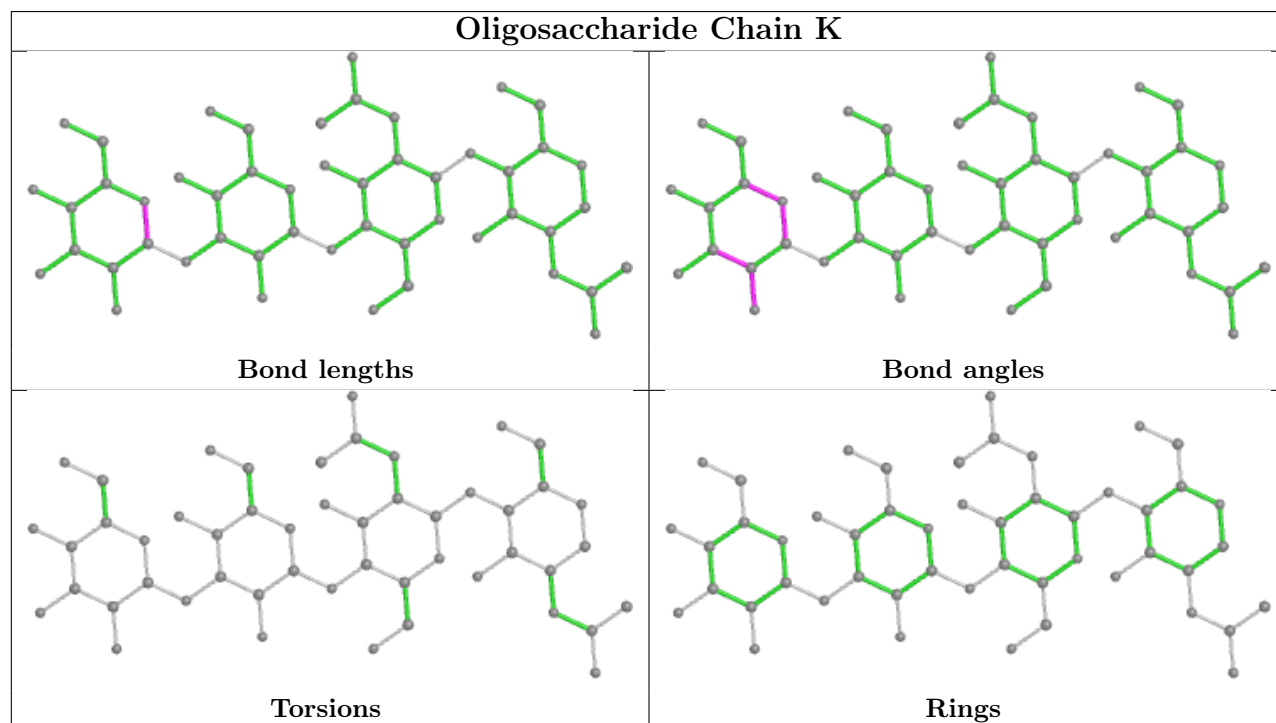
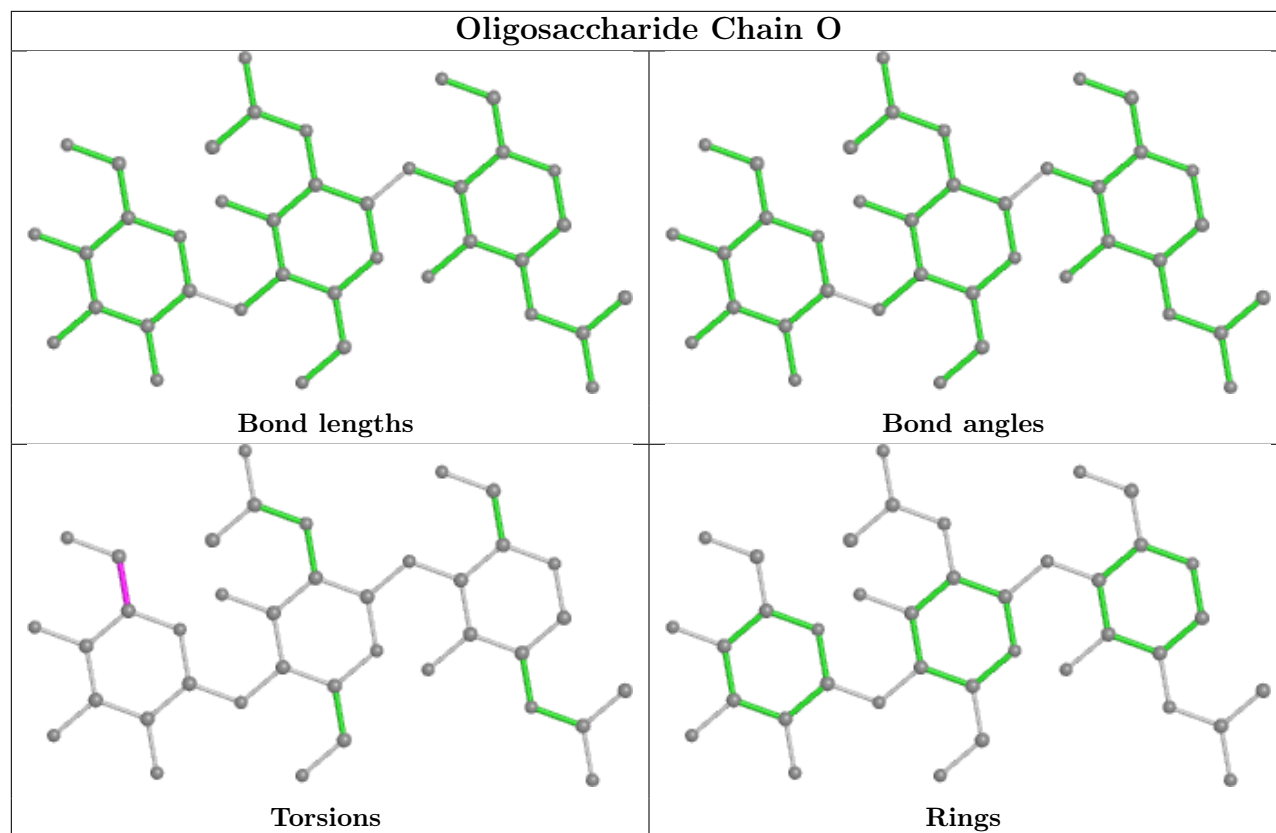


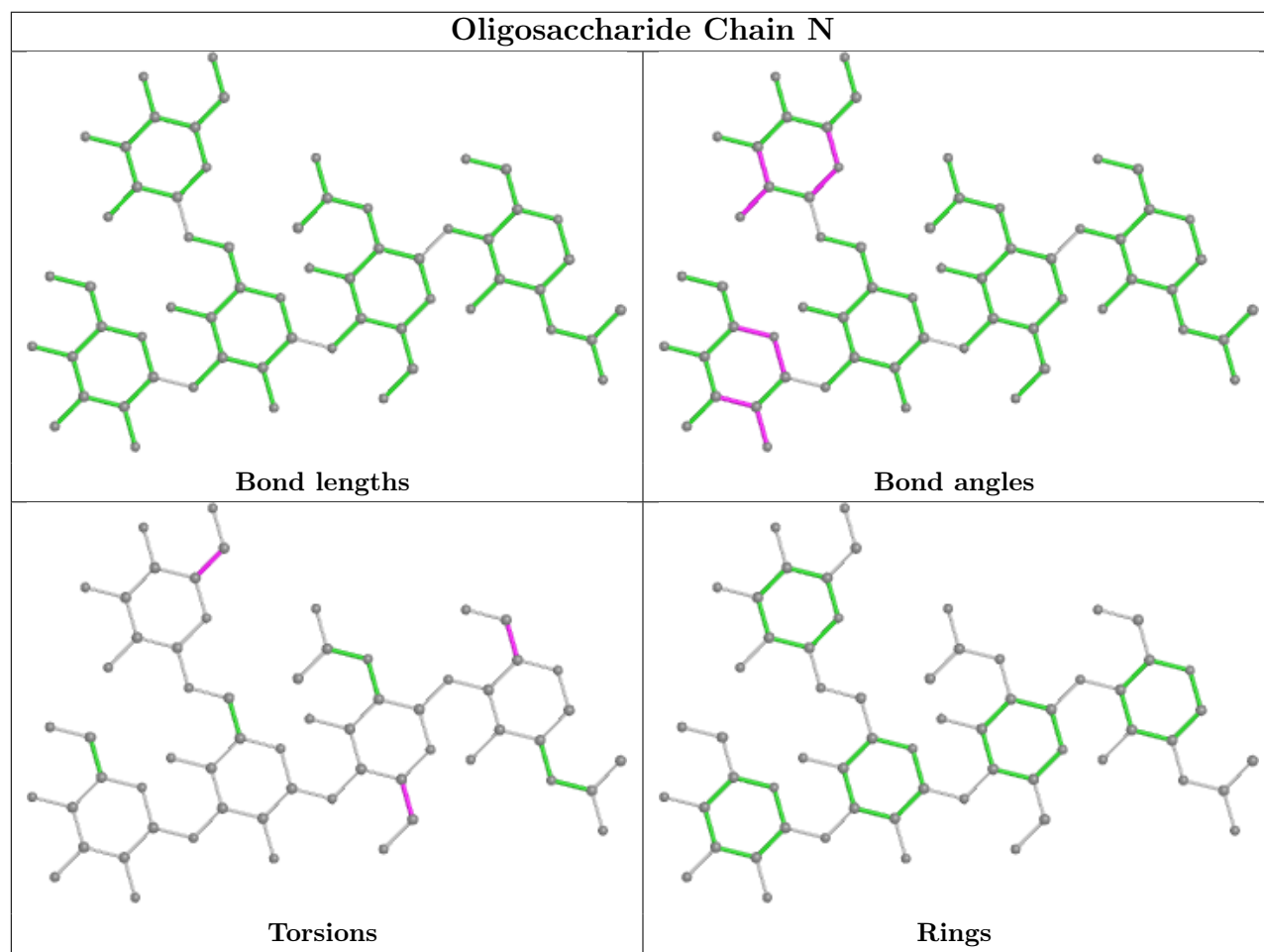
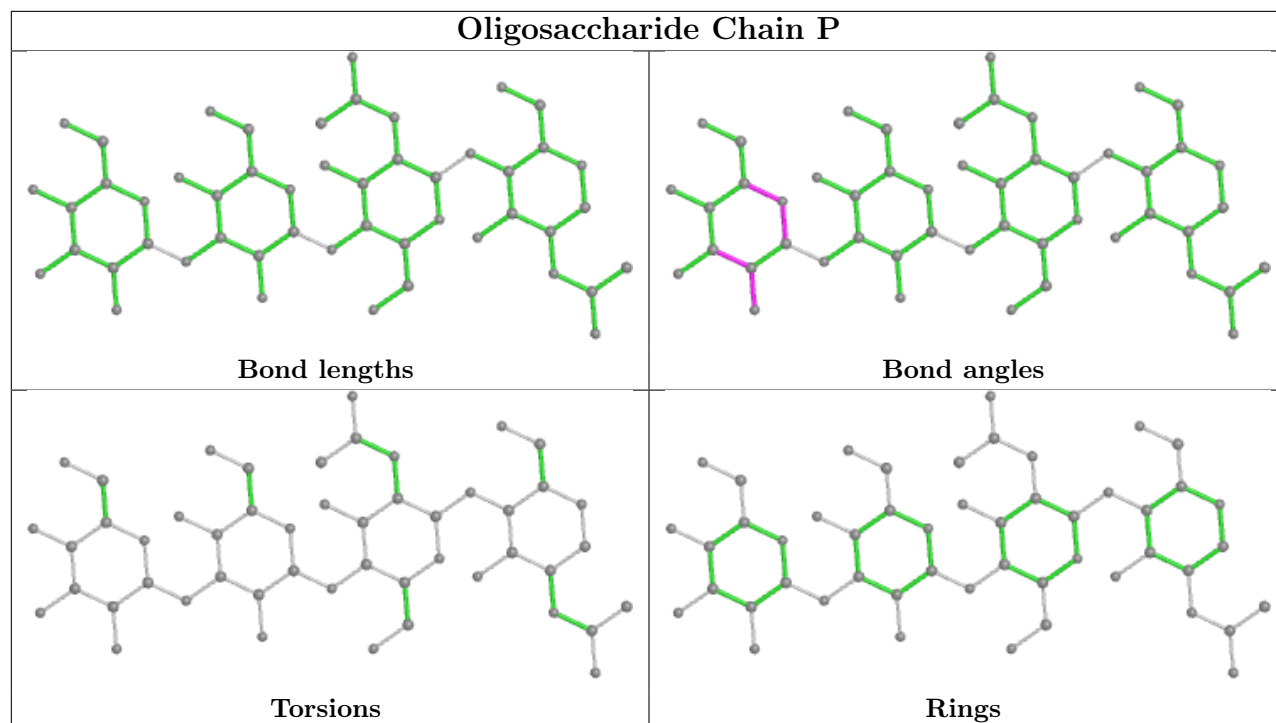












## 5.6 Ligand geometry

30 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$
8	NAG	A	1006	1	14,14,15	0.21	0	17,19,21	0.42	0
8	NAG	C	909	1	14,14,15	0.22	0	17,19,21	0.41	0
7	MAN	B	1013	-	11,11,12	0.74	0	15,15,17	1.00	2 (13%)
7	MAN	B	1014	-	11,11,12	0.67	0	15,15,17	1.07	2 (13%)
7	MAN	D	914	-	11,11,12	0.70	0	15,15,17	1.08	2 (13%)
8	NAG	A	1016	1	14,14,15	0.20	0	17,19,21	0.41	0
8	NAG	B	1017	-	14,14,15	0.23	0	17,19,21	0.39	0
8	NAG	A	1009	1	14,14,15	0.23	0	17,19,21	0.39	0
8	NAG	B	1016	-	14,14,15	0.20	0	17,19,21	0.42	0
8	NAG	C	915	1	14,14,15	0.23	0	17,19,21	0.39	0
7	MAN	A	1005	-	11,11,12	0.68	0	15,15,17	1.05	2 (13%)
7	MAN	B	1005	-	11,11,12	0.71	0	15,15,17	1.07	2 (13%)
9	U57	A	1017	-	19,22,22	1.36	4 (21%)	24,31,31	1.78	5 (20%)
9	U57	C	917	-	19,22,22	1.36	4 (21%)	24,31,31	1.84	6 (25%)
8	NAG	B	1009	-	14,14,15	0.24	0	17,19,21	0.39	0
7	MAN	B	1004	-	11,11,12	0.73	0	15,15,17	0.99	2 (13%)
8	NAG	B	1015	1	14,14,15	0.19	0	17,19,21	0.42	0
7	MAN	C	914	-	11,11,12	0.70	0	15,15,17	1.02	2 (13%)
8	NAG	D	917	1	14,14,15	0.19	0	17,19,21	0.44	0
9	U57	B	1018	-	19,22,22	1.35	4 (21%)	24,31,31	1.74	5 (20%)
9	U57	D	918	-	19,22,22	1.36	4 (21%)	24,31,31	1.79	5 (20%)
8	NAG	D	915	1	14,14,15	0.20	0	17,19,21	0.41	0
7	MAN	C	913	-	11,11,12	0.73	0	15,15,17	1.01	2 (13%)
7	MAN	C	905	-	11,11,12	0.71	0	15,15,17	1.01	2 (13%)
8	NAG	C	916	1	14,14,15	0.20	0	17,19,21	0.44	0
8	NAG	A	1014	1	14,14,15	0.17	0	17,19,21	0.47	0
8	NAG	A	1015	1	14,14,15	0.26	0	17,19,21	0.40	0
8	NAG	D	916	-	14,14,15	0.52	0	17,19,21	0.47	0
7	MAN	A	1013	-	11,11,12	0.78	0	15,15,17	1.01	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	D	909	1	14,14,15	0.22	0	17,19,21	0.40	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
8	NAG	A	1006	1	-	0/6/23/26	0/1/1/1
9	U57	D	918	-	-	2/13/13/13	0/2/2/2
7	MAN	B	1013	-	-	2/2/19/22	0/1/1/1
7	MAN	B	1014	-	-	0/2/19/22	0/1/1/1
8	NAG	C	909	1	-	4/6/23/26	0/1/1/1
7	MAN	D	914	-	-	0/2/19/22	0/1/1/1
8	NAG	A	1016	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1017	-	-	0/6/23/26	0/1/1/1
8	NAG	A	1009	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1016	-	-	2/6/23/26	0/1/1/1
8	NAG	C	915	1	-	0/6/23/26	0/1/1/1
7	MAN	A	1005	-	-	0/2/19/22	0/1/1/1
7	MAN	B	1005	-	-	2/2/19/22	0/1/1/1
9	U57	A	1017	-	-	1/13/13/13	0/2/2/2
9	U57	C	917	-	-	2/13/13/13	0/2/2/2
8	NAG	B	1009	-	-	2/6/23/26	0/1/1/1
7	MAN	B	1004	-	-	0/2/19/22	0/1/1/1
8	NAG	B	1015	1	-	2/6/23/26	0/1/1/1
7	MAN	C	914	-	-	0/2/19/22	0/1/1/1
8	NAG	D	917	1	-	0/6/23/26	0/1/1/1
9	U57	B	1018	-	-	1/13/13/13	0/2/2/2
8	NAG	D	915	1	-	2/6/23/26	0/1/1/1
7	MAN	C	913	-	-	0/2/19/22	0/1/1/1
7	MAN	C	905	-	-	2/2/19/22	0/1/1/1
8	NAG	C	916	1	1/1/5/7	1/6/23/26	0/1/1/1
8	NAG	A	1014	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1015	1	-	2/6/23/26	0/1/1/1
8	NAG	D	916	-	-	2/6/23/26	0/1/1/1
7	MAN	A	1013	-	-	0/2/19/22	0/1/1/1
8	NAG	D	909	1	-	2/6/23/26	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1017	U57	C03-N05	2.74	1.36	1.32
9	D	918	U57	C03-N05	2.72	1.36	1.32
9	B	1018	U57	C03-N05	2.72	1.36	1.32
9	C	917	U57	C03-N05	2.69	1.36	1.32
9	A	1017	U57	C07-N08	2.32	1.38	1.33
9	C	917	U57	C07-N08	2.32	1.38	1.33
9	B	1018	U57	C07-N08	2.32	1.38	1.33
9	D	918	U57	C07-N08	2.32	1.38	1.33
9	C	917	U57	C01-N04	-2.29	1.33	1.37
9	C	917	U57	C18-N17	2.26	1.35	1.31
9	D	918	U57	C01-N04	-2.25	1.33	1.37
9	D	918	U57	C18-N17	2.23	1.35	1.31
9	B	1018	U57	C01-N04	-2.22	1.34	1.37
9	A	1017	U57	C18-N17	2.22	1.35	1.31
9	A	1017	U57	C01-N04	-2.21	1.34	1.37
9	B	1018	U57	C18-N17	2.21	1.35	1.31

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	917	U57	C03-C02-N17	4.85	124.84	120.58
9	D	918	U57	C03-C02-N17	4.58	124.61	120.58
9	A	1017	U57	C03-C02-N17	4.51	124.54	120.58
9	B	1018	U57	C03-C02-N17	4.37	124.42	120.58
9	C	917	U57	N04-C07-N05	-3.44	122.63	127.22
9	A	1017	U57	N04-C07-N05	-3.43	122.65	127.22
9	D	918	U57	N04-C07-N05	-3.37	122.72	127.22
9	B	1018	U57	N04-C07-N05	-3.34	122.77	127.22
9	B	1018	U57	C18-N17-C02	2.95	119.73	116.78
9	A	1017	U57	C18-N17-C02	2.95	119.72	116.78
9	D	918	U57	C18-N17-C02	2.94	119.72	116.78
9	C	917	U57	C18-N17-C02	2.92	119.70	116.78
9	C	917	U57	C20-C19-C18	-2.71	118.19	121.89
9	A	1017	U57	C20-C19-C18	-2.63	118.30	121.89
9	D	918	U57	C20-C19-C18	-2.61	118.33	121.89
9	B	1018	U57	C20-C19-C18	-2.60	118.33	121.89
9	C	917	U57	C07-N05-C03	2.43	119.98	114.54
7	B	1014	MAN	C1-O5-C5	2.38	115.42	112.19
9	D	918	U57	C07-N05-C03	2.37	119.84	114.54
7	C	914	MAN	C1-O5-C5	2.36	115.39	112.19
7	B	1013	MAN	C1-O5-C5	2.34	115.37	112.19
9	A	1017	U57	C07-N05-C03	2.34	119.79	114.54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1005	MAN	C1-O5-C5	2.32	115.34	112.19
9	B	1018	U57	C07-N05-C03	2.30	119.69	114.54
7	D	914	MAN	C1-O5-C5	2.30	115.31	112.19
7	C	914	MAN	O2-C2-C3	-2.28	105.56	110.14
7	B	1005	MAN	C1-O5-C5	2.28	115.28	112.19
7	B	1014	MAN	O2-C2-C3	-2.28	105.57	110.14
7	C	905	MAN	O2-C2-C3	-2.28	105.58	110.14
7	C	905	MAN	C1-O5-C5	2.27	115.27	112.19
7	C	913	MAN	C1-O5-C5	2.27	115.27	112.19
7	B	1013	MAN	O2-C2-C3	-2.26	105.61	110.14
7	C	913	MAN	O2-C2-C3	-2.25	105.63	110.14
7	B	1004	MAN	O2-C2-C3	-2.24	105.64	110.14
7	B	1004	MAN	C1-O5-C5	2.23	115.22	112.19
7	A	1005	MAN	O2-C2-C3	-2.23	105.68	110.14
7	B	1005	MAN	O2-C2-C3	-2.22	105.69	110.14
7	D	914	MAN	O2-C2-C3	-2.20	105.72	110.14
7	A	1013	MAN	O2-C2-C3	-2.16	105.81	110.14
9	C	917	U57	C19-C18-N17	2.15	122.75	121.46
7	A	1013	MAN	C1-O5-C5	2.10	115.04	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	C	916	NAG	C1

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1017	U57	C13-C09-C10-C11
7	B	1005	MAN	O5-C5-C6-O6
8	D	916	NAG	O5-C5-C6-O6
8	B	1015	NAG	C4-C5-C6-O6
8	D	915	NAG	C4-C5-C6-O6
8	D	915	NAG	O5-C5-C6-O6
8	A	1014	NAG	C4-C5-C6-O6
8	D	916	NAG	C4-C5-C6-O6
8	A	1014	NAG	O5-C5-C6-O6
7	B	1005	MAN	C4-C5-C6-O6
8	B	1015	NAG	O5-C5-C6-O6
8	A	1015	NAG	C4-C5-C6-O6
8	B	1016	NAG	C4-C5-C6-O6
8	C	909	NAG	C8-C7-N2-C2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	C	909	NAG	O7-C7-N2-C2
8	A	1009	NAG	C8-C7-N2-C2
8	A	1009	NAG	O7-C7-N2-C2
8	B	1009	NAG	C8-C7-N2-C2
8	B	1009	NAG	O7-C7-N2-C2
8	D	909	NAG	C8-C7-N2-C2
8	D	909	NAG	O7-C7-N2-C2
8	A	1015	NAG	O5-C5-C6-O6
8	B	1016	NAG	O5-C5-C6-O6
7	C	905	MAN	O5-C5-C6-O6
8	C	909	NAG	O5-C5-C6-O6
7	B	1013	MAN	O5-C5-C6-O6
8	C	909	NAG	C4-C5-C6-O6
7	C	905	MAN	C4-C5-C6-O6
9	C	917	U57	C10-C11-C12-C15
9	D	918	U57	C13-C09-C10-C11
9	C	917	U57	C09-C10-C11-C12
7	B	1013	MAN	C4-C5-C6-O6
8	C	916	NAG	C4-C5-C6-O6
9	B	1018	U57	C10-C09-C13-O14
9	D	918	U57	C10-C09-C13-O14

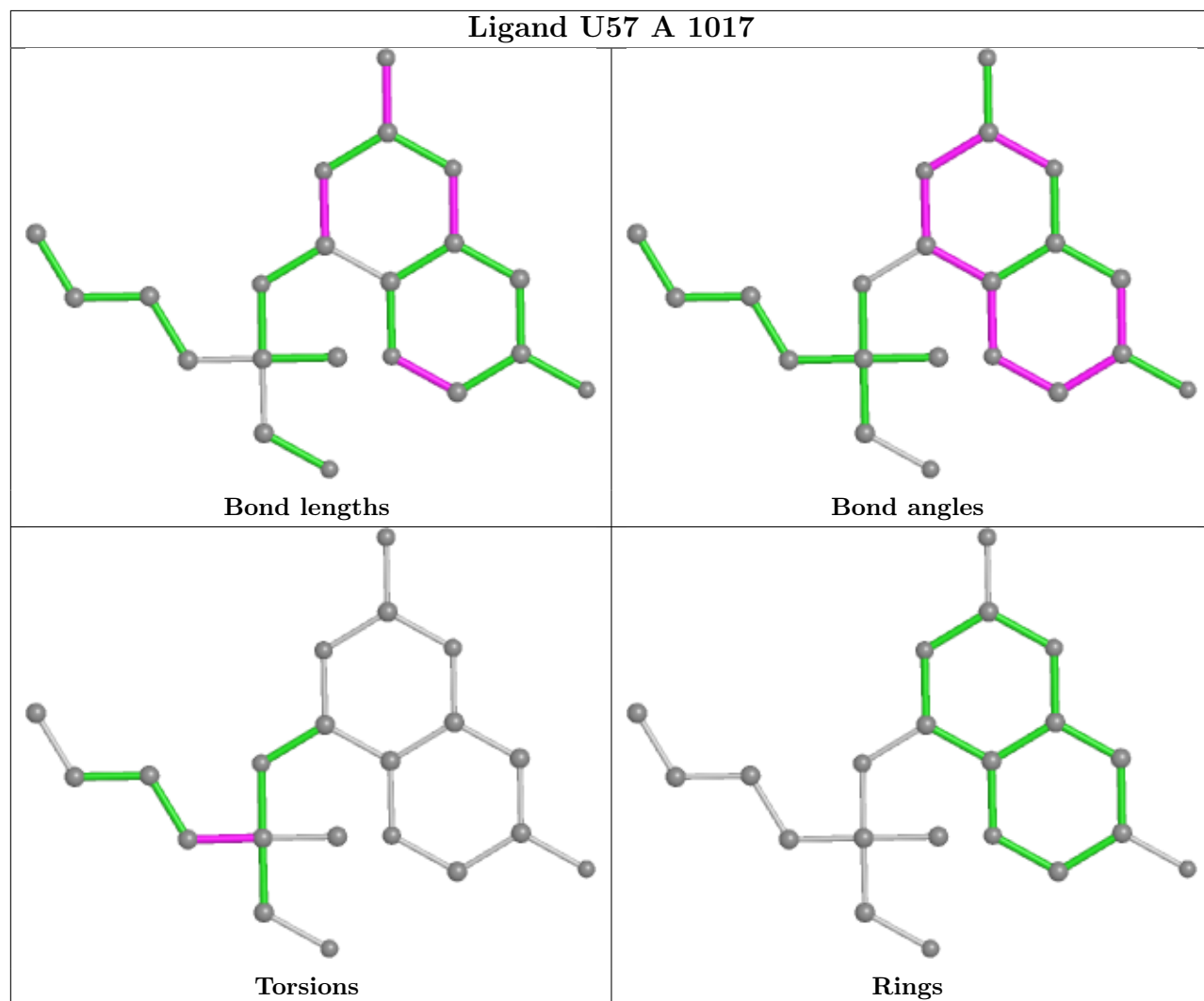
There are no ring outliers.

6 monomers are involved in 19 short contacts:

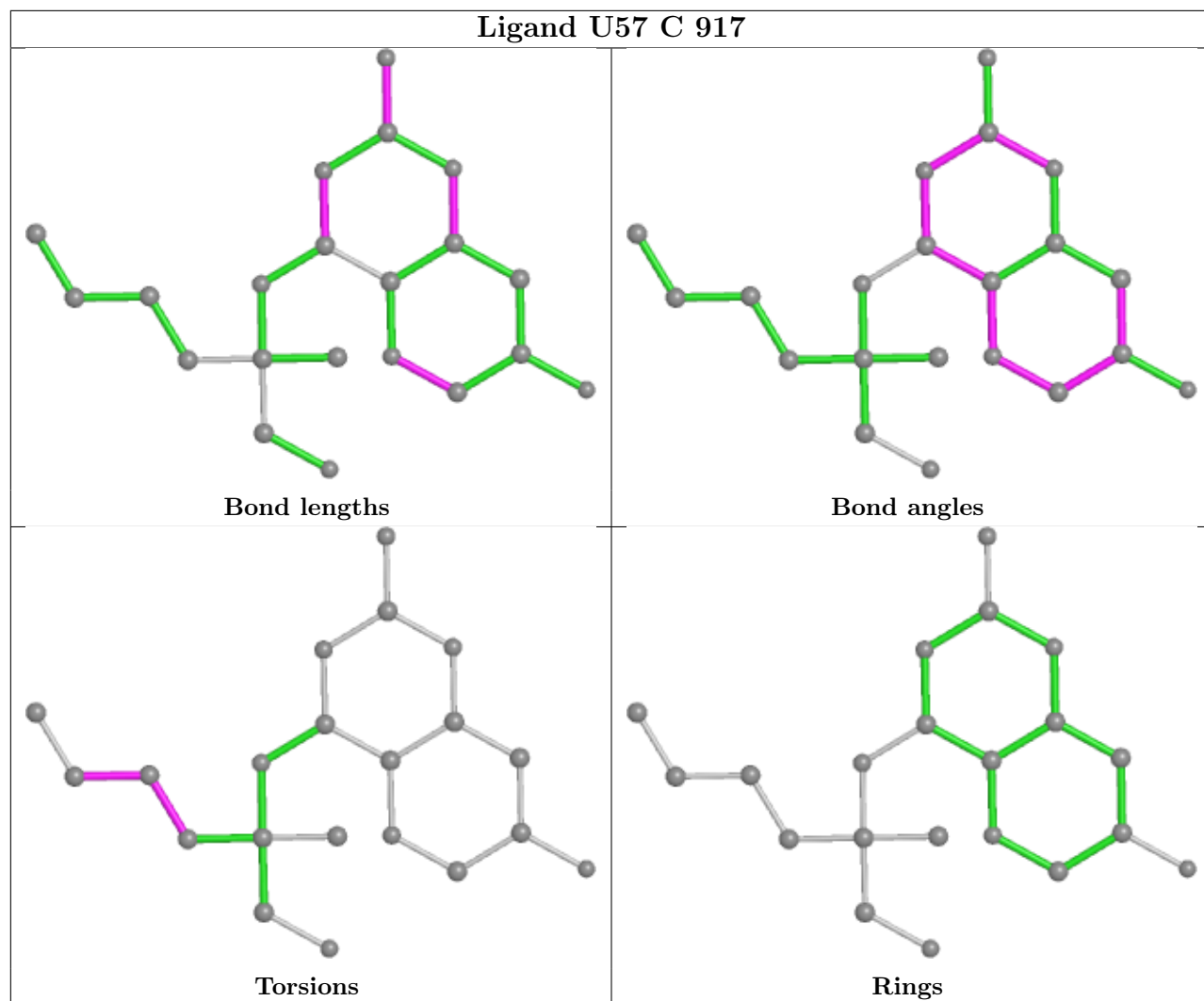
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1016	NAG	3	0
7	B	1004	MAN	2	0
7	C	913	MAN	3	0
7	C	905	MAN	3	0
8	D	916	NAG	5	1
7	A	1013	MAN	2	0

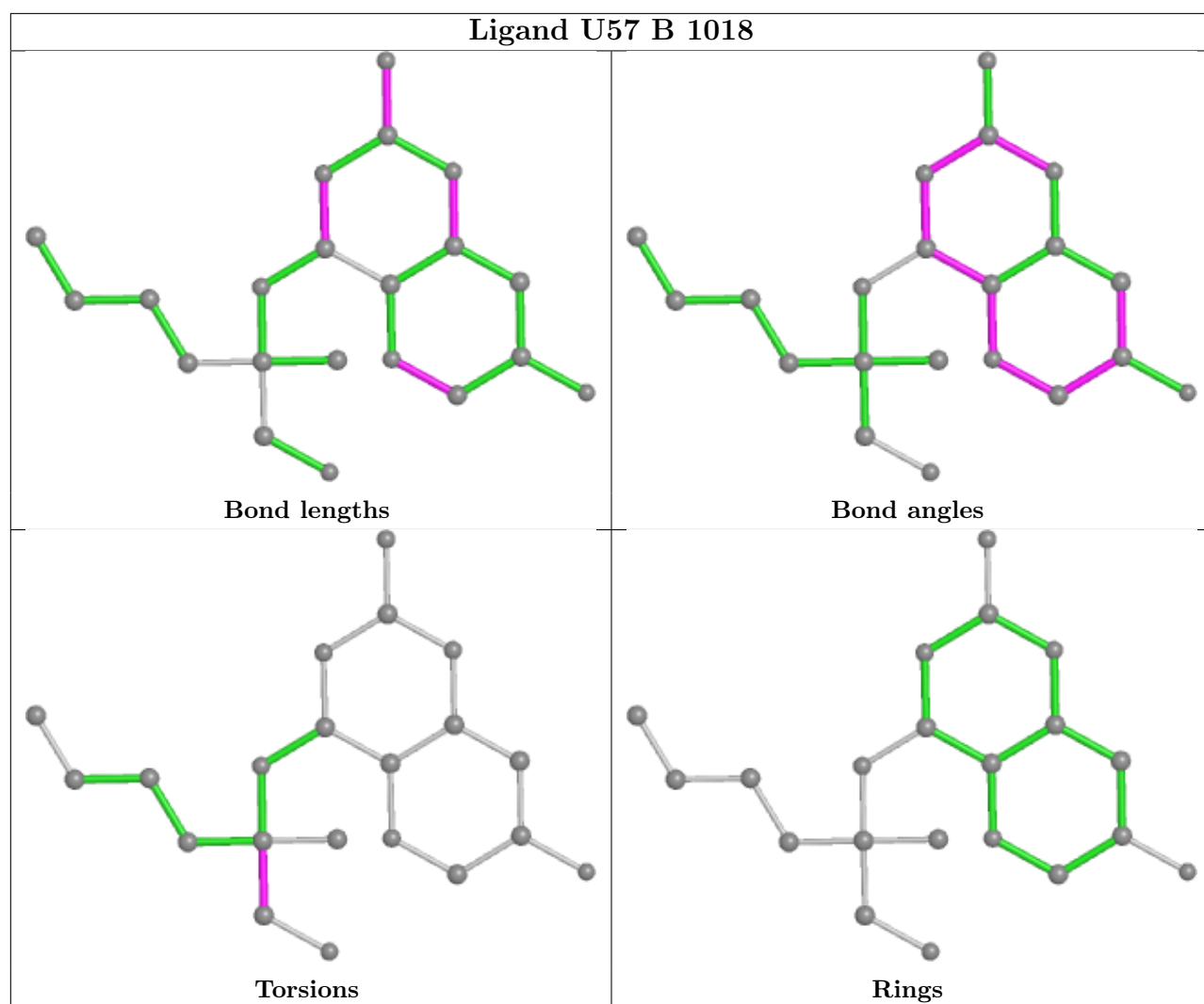
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

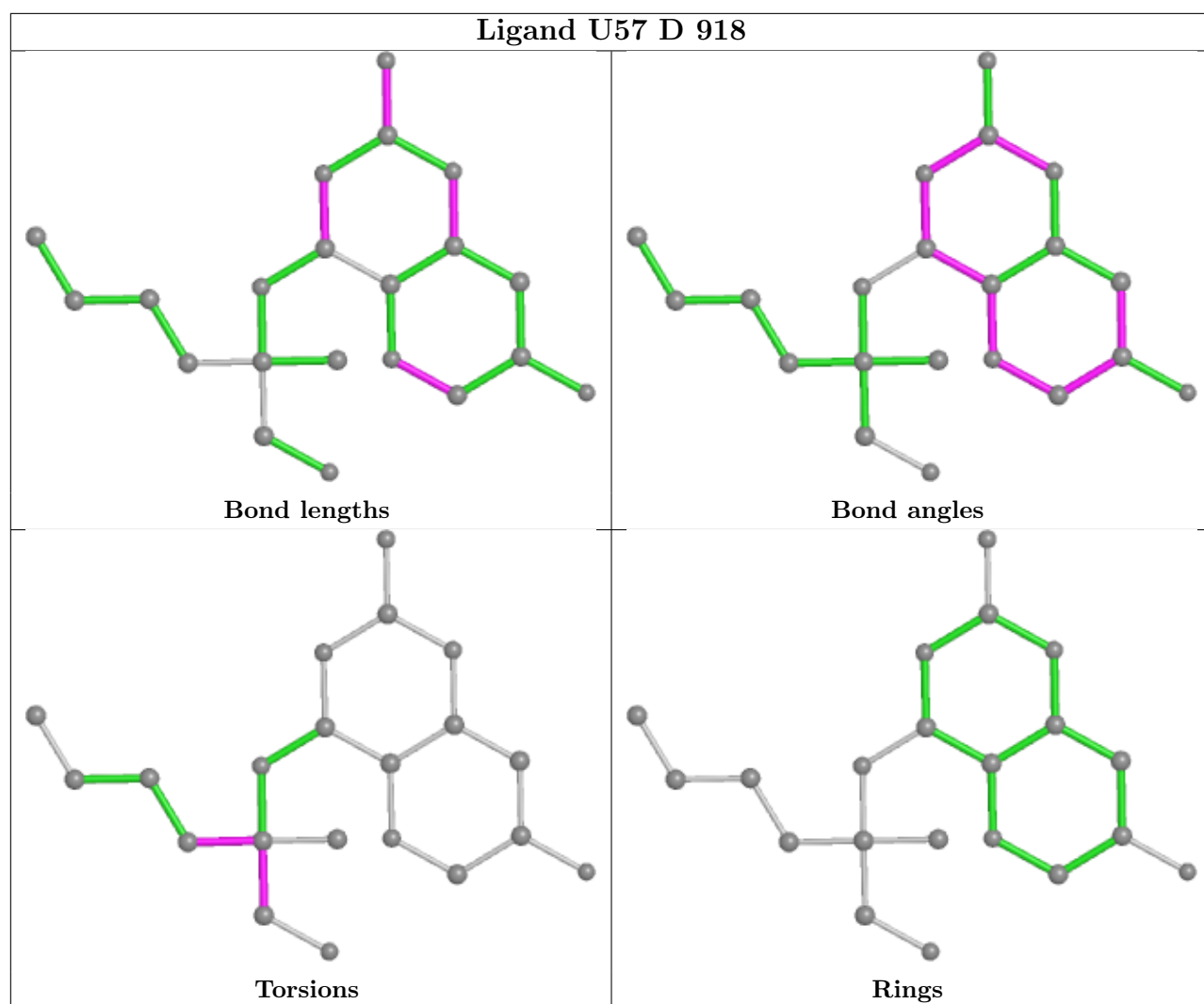
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## Ligand U57 C 917







## 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	743/811 (91%)	-0.10	5 (0%) 87 89	31, 47, 74, 105	0
1	B	751/811 (92%)	0.10	17 (2%) 60 63	31, 52, 91, 125	0
1	C	681/811 (83%)	0.24	36 (5%) 26 28	34, 58, 95, 130	0
1	D	708/811 (87%)	0.25	36 (5%) 28 29	33, 61, 93, 113	0
All	All	2883/3244 (88%)	0.11	94 (3%) 46 50	31, 54, 91, 130	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	86	LEU	6.3
1	D	814	ILE	5.5
1	C	64	TYR	5.3
1	C	166	ILE	4.5
1	D	459	PHE	4.4
1	B	760	THR	4.0
1	B	780	ILE	3.9
1	C	45	VAL	3.9
1	C	664	ALA	3.9
1	C	690	LEU	3.8
1	D	138	PRO	3.7
1	D	35	PRO	3.7
1	B	124	LEU	3.6
1	D	416	ASN	3.6
1	B	761	THR	3.6
1	C	87	GLN	3.5
1	D	776	CYS	3.5
1	C	47	ALA	3.4
1	A	702[A]	PHE	3.3
1	B	45	VAL	3.3
1	D	141	PRO	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	46	ILE	3.3
1	C	43	ASP	3.2
1	D	246	ILE	3.2
1	D	244	GLY	3.1
1	C	433	LEU	3.1
1	C	688	PRO	3.1
1	D	54	LEU	3.1
1	B	85	GLY	3.1
1	B	64	TYR	3.1
1	C	65	VAL	3.0
1	C	88	ASN	3.0
1	D	186	VAL	2.9
1	B	41	GLN	2.9
1	C	38	GLU	2.9
1	C	42	ASN	2.8
1	C	689	ARG	2.8
1	D	98	PRO	2.8
1	D	49	CYS	2.8
1	D	75	ILE	2.8
1	C	46	ILE	2.7
1	C	31	SER	2.7
1	C	86	LEU	2.7
1	C	32	ARG	2.6
1	D	307	PHE	2.6
1	D	783	PHE	2.6
1	A	61	VAL	2.6
1	D	224	LEU	2.5
1	C	39	LYS	2.5
1	D	36	CYS	2.5
1	D	213	LEU	2.5
1	C	44	SER	2.5
1	C	765	SER	2.5
1	C	62	GLY	2.5
1	B	42	ASN	2.4
1	B	59	GLN	2.4
1	D	433	LEU	2.4
1	D	766	MET	2.4
1	D	160	ASN	2.4
1	B	144	LEU	2.4
1	C	70	LEU	2.4
1	C	798	LEU	2.4
1	C	63	LYS	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	417	PHE	2.4
1	B	733	SER	2.3
1	D	137	LEU	2.3
1	D	70	LEU	2.3
1	C	41	GLN	2.3
1	D	219	LYS	2.3
1	D	37	ASP	2.3
1	D	728	PRO	2.3
1	B	810	ARG	2.3
1	C	695	LEU	2.2
1	D	78	ILE	2.2
1	D	34	TYR	2.2
1	D	795	ILE	2.2
1	C	678	PHE	2.2
1	B	791	LEU	2.2
1	C	83	PHE	2.2
1	A	100	VAL	2.1
1	C	92	ILE	2.1
1	B	734	GLU	2.1
1	D	278	ILE	2.1
1	C	127	LEU	2.1
1	C	124	LEU	2.1
1	D	55	GLN	2.1
1	C	200	LEU	2.1
1	D	245	LEU	2.0
1	C	796	PRO	2.0
1	A	732	LEU	2.0
1	D	159	TYR	2.0
1	C	679	PHE	2.0
1	D	135	ASN	2.0
1	A	678	PHE	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](#)

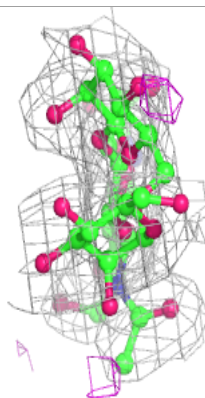
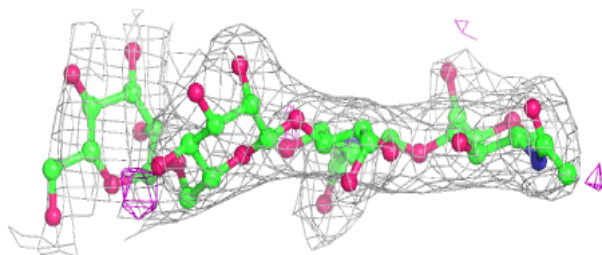
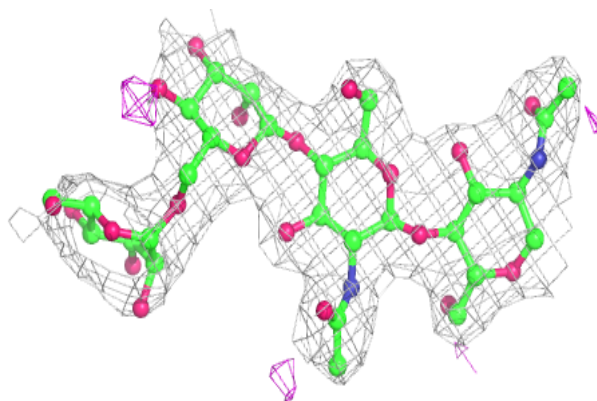
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BMA	L	3	11/12	0.80	0.20	83,91,100,102	0
4	BMA	I	3	11/12	0.83	0.17	77,87,94,101	0
6	MAN	N	5	11/12	0.84	0.15	78,87,95,102	0
3	BMA	F	2	11/12	0.84	0.21	72,80,90,92	0
4	BMA	O	3	11/12	0.86	0.18	93,98,104,104	0
5	MAN	P	4	11/12	0.88	0.26	87,95,107,108	0
6	MAN	N	4	11/12	0.89	0.15	70,81,89,94	0
2	MAN	E	4	11/12	0.90	0.15	67,73,85,99	0
5	BMA	K	3	11/12	0.92	0.13	52,62,72,73	0
5	MAN	K	4	11/12	0.92	0.18	59,77,83,83	0
4	NAG	L	2	14/15	0.92	0.16	54,64,82,86	0
6	BMA	N	3	11/12	0.92	0.09	67,69,80,83	0
4	BMA	H	3	11/12	0.94	0.13	57,63,69,72	0
4	NAG	O	2	14/15	0.94	0.14	61,71,85,92	0
2	BMA	E	3	11/12	0.94	0.12	47,59,68,69	0
4	NAG	M	2	14/15	0.94	0.14	46,58,73,84	0
4	BMA	G	3	11/12	0.94	0.10	50,61,71,72	0
5	BMA	P	3	11/12	0.95	0.10	53,70,79,87	0
5	NAG	K	2	14/15	0.95	0.15	41,49,56,56	0
4	BMA	J	3	11/12	0.95	0.14	56,67,79,83	0
4	NAG	I	2	14/15	0.95	0.14	46,56,69,74	0
4	NAG	H	2	14/15	0.95	0.12	35,47,56,60	0
4	NAG	L	1	14/15	0.95	0.18	41,48,53,57	0
3	NAG	F	1	14/15	0.95	0.15	44,56,68,72	0
6	NAG	N	2	14/15	0.95	0.13	44,58,68,73	0
4	NAG	M	1	14/15	0.96	0.13	40,50,54,54	0
4	NAG	H	1	14/15	0.96	0.16	35,46,55,56	0
6	NAG	N	1	14/15	0.96	0.17	46,50,58,64	0
5	NAG	P	1	14/15	0.96	0.17	29,35,42,44	0
5	NAG	P	2	14/15	0.96	0.18	36,39,54,62	0
2	NAG	E	1	14/15	0.97	0.19	30,34,39,48	0
2	NAG	E	2	14/15	0.97	0.11	29,39,51,53	0
4	NAG	G	1	14/15	0.97	0.12	23,37,42,48	0
4	BMA	M	3	11/12	0.97	0.16	76,83,96,101	0
5	NAG	K	1	14/15	0.97	0.16	29,41,45,46	0
4	NAG	J	2	14/15	0.97	0.12	28,43,51,58	0
4	NAG	I	1	14/15	0.97	0.17	30,36,45,47	0
4	NAG	G	2	14/15	0.97	0.14	29,45,53,56	0
4	NAG	O	1	14/15	0.98	0.18	36,42,52,52	0
4	NAG	J	1	14/15	0.98	0.12	28,39,41,43	0

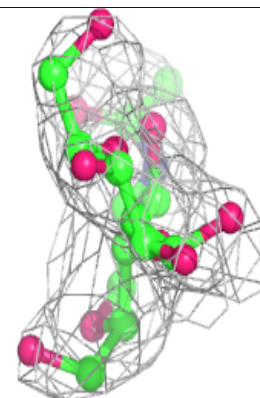
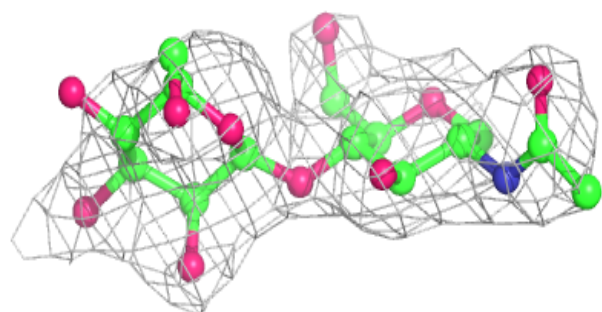
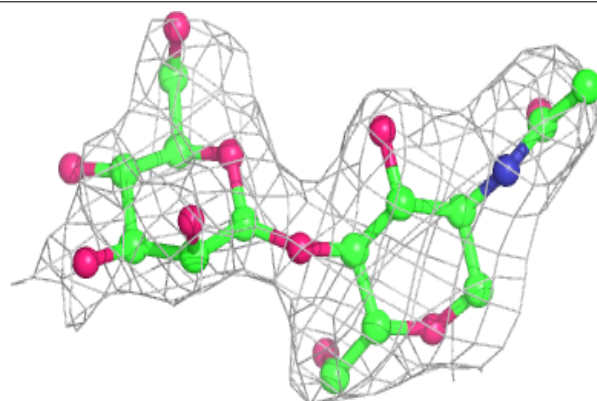
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain E:**

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

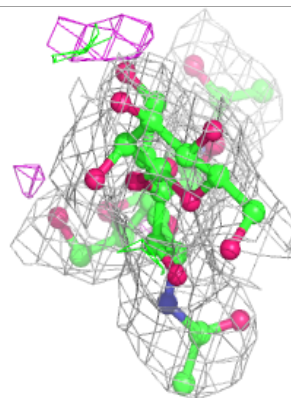
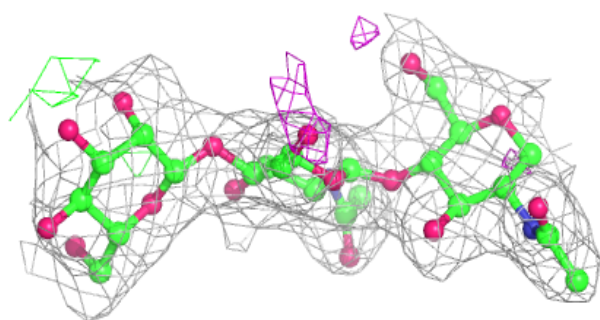
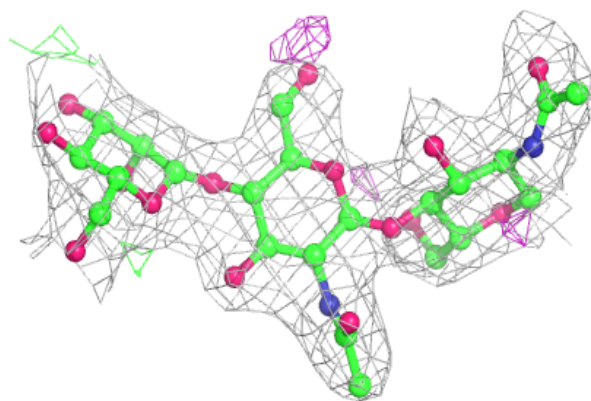
**Electron density around Chain F:**

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

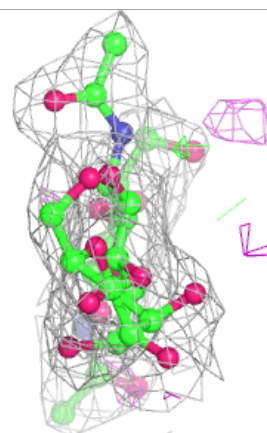
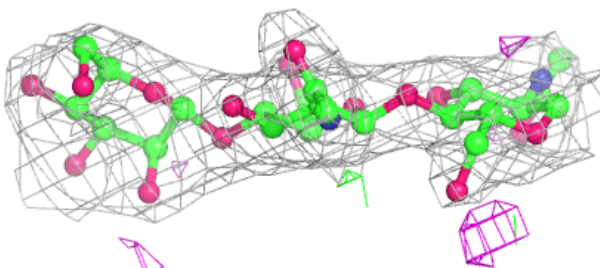
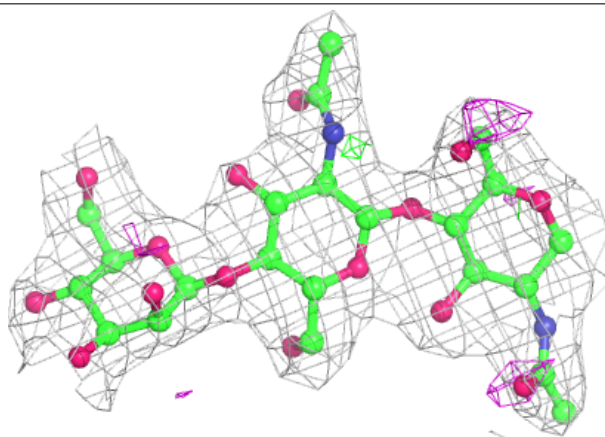


**Electron density around Chain G:**

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

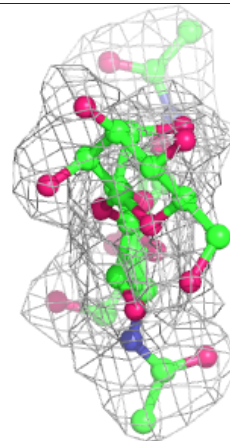
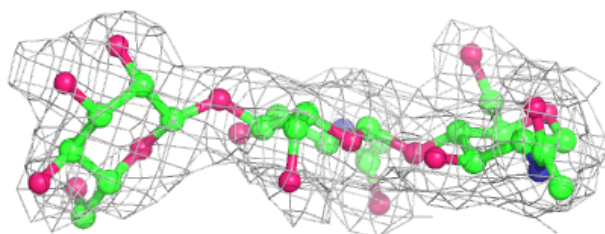
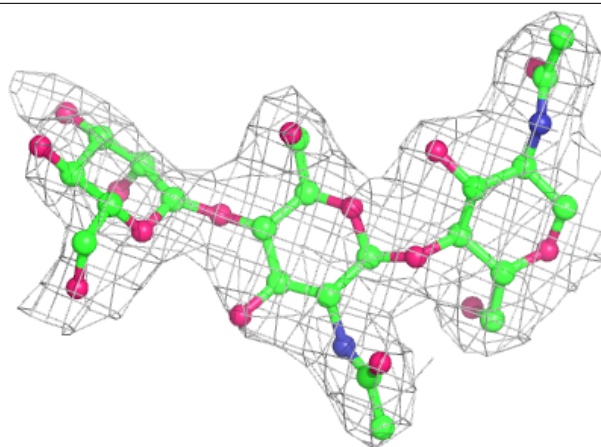
**Electron density around Chain H:**

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

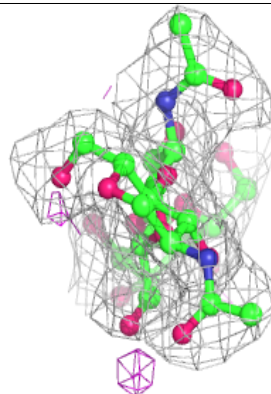
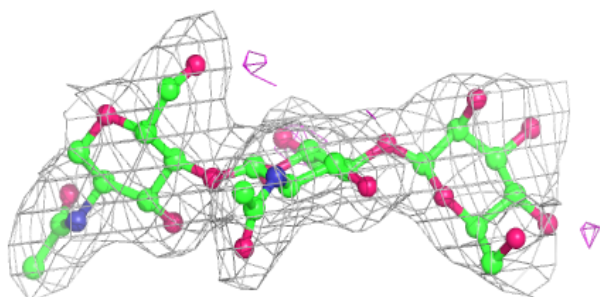
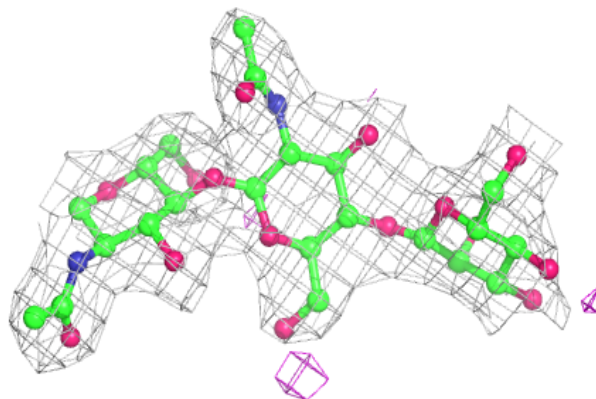


**Electron density around Chain I:**

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

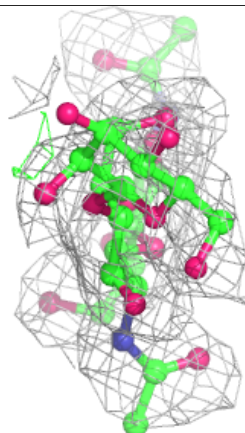
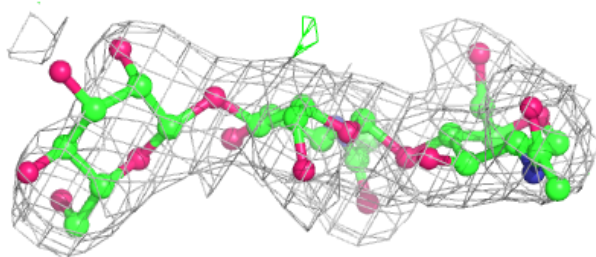
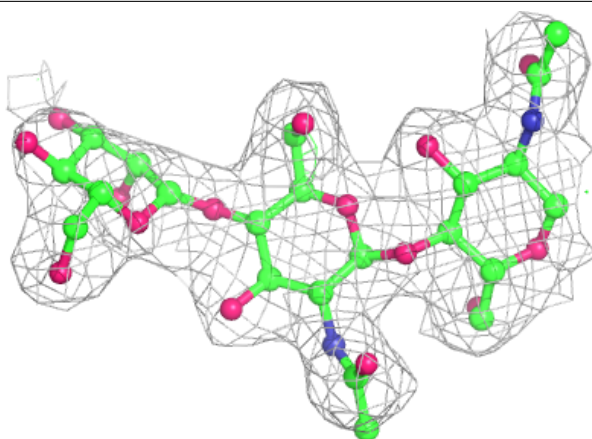
**Electron density around Chain J:**

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

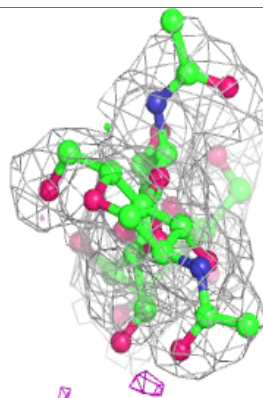
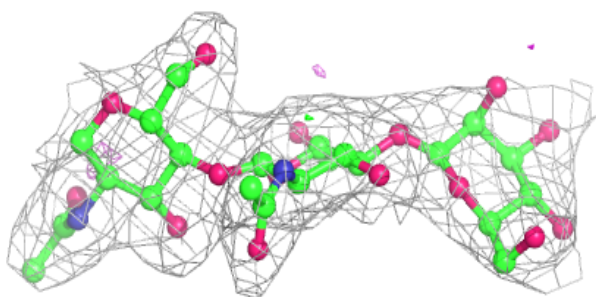
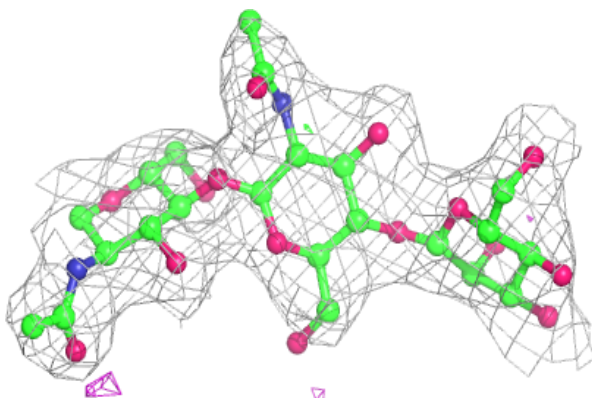


**Electron density around Chain L:**

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

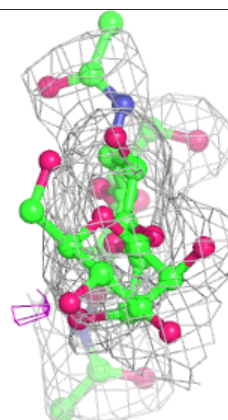
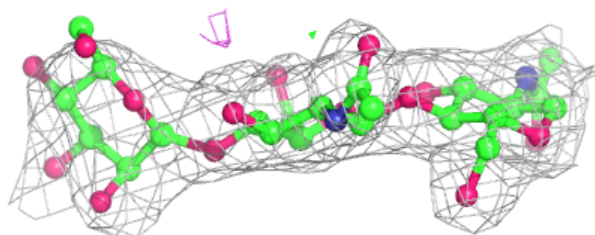
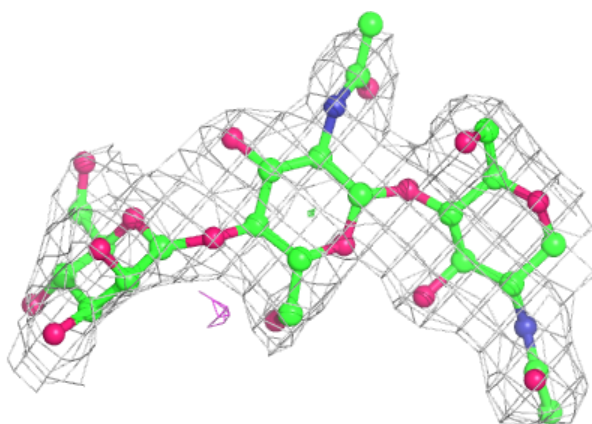
**Electron density around Chain M:**

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

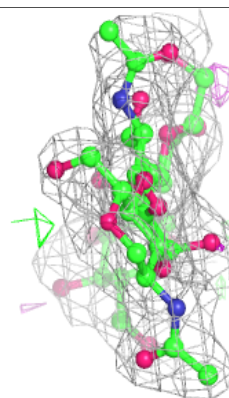
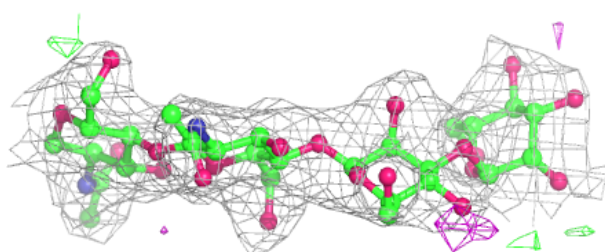
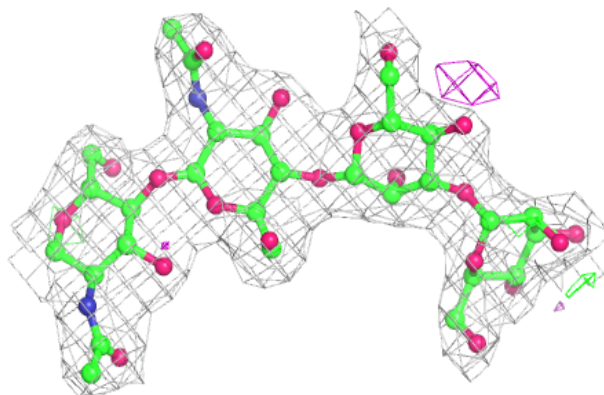


**Electron density around Chain O:**

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

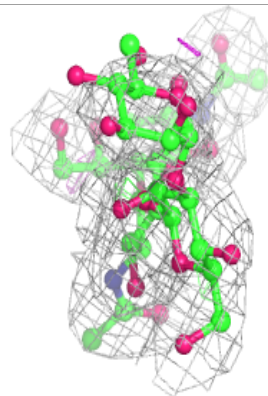
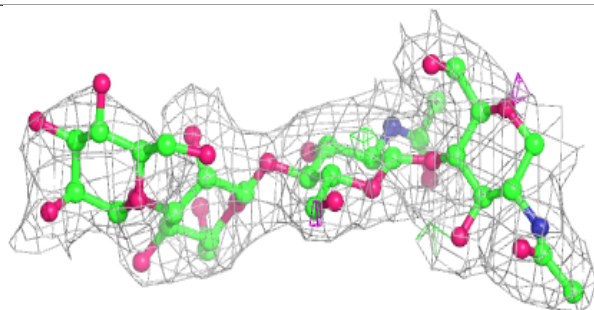
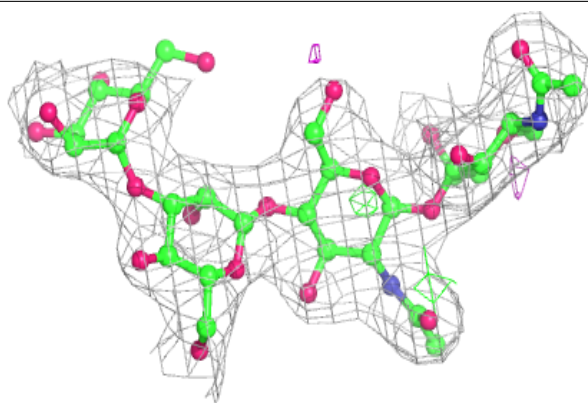
**Electron density around Chain K:**

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

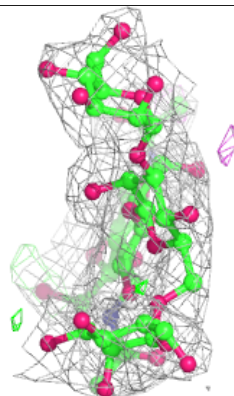
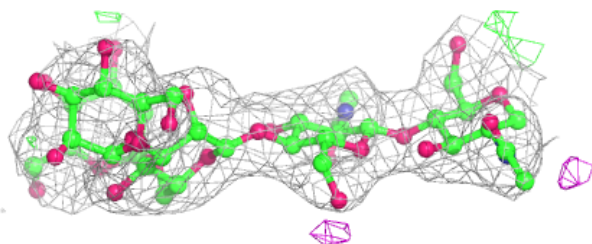
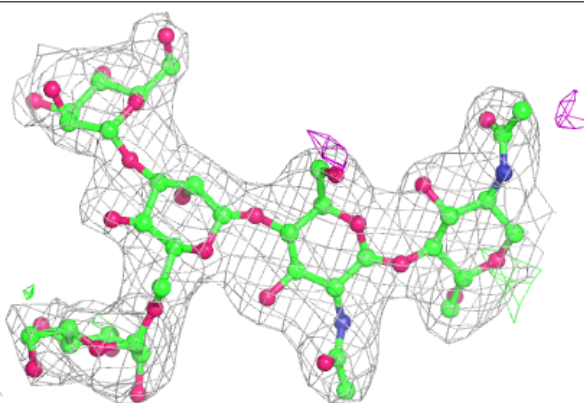


**Electron density around Chain P:**

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

**Electron density around Chain N:**

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



## 6.4 Ligands ⓘ

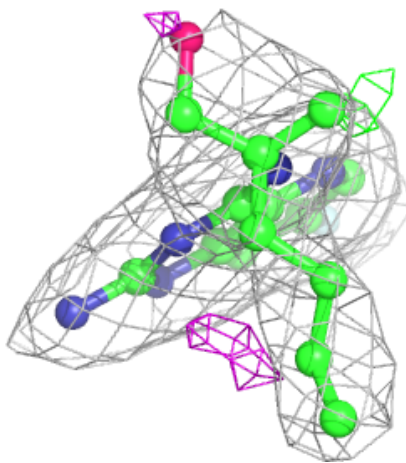
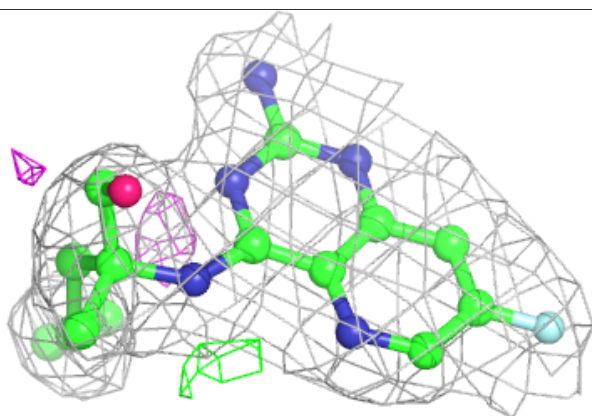
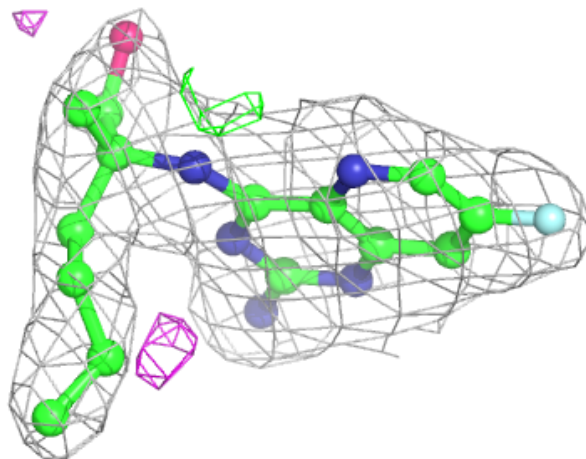
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	NAG	B	1016	14/15	0.37	0.66	95,104,122,123	0
7	MAN	C	913	11/12	0.60	0.28	81,102,110,110	0
7	MAN	B	1013	11/12	0.69	0.29	84,97,100,100	0
7	MAN	D	914	11/12	0.70	0.20	78,90,103,111	0
8	NAG	D	916	14/15	0.71	0.38	72,85,103,105	0
7	MAN	C	914	11/12	0.76	0.28	92,107,113,117	0
7	MAN	B	1005	11/12	0.82	0.15	73,81,91,93	0
8	NAG	C	915	14/15	0.82	0.25	82,95,104,105	0
7	MAN	B	1004	11/12	0.83	0.18	54,67,73,76	0
8	NAG	A	1014	14/15	0.84	0.17	67,74,83,91	0
8	NAG	B	1009	14/15	0.84	0.18	71,76,92,93	0
7	MAN	B	1014	11/12	0.85	0.15	72,85,90,92	0
8	NAG	D	915	14/15	0.86	0.22	64,79,88,90	0
8	NAG	B	1015	14/15	0.86	0.20	49,63,74,85	0
7	MAN	C	905	11/12	0.89	0.13	81,84,92,96	0
7	MAN	A	1013	11/12	0.89	0.12	77,83,90,91	0
8	NAG	C	916	14/15	0.91	0.12	72,82,91,96	0
8	NAG	D	917	14/15	0.91	0.16	51,58,72,75	0
8	NAG	A	1009	14/15	0.92	0.17	55,68,85,98	0
7	MAN	A	1005	11/12	0.93	0.11	49,61,67,68	0
8	NAG	C	909	14/15	0.93	0.14	63,71,84,92	0
8	NAG	A	1015	14/15	0.93	0.18	52,57,66,67	0
8	NAG	D	909	14/15	0.93	0.14	56,69,78,93	0
8	NAG	A	1016	14/15	0.94	0.17	51,62,67,73	0
9	U57	C	917	21/21	0.95	0.17	41,51,60,76	0
8	NAG	B	1017	14/15	0.95	0.17	47,57,64,66	0
9	U57	D	918	21/21	0.96	0.16	33,39,44,53	0
9	U57	A	1017	21/21	0.97	0.18	31,38,47,55	0
8	NAG	A	1006	14/15	0.97	0.15	34,39,45,45	0
9	U57	B	1018	21/21	0.98	0.17	34,39,45,53	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.

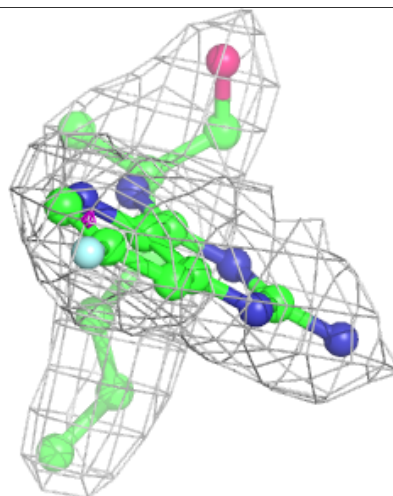
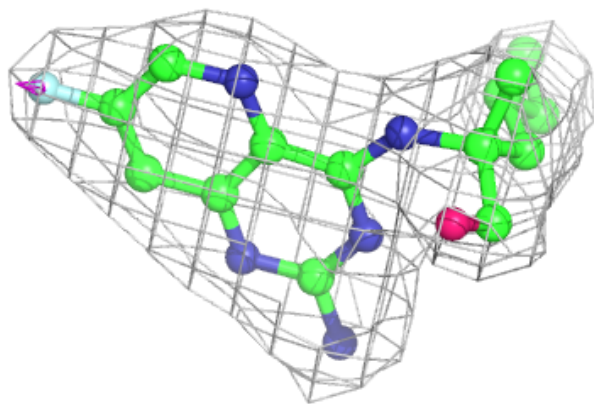
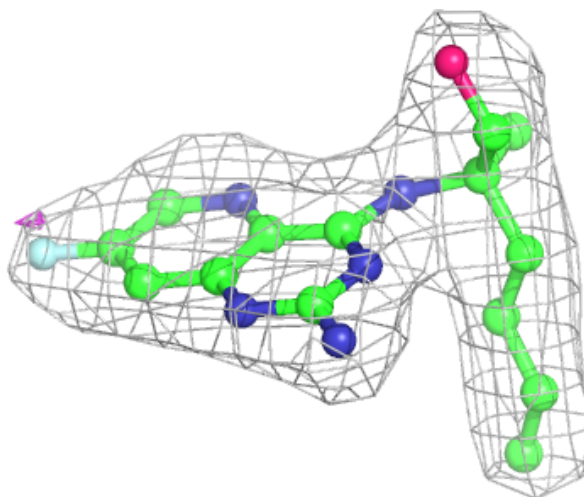
**Electron density around U57 C 917:**

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



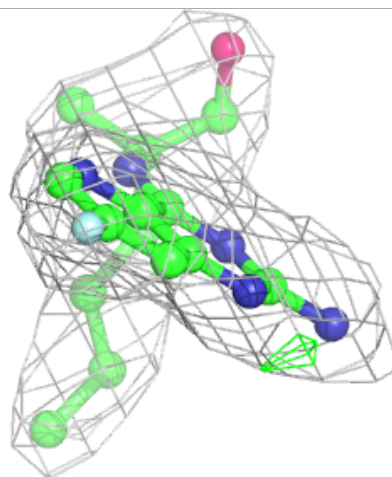
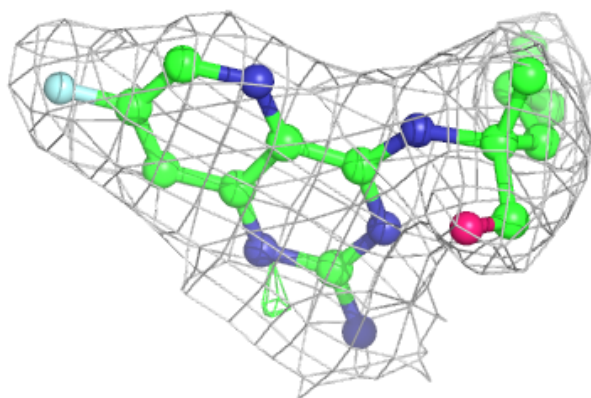
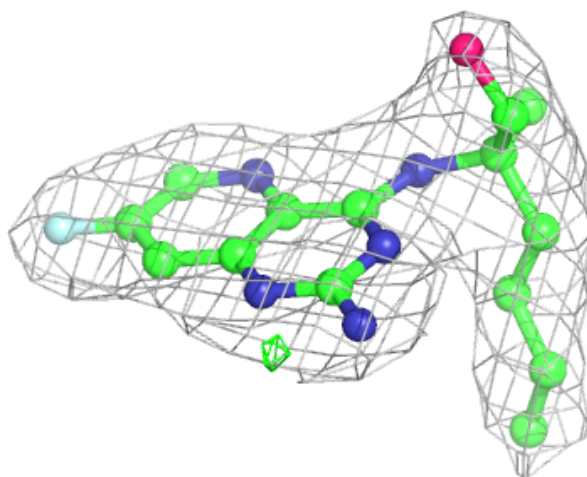
**Electron density around U57 D 918:**

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



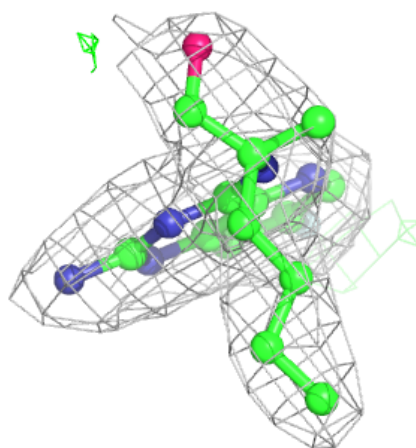
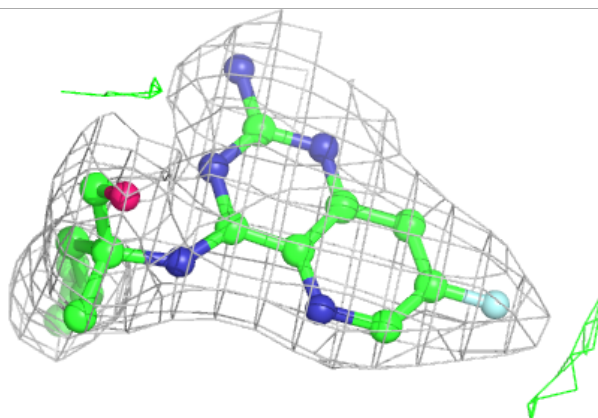
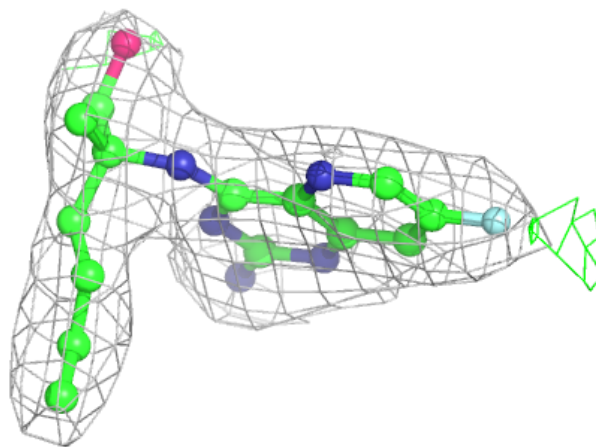
**Electron density around U57 A 1017:**

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



**Electron density around U57 B 1018:**

$2mF_o-DF_c$  (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.