



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2024 – 11:51 PM EDT

PDB ID : 4R08  
Title : Crystal structure of human TLR8 in complex with ssRNA40  
Authors : Tanji, H.; Ohto, U.; Shimizu, T.  
Deposited on : 2014-07-30  
Resolution : 2.40 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

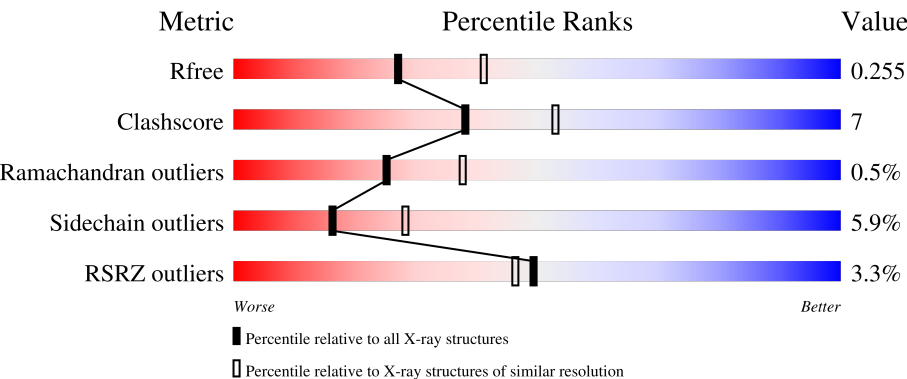
MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 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 2.40 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>	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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>77%</div><div>14%</div><div>8%</div></div>
1	B	811	<div><div>75%</div><div>15%</div><div>9%</div></div>
1	C	811	<div><div>7%</div><div>66%</div><div>20%</div><div>10%</div></div>
1	D	811	<div><div>3%</div><div>72%</div><div>18%</div><div>8%</div></div>
2	E	3	<div><div>67%</div><div>33%</div></div>

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Mol	Chain	Length	Quality of chain
2	F	3	 33% 67%
2	H	3	 33% 67%
2	I	3	 100%
2	K	3	 100%
2	L	3	 33% 67%
2	N	3	 67% 33%
2	O	3	 33% 67%
3	G	2	 100%
3	J	2	 100%
3	M	2	 100%
3	P	2	 100%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 25676 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	4	0	0
			5992	3835	1017	1121	19			
1	B	737	Total	C	N	O	S	4	0	0
			5941	3806	1009	1107	19			
1	C	731	Total	C	N	O	S	4	0	0
			5898	3779	1000	1100	19			
1	D	743	Total	C	N	O	S	4	0	0
			5989	3834	1016	1120	19			

There are 40 discrepancies between the modelled and reference sequences:

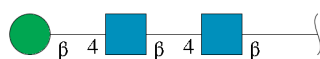
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ARG	-	expression tag	UNP Q9NR97
A	23	SER	-	expression tag	UNP Q9NR97
A	24	PRO	-	expression tag	UNP Q9NR97
A	25	TRP	-	expression tag	UNP Q9NR97
A	828	GLU	-	expression tag	UNP Q9NR97
A	829	PHE	-	expression tag	UNP Q9NR97
A	830	LEU	-	expression tag	UNP Q9NR97
A	831	VAL	-	expression tag	UNP Q9NR97
A	832	PRO	-	expression tag	UNP Q9NR97
A	833	ARG	-	expression tag	UNP Q9NR97
B	22	ARG	-	expression tag	UNP Q9NR97
B	23	SER	-	expression tag	UNP Q9NR97
B	24	PRO	-	expression tag	UNP Q9NR97
B	25	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	22	ARG	-	expression tag	UNP Q9NR97

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Chain	Residue	Modelled	Actual	Comment	Reference
C	23	SER	-	expression tag	UNP Q9NR97
C	24	PRO	-	expression tag	UNP Q9NR97
C	25	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	22	ARG	-	expression tag	UNP Q9NR97
D	23	SER	-	expression tag	UNP Q9NR97
D	24	PRO	-	expression tag	UNP Q9NR97
D	25	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 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	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	L	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

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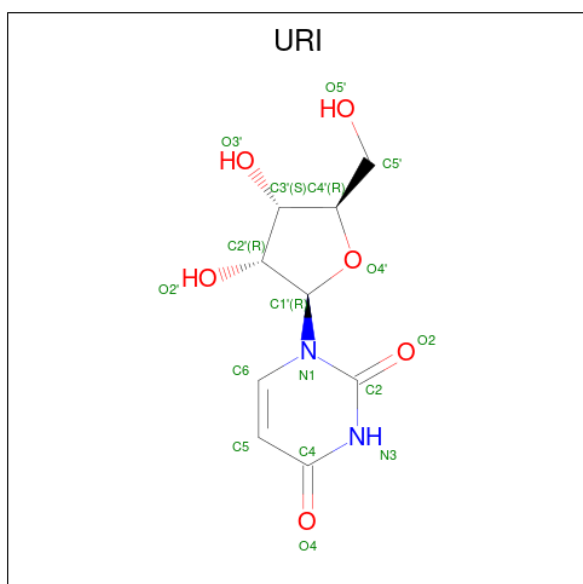
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	O	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 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
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is URIDINE (three-letter code: URI) (formula: C<sub>9</sub>H<sub>12</sub>N<sub>2</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	9	2	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			17	9	2	6		
4	C	1	Total	C	N	O	0	0
			17	9	2	6		
4	D	1	Total	C	N	O	0	0
			17	9	2	6		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



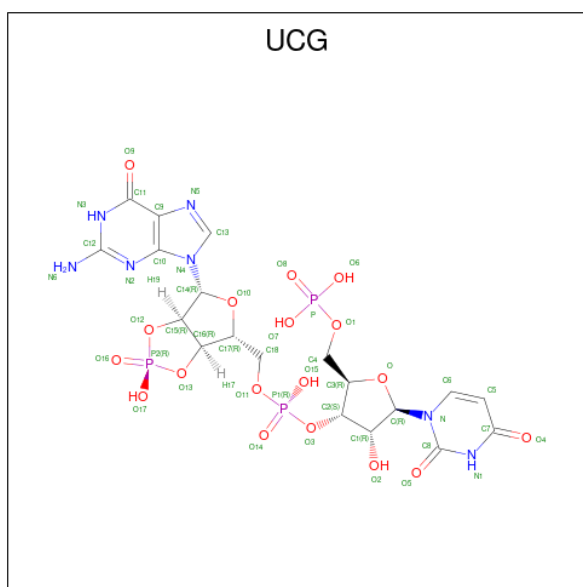
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1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

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

- Molecule 6 is 3'-O-[(R)-{[(2R,3aR,4R,6R,6aR)-6-(2-amino-6-oxo-1,6-dihydro-9H-purin-9-yl)-2-hydroxy-2-oxidotetrahydrofuro[3,4-d][1,3,2]dioxaphosphol-4-yl]methoxy}(hydroxy)phosphoryl]uridine 5'-(dihydrogen phosphate) (three-letter code: UCG) (formula: C<sub>19</sub>H<sub>24</sub>N<sub>7</sub>O<sub>18</sub>P<sub>3</sub>).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			47	19	7	18	3		
6	B	1	Total	C	N	O	P	0	0
			47	19	7	18	3		
6	C	1	Total	C	N	O	P	0	0
			47	19	7	18	3		
6	D	1	Total	C	N	O	P	0	0
			47	19	7	18	3		

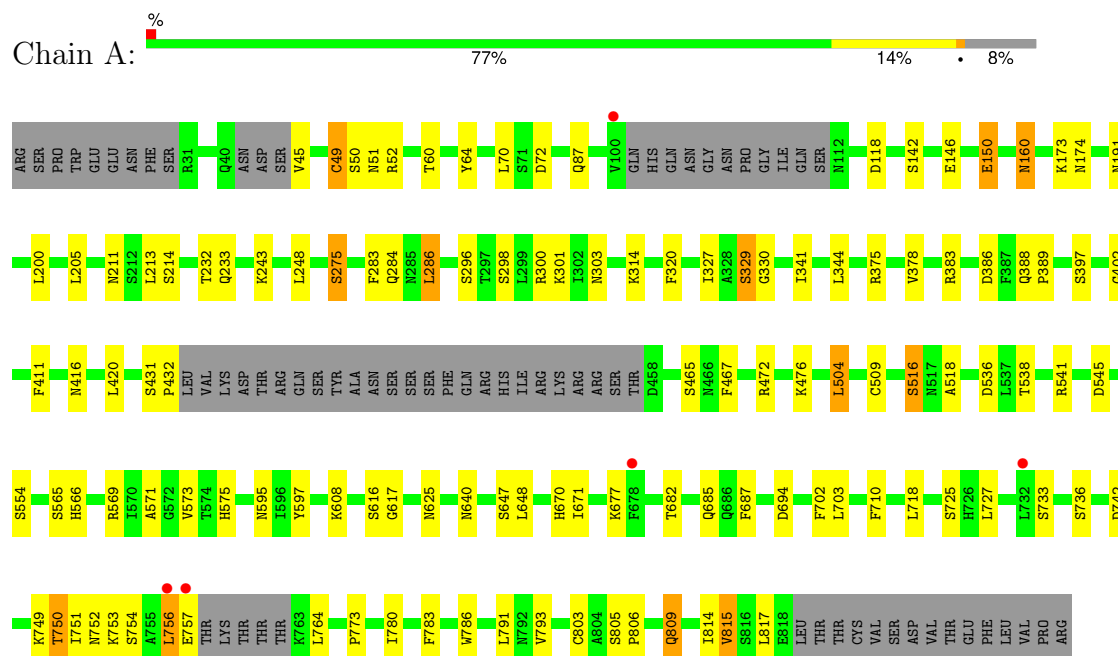
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	300	Total	O	0	0
			300	300		
7	B	250	Total	O	0	0
			250	250		
7	C	192	Total	O	0	0
			192	192		
7	D	182	Total	O	0	0
			182	182		

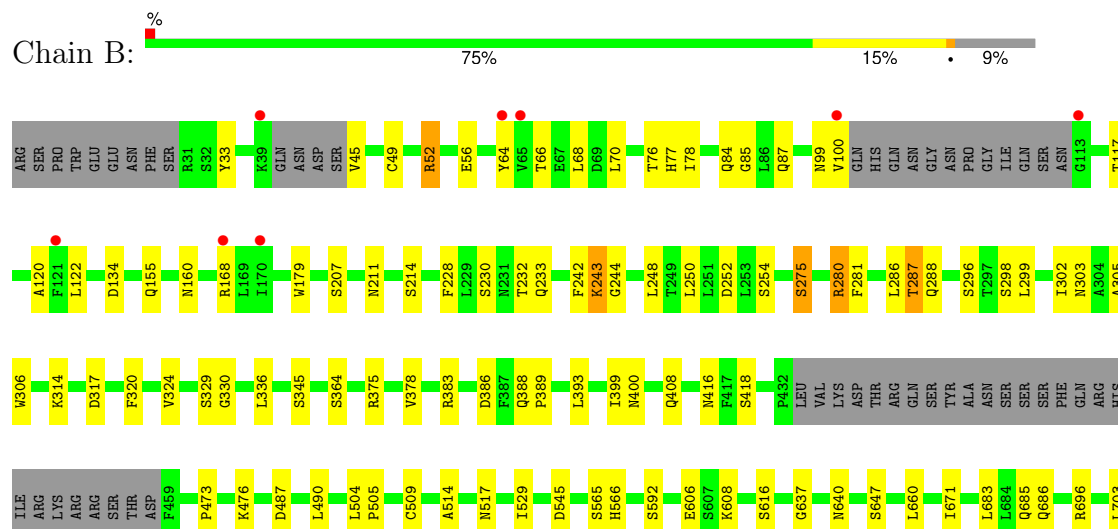
### 3 Residue-property plots

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

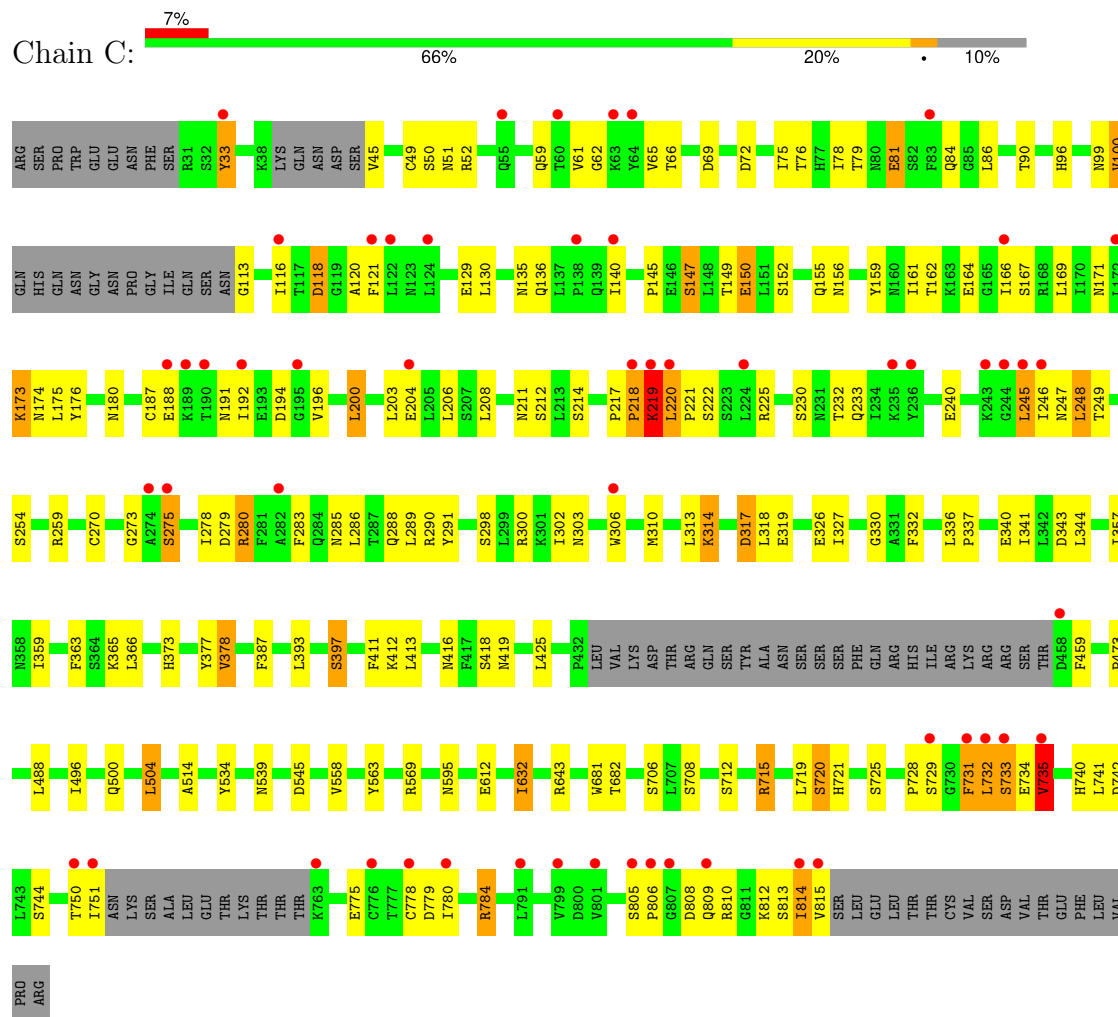
#### • Molecule 1: Toll-like receptor 8



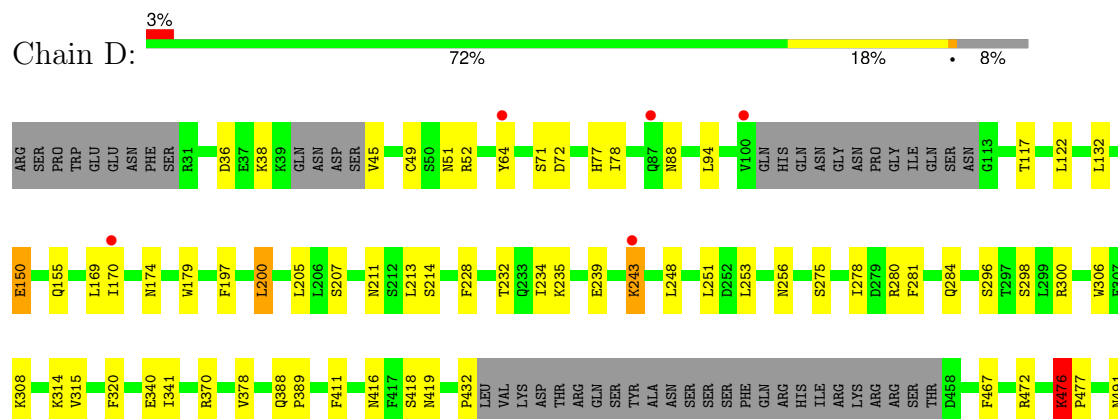
#### • Molecule 1: Toll-like receptor 8

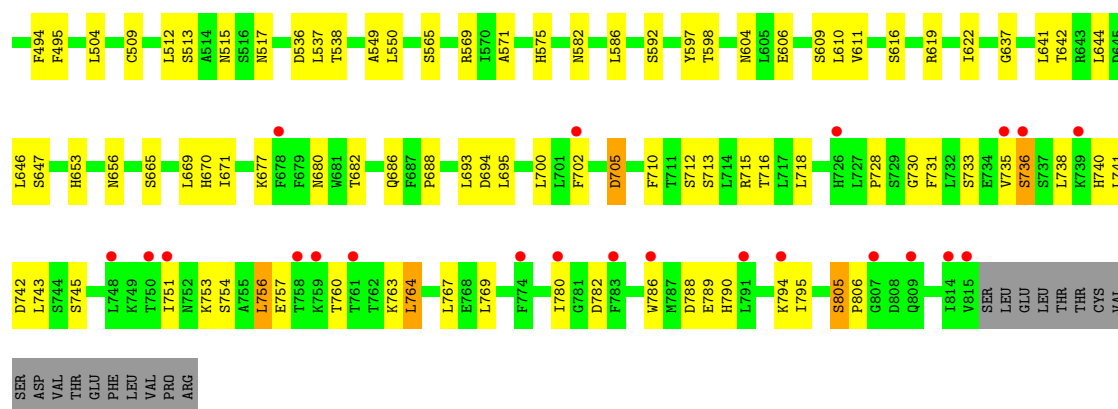


- Molecule 1: Toll-like receptor 8



- Molecule 1: Toll-like receptor 8





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

Chain E: 67% 33%



- Molecule 2: 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%



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

Chain H: 33% 67%



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

Chain K: 100%



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

Chain L:  33% 67%



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

Chain N:  67% 33%



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

Chain O:  33% 67%



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

Chain G:  100%



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

Chain J:  100%



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

Chain M:  100%



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

Chain P:  100%

MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.32Å 139.69Å 167.57Å 90.00° 91.44° 90.00°	Depositor
Resolution (Å)	40.98 – 2.40 40.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.8 (40.98-2.40) 92.9 (40.98-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.190 , 0.258 0.194 , 0.255	Depositor DCC
$R_{free}$ test set	7227 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.6	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	25676	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: URI, BMA, NAG, UCG

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	0.49	0/6115	0.64	0/8289
1	B	0.48	1/6064 (0.0%)	0.60	0/8220
1	C	0.45	0/6021	0.58	0/8164
1	D	0.48	1/6113 (0.0%)	0.61	2/8289 (0.0%)
All	All	0.48	2/24313 (0.0%)	0.61	2/32962 (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	C	0	2
1	D	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	476	LYS	CB-CG	-11.87	1.20	1.52
1	B	476	LYS	CB-CG	-6.11	1.36	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	805	SER	C-N-CD	-6.52	106.25	120.60
1	D	476	LYS	CA-CB-CG	6.21	127.06	113.40

There are no chirality outliers.

All (3) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	C	218	PRO	Peptide
1	C	735	VAL	Peptide
1	D	169	LEU	Peptide

## 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	5992	0	5972	57	0
1	B	5941	0	5931	67	0
1	C	5898	0	5878	126	0
1	D	5989	0	5978	84	0
2	E	39	0	34	2	0
2	F	39	0	34	0	0
2	H	39	0	34	0	0
2	I	39	0	34	0	0
2	K	39	0	34	0	0
2	L	39	0	34	0	0
2	N	39	0	34	2	0
2	O	39	0	34	0	0
3	G	28	0	25	0	0
3	J	28	0	25	0	0
3	M	28	0	25	0	0
3	P	28	0	25	0	0
4	A	17	0	12	0	0
4	B	17	0	12	0	0
4	C	17	0	12	0	0
4	D	17	0	12	0	0
5	A	70	0	65	1	0
5	B	70	0	65	2	0
5	C	56	0	52	0	0
5	D	56	0	52	1	0
6	A	47	0	20	2	0
6	B	47	0	20	1	0
6	C	47	0	20	3	0
6	D	47	0	20	1	0
7	A	300	0	0	6	0
7	B	250	0	0	5	0
7	C	192	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	182	0	0	4	0
All	All	25676	0	24493	336	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 7.

All (336) 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:C:219:LYS:HA	1:C:220:LEU:HB2	1.26	1.09
1:B:280:ARG:O	1:B:280:ARG:HD3	1.66	0.94
1:C:219:LYS:HA	1:C:220:LEU:CB	2.03	0.88
1:C:219:LYS:CA	1:C:220:LEU:HB2	2.08	0.81
1:C:708:SER:HB3	1:C:734:GLU:HG3	1.62	0.81
1:A:536:ASP:OD2	7:A:1049:HOH:O	1.97	0.80
1:C:99:ASN:O	1:C:100:VAL:HG13	1.80	0.80
1:C:303:ASN:OD1	7:C:1188:HOH:O	2.00	0.79
1:B:731:PHE:HA	1:B:734:GLU:HG3	1.66	0.76
1:B:280:ARG:HD3	1:B:280:ARG:C	2.05	0.76
1:C:230:SER:OG	1:C:254:SER:OG	1.76	0.75
1:B:242:PHE:O	1:B:244:GLY:N	2.21	0.73
1:D:150:GLU:HG2	1:D:174:ASN:HB2	1.70	0.73
1:D:751:ILE:HG22	1:D:756:LEU:HD21	1.69	0.73
1:D:239:GLU:HG3	1:D:284:GLN:HE21	1.55	0.71
1:D:730:GLY:N	1:D:754:SER:O	2.24	0.70
1:B:732:LEU:HB2	1:B:755:ALA:O	1.91	0.70
1:C:219:LYS:NZ	1:C:240:GLU:O	2.25	0.70
1:B:487:ASP:OD2	7:B:1157:HOH:O	2.10	0.69
1:B:660:LEU:CD2	1:B:686:GLN:HG3	2.24	0.67
1:C:192:ILE:HG21	1:C:217:PRO:HB3	1.77	0.66
1:C:715:ARG:NH2	1:C:715:ARG:HG3	2.10	0.66
1:C:50:SER:O	1:C:52:ARG:HG3	1.96	0.65
1:D:622:ILE:O	7:D:1158:HOH:O	2.14	0.65
1:D:693:LEU:HD21	1:D:695:LEU:HD11	1.79	0.65
1:C:150:GLU:CG	1:C:174:ASN:HD22	2.11	0.64
1:D:205:LEU:HD23	1:D:205:LEU:C	2.18	0.64
1:C:732:LEU:C	1:C:734:GLU:H	2.02	0.63
1:C:715:ARG:HG3	1:C:715:ARG:HH21	1.62	0.63
1:B:383:ARG:HB2	1:B:386:ASP:OD2	1.99	0.63
1:D:416:ASN:ND2	7:D:1023:HOH:O	2.31	0.63
1:C:728:PRO:O	1:C:731:PHE:HB3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:720:SER:HB2	1:B:742:ASP:OD2	1.99	0.62
1:C:300:ARG:NE	7:C:1085:HOH:O	2.19	0.61
1:D:736:SER:OG	1:D:760:THR:HG21	2.01	0.61
1:C:270:CYS:O	1:C:273:GLY:N	2.32	0.60
1:D:751:ILE:CG2	1:D:756:LEU:HD21	2.32	0.60
1:A:49:CYS:HB3	1:A:70:LEU:HD23	1.83	0.60
1:D:467:PHE:HB3	2:N:1:NAG:H81	1.84	0.60
1:A:383:ARG:HB2	1:A:386:ASP:OD2	2.02	0.59
1:A:411:PHE:HB3	1:A:504:LEU:HD13	1.84	0.59
1:A:160:ASN:ND2	1:A:191:ASN:OD1	2.36	0.59
1:B:299:LEU:HD13	1:B:302:ILE:CD1	2.32	0.59
1:D:275:SER:HA	1:D:298:SER:HB2	1.83	0.59
1:D:536:ASP:OD1	1:D:538:THR:HG23	2.03	0.58
1:A:205:LEU:HD23	1:A:205:LEU:C	2.24	0.58
1:C:81:GLU:O	1:C:84:GLN:HB3	2.03	0.58
1:D:411:PHE:HB3	1:D:504:LEU:HD13	1.86	0.58
1:B:84:GLN:HG2	1:B:85:GLY:N	2.19	0.57
1:B:99:ASN:O	1:B:100:VAL:HB	2.04	0.57
1:C:162:THR:O	1:C:196:VAL:HG21	2.04	0.57
1:C:595:ASN:HB3	7:C:1042:HOH:O	2.05	0.57
1:C:326:GLU:OE1	1:C:330:GLY:HA2	2.04	0.57
1:D:211:ASN:O	1:D:232:THR:HA	2.05	0.57
1:C:341:ILE:HD12	6:C:901:UCG:C8	2.36	0.56
1:C:280:ARG:O	1:C:280:ARG:HD3	2.06	0.56
1:C:219:LYS:HG3	1:C:220:LEU:O	2.05	0.56
1:B:287:THR:HG22	1:B:288:GLN:HE21	1.71	0.56
1:A:687:PHE:O	7:A:1132:HOH:O	2.18	0.56
1:C:79:THR:C	1:C:120:ALA:HB1	2.27	0.56
1:C:317:ASP:OD1	1:C:319:GLU:OE1	2.24	0.55
1:D:207:SER:HA	1:D:228:PHE:HB2	1.88	0.55
1:A:211:ASN:O	1:A:232:THR:HA	2.06	0.55
1:A:518:ALA:HA	1:A:541:ARG:O	2.05	0.55
1:C:249:THR:HA	1:C:288:GLN:O	2.07	0.55
1:C:731:PHE:O	1:C:734:GLU:HB2	2.07	0.55
1:A:752:ASN:HB2	1:A:754:SER:OG	2.05	0.54
1:B:211:ASN:O	1:B:232:THR:HA	2.07	0.54
1:C:66:THR:O	1:C:90:THR:HG22	2.07	0.54
1:B:345:SER:HB3	1:B:375:ARG:HB2	1.89	0.54
1:D:741:LEU:HD21	1:D:743:LEU:HD11	1.88	0.54
1:B:280:ARG:C	1:B:280:ARG:CD	2.76	0.54
1:C:45:VAL:CG1	1:C:65:VAL:HA	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:731:PHE:C	1:C:731:PHE:CD2	2.81	0.53
1:C:303:ASN:HB3	1:C:306:TRP:CE2	2.44	0.53
1:A:805:SER:HB2	1:A:806:PRO:HA	1.91	0.53
1:B:52:ARG:HG2	1:B:799:VAL:HG21	1.91	0.53
1:B:275:SER:HA	1:B:298:SER:HB2	1.91	0.52
1:B:660:LEU:HD22	1:B:686:GLN:HG3	1.90	0.52
1:D:767:LEU:O	1:D:795:ILE:HD13	2.10	0.52
1:A:467:PHE:HB3	2:E:1:NAG:H81	1.90	0.52
1:C:61:VAL:HG12	1:C:62:GLY:O	2.10	0.52
1:C:219:LYS:HG3	1:C:220:LEU:HB2	1.90	0.52
1:D:296:SER:HA	1:D:320:PHE:O	2.10	0.52
1:A:608:LYS:O	1:A:640:ASN:HB2	2.09	0.52
1:C:218:PRO:O	1:C:219:LYS:O	2.28	0.52
1:C:377:TYR:O	1:C:378:VAL:HB	2.10	0.52
1:B:324:VAL:HG23	7:B:1009:HOH:O	2.10	0.51
1:C:59:GLN:HG3	1:C:84:GLN:NE2	2.24	0.51
1:C:411:PHE:O	7:C:1068:HOH:O	2.19	0.51
1:D:604:ASN:HB3	7:D:1116:HOH:O	2.09	0.51
1:A:341:ILE:HD11	6:A:915:UCG:C5	2.40	0.51
1:B:207:SER:HA	1:B:228:PHE:HB2	1.92	0.51
1:A:750:THR:OG1	1:A:751:ILE:N	2.36	0.51
1:A:411:PHE:HB3	1:A:504:LEU:CD1	2.41	0.51
1:C:118:ASP:OD1	1:C:118:ASP:N	2.44	0.51
1:A:803:CYS:HB2	1:A:809:GLN:O	2.12	0.50
1:D:341:ILE:HD12	6:D:902:UCG:H5	1.92	0.50
1:C:341:ILE:HD13	6:C:901:UCG:H5	1.93	0.50
1:D:549:ALA:O	1:D:550:LEU:HB2	2.12	0.50
1:D:741:LEU:HD23	1:D:767:LEU:CD1	2.41	0.50
1:A:670:HIS:HA	1:A:694:ASP:HB3	1.94	0.50
1:C:343:ASP:HA	1:C:373:HIS:HB2	1.94	0.50
1:C:732:LEU:C	1:C:732:LEU:HD22	2.31	0.50
1:D:571:ALA:HB2	1:D:597:TYR:OH	2.12	0.50
5:B:911:NAG:H81	7:B:1181:HOH:O	2.12	0.50
1:C:159:TYR:CE1	1:C:187:CYS:HB2	2.47	0.50
1:C:473:PRO:HA	6:C:901:UCG:O17	2.12	0.50
1:D:682:THR:HA	1:D:710:PHE:CD1	2.47	0.50
1:A:571:ALA:HB2	1:A:597:TYR:OH	2.12	0.49
1:C:225:ARG:HA	1:C:247:ASN:O	2.11	0.49
1:B:68:LEU:HD21	1:B:70:LEU:HD11	1.95	0.49
1:B:703:LEU:CD2	1:B:724:ILE:HG21	2.43	0.49
1:C:314:LYS:HD3	1:C:340:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:728:PRO:O	1:D:731:PHE:HB2	2.12	0.49
1:D:278:ILE:HB	1:D:306:TRP:CZ2	2.48	0.49
1:C:200:LEU:O	1:C:221:PRO:HG3	2.12	0.49
1:D:688:PRO:O	1:D:713:SER:CB	2.61	0.49
1:B:134:ASP:HA	1:B:155:GLN:O	2.13	0.48
1:C:303:ASN:HB3	1:C:306:TRP:CD2	2.48	0.48
1:C:732:LEU:HD13	1:C:733:SER:N	2.27	0.48
1:D:155:GLN:HA	1:D:179:TRP:O	2.12	0.48
1:A:329:SER:OG	1:A:330:GLY:N	2.44	0.48
1:D:677:LYS:O	1:D:700:LEU:HD23	2.14	0.48
1:C:514:ALA:HA	1:C:539:ASN:O	2.14	0.48
1:D:51:ASN:HA	1:D:72:ASP:O	2.13	0.48
1:B:250:LEU:HD23	1:B:250:LEU:C	2.34	0.48
1:C:45:VAL:HG11	1:C:65:VAL:HA	1.95	0.48
1:D:718:LEU:HA	1:D:742:ASP:HB3	1.96	0.48
1:B:45:VAL:HG11	1:B:64:TYR:O	2.14	0.47
1:D:705:ASP:HA	1:D:728:PRO:HB2	1.96	0.47
1:A:146:GLU:O	1:A:146:GLU:HG2	2.13	0.47
1:B:616:SER:HA	1:B:647:SER:O	2.13	0.47
1:C:813:SER:O	1:C:815:VAL:N	2.46	0.47
1:D:512:LEU:HB2	1:D:537:LEU:HD23	1.97	0.47
1:A:303:ASN:ND2	7:A:1278:HOH:O	2.44	0.47
1:C:49:CYS:HA	1:C:52:ARG:NE	2.29	0.47
1:C:152:SER:HA	1:C:176:TYR:HB2	1.96	0.47
1:C:206:LEU:HD21	1:C:208:LEU:HD11	1.96	0.47
1:C:359:ILE:HG23	1:C:363:PHE:CD1	2.49	0.47
1:A:51:ASN:HA	1:A:72:ASP:O	2.14	0.47
5:A:914:NAG:H81	7:A:1167:HOH:O	2.15	0.47
1:B:77:HIS:O	1:B:78:ILE:HD13	2.14	0.47
1:C:49:CYS:HB3	1:C:69:ASP:O	2.15	0.47
1:C:129:GLU:HA	1:C:150:GLU:O	2.14	0.47
1:D:786:TRP:O	1:D:790:HIS:ND1	2.48	0.47
1:C:33:TYR:HE1	1:C:813:SER:OG	1.98	0.47
1:C:155:GLN:HG3	1:C:459:PHE:CZ	2.50	0.47
1:C:175:LEU:HB2	1:C:203:LEU:HD11	1.97	0.47
1:D:597:TYR:HB3	1:D:619:ARG:HB2	1.96	0.47
1:D:606:GLU:HG2	1:D:637:GLY:HA3	1.97	0.46
1:B:683:LEU:HD21	5:B:914:NAG:O5	2.15	0.46
1:C:150:GLU:HG2	1:C:174:ASN:HD22	1.80	0.46
1:A:45:VAL:HG11	1:A:64:TYR:HD2	1.80	0.46
1:B:608:LYS:O	1:B:640:ASN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:HIS:O	1:D:78:ILE:HD13	2.15	0.46
1:C:49:CYS:HA	1:C:52:ARG:HE	1.80	0.46
1:B:230:SER:HA	1:B:254:SER:O	2.15	0.46
1:C:720:SER:HA	1:C:744:SER:O	2.15	0.46
1:B:809:GLN:O	1:B:810:ARG:C	2.54	0.46
1:C:750:THR:HG22	1:C:751:ILE:N	2.30	0.46
1:D:586:LEU:O	1:D:610:LEU:HA	2.16	0.46
1:D:592:SER:HA	1:D:616:SER:O	2.16	0.46
1:C:336:LEU:N	1:C:337:PRO:CD	2.79	0.46
1:C:539:ASN:HA	1:C:563:TYR:O	2.16	0.46
1:C:814:ILE:HG13	1:C:815:VAL:N	2.31	0.46
1:C:806:PRO:O	1:C:809:GLN:N	2.43	0.46
1:C:366:LEU:O	1:C:393:LEU:HD22	2.16	0.46
1:D:656:ASN:HD21	1:D:680:ASN:HD22	1.63	0.46
1:D:763:LYS:HE3	1:D:763:LYS:HA	1.97	0.46
1:B:242:PHE:O	1:B:243:LYS:C	2.54	0.45
1:C:113:GLY:HA2	1:C:136:GLN:HB2	1.98	0.45
1:D:767:LEU:HD21	1:D:769:LEU:HD11	1.98	0.45
1:C:775:GLU:HA	1:C:805:SER:O	2.16	0.45
1:A:809:GLN:HA	1:A:809:GLN:HE21	1.81	0.45
1:B:490:LEU:HD23	1:B:514:ALA:HB1	1.99	0.45
1:B:685:GLN:HE21	1:B:710:PHE:HD1	1.65	0.45
1:C:150:GLU:HG2	1:C:174:ASN:HB2	1.99	0.45
1:D:705:ASP:OD1	1:D:705:ASP:N	2.46	0.45
1:C:632:ILE:HD13	1:C:632:ILE:HA	1.72	0.45
1:B:388:GLN:CB	1:B:389:PRO:HD3	2.47	0.45
1:D:94:LEU:HB2	1:D:132:LEU:HD23	1.98	0.45
1:D:670:HIS:HA	1:D:694:ASP:HB3	1.99	0.45
1:C:720:SER:OG	1:C:721:HIS:HD2	2.00	0.45
1:C:732:LEU:C	1:C:734:GLU:N	2.68	0.45
1:D:432:PRO:HG3	1:D:495:PHE:O	2.17	0.45
1:C:327:ILE:HG12	1:C:344:LEU:HD13	1.99	0.45
1:B:784:ARG:HD3	1:B:814:ILE:O	2.17	0.45
1:D:786:TRP:O	1:D:790:HIS:HB2	2.16	0.45
1:A:516:SER:O	1:A:516:SER:OG	2.29	0.44
1:A:727:LEU:HD12	1:A:751:ILE:HG12	1.99	0.44
1:B:696:ARG:HG2	1:B:720:SER:HB3	1.99	0.44
1:C:140:ILE:HG21	1:C:166:ILE:HD11	1.98	0.44
1:D:756:LEU:N	1:D:756:LEU:HD23	2.32	0.44
1:D:789:GLU:O	1:D:790:HIS:ND1	2.49	0.44
1:B:314:LYS:HG3	7:B:1109:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:LEU:C	1:D:205:LEU:CD2	2.86	0.44
1:A:300:ARG:NE	7:A:1172:HOH:O	2.15	0.44
1:C:145:PRO:O	1:C:169:LEU:HD22	2.17	0.44
1:C:808:ASP:O	1:C:812:LYS:NZ	2.49	0.44
1:D:197:PHE:HA	1:D:200:LEU:HD22	2.00	0.44
1:D:388:GLN:N	1:D:389:PRO:CD	2.80	0.44
1:A:214:SER:HA	1:A:233:GLN:O	2.18	0.44
1:A:671:ILE:O	1:A:671:ILE:HG22	2.18	0.44
1:D:754:SER:O	1:D:757:GLU:HB2	2.18	0.44
1:B:280:ARG:HD2	1:B:281:PHE:CE2	2.53	0.44
1:B:296:SER:HA	1:B:320:PHE:O	2.17	0.44
1:A:616:SER:HA	1:A:647:SER:O	2.18	0.44
1:C:778:CYS:O	1:C:779:ASP:C	2.56	0.43
1:A:283:PHE:HA	1:A:286:LEU:HD22	1.98	0.43
1:C:731:PHE:C	1:C:734:GLU:HB2	2.39	0.43
1:D:239:GLU:HG3	1:D:284:GLN:NE2	2.30	0.43
1:D:513:SER:HA	1:D:538:THR:O	2.18	0.43
1:A:749:LYS:HA	1:A:773:PRO:O	2.18	0.43
1:B:155:GLN:HA	1:B:179:TRP:O	2.17	0.43
1:B:280:ARG:NH2	1:B:305:ALA:HB1	2.33	0.43
1:C:51:ASN:HA	1:C:72:ASP:O	2.18	0.43
1:C:731:PHE:HA	1:C:734:GLU:OE2	2.19	0.43
1:D:467:PHE:CB	2:N:1:NAG:H81	2.49	0.43
1:D:745:SER:C	7:D:1096:HOH:O	2.56	0.43
1:A:718:LEU:HA	1:A:742:ASP:HB3	2.00	0.43
1:C:290:ARG:HB2	1:C:291:TYR:CD1	2.53	0.43
1:C:496:ILE:HG23	1:C:500:GLN:HB3	2.01	0.43
1:C:612:GLU:OE2	1:C:643:ARG:NH1	2.52	0.43
1:B:303:ASN:HB3	1:B:306:TRP:CE2	2.54	0.43
1:C:121:PHE:CE2	1:C:130:LEU:HD21	2.53	0.43
1:C:156:ASN:O	1:C:180:ASN:OD1	2.37	0.43
1:D:611:VAL:O	1:D:641:LEU:HD12	2.19	0.43
1:B:364:SER:HA	1:B:393:LEU:HD21	2.00	0.43
1:C:161:ILE:HG22	1:C:196:VAL:HG11	2.00	0.43
1:C:222:SER:HA	1:C:245:LEU:HD23	2.00	0.43
1:C:411:PHE:HB3	1:C:504:LEU:HD13	2.00	0.43
1:B:399:ILE:HG23	1:B:399:ILE:O	2.18	0.43
1:B:400:ASN:OD1	1:B:400:ASN:C	2.57	0.43
1:C:75:ILE:HG21	1:C:78:ILE:HD11	2.01	0.43
1:C:740:HIS:HD2	1:C:741:LEU:N	2.15	0.43
1:D:314:LYS:HG2	1:D:315:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LEU:O	1:A:214:SER:HB2	2.19	0.43
1:A:388:GLN:N	1:A:389:PRO:CD	2.82	0.43
1:C:194:ASP:C	1:C:194:ASP:OD2	2.57	0.43
1:C:233:GLN:HA	7:C:1094:HOH:O	2.18	0.43
1:C:539:ASN:HB3	7:C:1141:HOH:O	2.18	0.43
1:C:612:GLU:HA	1:C:643:ARG:O	2.19	0.43
1:D:370:ARG:NH2	5:D:909:NAG:H81	2.34	0.43
1:A:467:PHE:CB	2:E:1:NAG:H81	2.49	0.42
1:A:536:ASP:OD1	1:A:538:THR:HG23	2.18	0.42
1:B:214:SER:HA	1:B:233:GLN:O	2.19	0.42
1:C:289:LEU:HD23	1:C:310:MET:SD	2.58	0.42
1:C:545:ASP:CG	1:C:545:ASP:O	2.56	0.42
1:C:731:PHE:O	1:C:734:GLU:CB	2.67	0.42
1:A:150:GLU:HG2	1:A:174:ASN:HB2	2.00	0.42
1:C:534:TYR:CE2	1:C:558:VAL:HG11	2.54	0.42
1:C:784:ARG:HE	1:C:784:ARG:HA	1.84	0.42
1:D:565:SER:HB3	1:D:569:ARG:NH1	2.35	0.42
1:D:616:SER:HA	1:D:647:SER:O	2.19	0.42
1:A:388:GLN:HB2	1:A:389:PRO:HD3	2.02	0.42
1:A:420:LEU:HD23	1:A:420:LEU:HA	1.85	0.42
1:B:336:LEU:HD23	7:B:1046:HOH:O	2.18	0.42
1:C:275:SER:HA	1:C:298:SER:HB2	2.02	0.42
1:A:275:SER:HA	1:A:298:SER:HB2	2.01	0.42
1:C:149:THR:HA	1:C:171:ASN:O	2.20	0.42
1:C:357:ILE:HG13	1:C:377:TYR:CZ	2.55	0.42
1:D:38:LYS:O	1:D:45:VAL:HA	2.19	0.42
1:D:251:LEU:HD21	1:D:253:LEU:HD11	2.00	0.42
1:A:565:SER:O	1:A:566:HIS:C	2.58	0.42
1:C:225:ARG:O	1:C:248:LEU:HD22	2.19	0.42
1:D:280:ARG:HG3	1:D:281:PHE:CD1	2.54	0.42
1:A:545:ASP:CG	1:A:545:ASP:O	2.57	0.42
1:A:764:LEU:O	1:A:793:VAL:HG22	2.19	0.42
1:B:545:ASP:CG	1:B:545:ASP:O	2.58	0.42
1:B:784:ARG:HH12	1:B:817:LEU:HB2	1.84	0.42
1:D:213:LEU:O	1:D:214:SER:HB2	2.19	0.42
1:A:296:SER:HA	1:A:320:PHE:O	2.20	0.42
1:A:431:SER:HB2	1:A:432:PRO:CD	2.49	0.42
1:A:783:PHE:O	1:A:786:TRP:HB3	2.20	0.42
1:C:211:ASN:O	1:C:232:THR:HA	2.19	0.42
1:D:611:VAL:HG13	1:D:642:THR:OG1	2.20	0.42
1:C:135:ASN:O	1:C:136:GLN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:SER:O	1:D:72:ASP:HB2	2.19	0.41
1:D:716:THR:HG23	1:D:740:HIS:HB3	2.01	0.41
1:D:491:ASN:O	1:D:515:ASN:HA	2.20	0.41
1:D:598:THR:HG23	1:D:598:THR:O	2.19	0.41
1:C:283:PHE:HA	1:C:286:LEU:HD22	2.03	0.41
1:C:318:LEU:HB2	1:C:344:LEU:HD23	2.01	0.41
1:D:234:ILE:O	1:D:256:ASN:HB3	2.20	0.41
1:D:575:HIS:CE1	1:D:598:THR:HG23	2.55	0.41
1:D:669:LEU:HD21	1:D:671:ILE:HD11	2.02	0.41
1:A:375:ARG:HA	1:A:402:GLY:O	2.21	0.41
1:A:685:GLN:HG3	1:A:710:PHE:HA	2.03	0.41
1:A:814:ILE:HG13	1:A:815:VAL:N	2.35	0.41
1:B:117:THR:OG1	1:B:120:ALA:HB2	2.20	0.41
1:C:219:LYS:CG	1:C:220:LEU:HB2	2.50	0.41
1:C:397:SER:HA	1:C:419:ASN:O	2.21	0.41
1:D:743:LEU:HB2	1:D:769:LEU:HD23	2.03	0.41
1:A:569:ARG:NH1	7:A:1096:HOH:O	2.37	0.41
1:B:671:ILE:O	1:B:671:ILE:HG22	2.21	0.41
1:B:703:LEU:HD11	1:B:719:LEU:HD13	2.01	0.41
1:B:45:VAL:HG13	1:B:45:VAL:O	2.21	0.41
1:B:592:SER:HA	1:B:616:SER:O	2.21	0.41
1:B:606:GLU:HG2	1:B:637:GLY:HA3	2.03	0.41
1:D:340:GLU:C	1:D:341:ILE:HG12	2.40	0.41
1:B:45:VAL:HG21	1:B:64:TYR:HD2	1.86	0.41
1:D:780:ILE:O	1:D:782:ASP:N	2.53	0.41
1:A:327:ILE:HD11	1:A:344:LEU:HD22	2.02	0.41
1:B:280:ARG:NH2	1:B:305:ALA:CB	2.84	0.41
1:B:329:SER:OG	1:B:330:GLY:N	2.54	0.41
1:B:517:ASN:OD1	1:B:517:ASN:C	2.59	0.41
1:B:529:ILE:HG13	1:B:529:ILE:O	2.21	0.41
1:C:302:ILE:HG21	1:C:332:PHE:CD2	2.56	0.41
1:C:413:LEU:C	1:C:413:LEU:HD12	2.41	0.41
1:C:719:LEU:HB2	1:C:742:ASP:O	2.21	0.41
1:D:644:LEU:HD21	1:D:646:LEU:HD21	2.02	0.41
1:A:573:VAL:O	1:A:575:HIS:CE1	2.74	0.41
1:A:756:LEU:O	1:A:757:GLU:C	2.60	0.41
1:C:173:LYS:O	1:C:204:GLU:N	2.40	0.41
1:C:300:ARG:CD	7:C:1085:HOH:O	2.63	0.41
1:B:33:TYR:CD2	1:B:33:TYR:C	2.95	0.40
1:C:96:HIS:HB3	1:C:99:ASN:OD1	2.21	0.40
1:C:425:LEU:HB2	1:C:488:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:720:SER:HB3	1:C:742:ASP:OD2	2.20	0.40
1:A:617:GLY:HA2	1:A:648:LEU:O	2.21	0.40
1:B:228:PHE:HA	1:B:252:ASP:HB3	2.03	0.40
1:B:565:SER:O	1:B:566:HIS:C	2.59	0.40
1:D:738:LEU:O	1:D:764:LEU:HD12	2.21	0.40
1:C:740:HIS:CD2	1:C:740:HIS:C	2.94	0.40
1:A:341:ILE:HD11	6:A:915:UCG:C6	2.51	0.40
1:B:473:PRO:HA	6:B:915:UCG:O17	2.21	0.40
1:C:147:SER:HA	1:C:171:ASN:HD22	1.86	0.40
1:C:313:LEU:HD23	1:C:336:LEU:CD2	2.52	0.40
1:C:732:LEU:O	1:C:734:GLU:N	2.48	0.40
1:D:671:ILE:HB	1:D:695:LEU:HD23	2.03	0.40
1:D:688:PRO:O	1:D:713:SER:OG	2.37	0.40
1:B:805:SER:HB2	1:B:806:PRO:HA	2.02	0.40
1:C:813:SER:O	1:C:814:ILE:C	2.60	0.40
1:D:476:LYS:HA	1:D:477:PRO:HD2	1.84	0.40
1:D:494:PHE:O	1:D:517:ASN:HA	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	733/811 (90%)	672 (92%)	59 (8%)	2 (0%)	37	51
1	B	727/811 (90%)	669 (92%)	53 (7%)	5 (1%)	19	29
1	C	721/811 (89%)	643 (89%)	72 (10%)	6 (1%)	16	26
1	D	735/811 (91%)	671 (91%)	61 (8%)	3 (0%)	30	44
All	All	2916/3244 (90%)	2655 (91%)	245 (8%)	16 (0%)	25	38

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	243	LYS
1	C	220	LEU
1	C	219	LYS
1	C	733	SER
1	D	243	LYS
1	B	754	SER
1	A	284	GLN
1	B	505	PRO
1	C	378	VAL
1	A	378	VAL
1	B	378	VAL
1	B	773	PRO
1	D	378	VAL
1	C	735	VAL
1	C	814	ILE
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	690/755 (91%)	646 (94%)	44 (6%)	14	24
1	B	684/755 (91%)	656 (96%)	28 (4%)	26	44
1	C	679/755 (90%)	627 (92%)	52 (8%)	10	17
1	D	690/755 (91%)	652 (94%)	38 (6%)	18	31
All	All	2743/3020 (91%)	2581 (94%)	162 (6%)	16	28

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	CYS
1	A	50	SER
1	A	52	ARG
1	A	60	THR
1	A	87	GLN
1	A	118	ASP

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Mol	Chain	Res	Type
1	A	142	SER
1	A	150	GLU
1	A	160	ASN
1	A	173	LYS
1	A	200	LEU
1	A	243	LYS
1	A	248	LEU
1	A	275	SER
1	A	286	LEU
1	A	301	LYS
1	A	314	LYS
1	A	329	SER
1	A	397	SER
1	A	416	ASN
1	A	465	SER
1	A	472	ARG
1	A	476	LYS
1	A	504	LEU
1	A	509	CYS
1	A	516	SER
1	A	554	SER
1	A	595	ASN
1	A	625	ASN
1	A	677	LYS
1	A	682	THR
1	A	702	PHE
1	A	703	LEU
1	A	725	SER
1	A	733	SER
1	A	736	SER
1	A	750	THR
1	A	753	LYS
1	A	756	LEU
1	A	780	ILE
1	A	791	LEU
1	A	809	GLN
1	A	815	VAL
1	A	817	LEU
1	B	49	CYS
1	B	52	ARG
1	B	56	GLU
1	B	66	THR

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Mol	Chain	Res	Type
1	B	76	THR
1	B	87	GLN
1	B	122	LEU
1	B	160	ASN
1	B	168	ARG
1	B	248	LEU
1	B	275	SER
1	B	280	ARG
1	B	286	LEU
1	B	287	THR
1	B	317	ASP
1	B	408	GLN
1	B	416	ASN
1	B	418	SER
1	B	504	LEU
1	B	509	CYS
1	B	727	LEU
1	B	733	SER
1	B	750	THR
1	B	754	SER
1	B	765	SER
1	B	780	ILE
1	B	794	LYS
1	B	817	LEU
1	C	33	TYR
1	C	76	THR
1	C	81	GLU
1	C	86	LEU
1	C	100	VAL
1	C	116	ILE
1	C	118	ASP
1	C	147	SER
1	C	150	GLU
1	C	164	GLU
1	C	167	SER
1	C	173	LYS
1	C	188	GLU
1	C	191	ASN
1	C	200	LEU
1	C	212	SER
1	C	214	SER
1	C	219	LYS

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Mol	Chain	Res	Type
1	C	245	LEU
1	C	246	ILE
1	C	248	LEU
1	C	259	ARG
1	C	275	SER
1	C	278	ILE
1	C	279	ASP
1	C	280	ARG
1	C	285	ASN
1	C	314	LYS
1	C	317	ASP
1	C	365	LYS
1	C	387	PHE
1	C	397	SER
1	C	412	LYS
1	C	416	ASN
1	C	418	SER
1	C	504	LEU
1	C	569	ARG
1	C	632	ILE
1	C	681	TRP
1	C	682	THR
1	C	706	SER
1	C	712	SER
1	C	715	ARG
1	C	720	SER
1	C	725	SER
1	C	729	SER
1	C	731	PHE
1	C	732	LEU
1	C	735	VAL
1	C	780	ILE
1	C	784	ARG
1	C	810	ARG
1	D	36	ASP
1	D	49	CYS
1	D	52	ARG
1	D	64	TYR
1	D	88	ASN
1	D	117	THR
1	D	122	LEU
1	D	150	GLU

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Mol	Chain	Res	Type
1	D	170	ILE
1	D	200	LEU
1	D	235	LYS
1	D	243	LYS
1	D	248	LEU
1	D	300	ARG
1	D	308	LYS
1	D	418	SER
1	D	419	ASN
1	D	472	ARG
1	D	476	LYS
1	D	509	CYS
1	D	582	ASN
1	D	609	SER
1	D	653	HIS
1	D	665	SER
1	D	686	GLN
1	D	702	PHE
1	D	705	ASP
1	D	712	SER
1	D	715	ARG
1	D	733	SER
1	D	735	VAL
1	D	736	SER
1	D	753	LYS
1	D	756	LEU
1	D	764	LEU
1	D	788	ASP
1	D	794	LYS
1	D	805	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	87	GLN
1	A	160	ASN
1	A	191	ASN
1	A	288	GLN
1	A	721	HIS
1	A	809	GLN
1	B	288	GLN

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Mol	Chain	Res	Type
1	B	312	HIS
1	B	503	ASN
1	C	84	GLN
1	C	174	ASN
1	C	202	ASN
1	C	284	GLN
1	C	285	ASN
1	C	721	HIS
1	D	123	ASN
1	D	247	ASN
1	D	284	GLN
1	D	416	ASN
1	D	581	GLN
1	D	629	ASN
1	D	656	ASN
1	D	661	ASN
1	D	686	GLN

### 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 ⓘ

32 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	2,1	14,14,15	0.96	1 (7%)	17,19,21	2.15	4 (23%)



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	0.68	0	17,19,21	1.28	2 (11%)
2	BMA	E	3	2	11,11,12	1.05	1 (9%)	15,15,17	1.67	5 (33%)
2	NAG	F	1	2,1	14,14,15	0.73	0	17,19,21	1.44	3 (17%)
2	NAG	F	2	2	14,14,15	0.67	0	17,19,21	1.01	0
2	BMA	F	3	2	11,11,12	0.54	0	15,15,17	1.52	2 (13%)
3	NAG	G	1	3,1	14,14,15	0.62	0	17,19,21	1.07	1 (5%)
3	NAG	G	2	3	14,14,15	0.71	1 (7%)	17,19,21	1.42	4 (23%)
2	NAG	H	1	2,1	14,14,15	0.79	0	17,19,21	1.33	4 (23%)
2	NAG	H	2	2	14,14,15	0.62	0	17,19,21	1.30	3 (17%)
2	BMA	H	3	2	11,11,12	0.25	0	15,15,17	0.53	0
2	NAG	I	1	2,1	14,14,15	0.77	0	17,19,21	1.53	5 (29%)
2	NAG	I	2	2	14,14,15	0.96	0	17,19,21	1.34	3 (17%)
2	BMA	I	3	2	11,11,12	0.44	0	15,15,17	0.98	1 (6%)
3	NAG	J	1	3,1	14,14,15	0.96	2 (14%)	17,19,21	1.87	3 (17%)
3	NAG	J	2	3	14,14,15	0.64	0	17,19,21	1.58	4 (23%)
2	NAG	K	1	2,1	14,14,15	0.56	0	17,19,21	1.40	4 (23%)
2	NAG	K	2	2	14,14,15	0.65	0	17,19,21	1.26	2 (11%)
2	BMA	K	3	2	11,11,12	0.70	0	15,15,17	1.34	2 (13%)
2	NAG	L	1	2,1	14,14,15	0.48	0	17,19,21	1.45	3 (17%)
2	NAG	L	2	2	14,14,15	0.78	0	17,19,21	0.86	0
2	BMA	L	3	2	11,11,12	0.52	0	15,15,17	0.90	1 (6%)
3	NAG	M	1	3,1	14,14,15	0.81	0	17,19,21	1.77	5 (29%)
3	NAG	M	2	3	14,14,15	0.56	0	17,19,21	1.45	3 (17%)
2	NAG	N	1	2,1	14,14,15	0.85	1 (7%)	17,19,21	1.91	4 (23%)
2	NAG	N	2	2	14,14,15	0.76	0	17,19,21	1.57	4 (23%)
2	BMA	N	3	2	11,11,12	0.94	1 (9%)	15,15,17	2.24	6 (40%)
2	NAG	O	1	2,1	14,14,15	0.72	0	17,19,21	1.00	1 (5%)
2	NAG	O	2	2	14,14,15	0.57	0	17,19,21	0.90	0
2	BMA	O	3	2	11,11,12	0.42	0	15,15,17	1.20	1 (6%)
3	NAG	P	1	3,1	14,14,15	0.68	0	17,19,21	1.32	2 (11%)
3	NAG	P	2	3	14,14,15	0.62	0	17,19,21	1.13	1 (5%)

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	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	1/2/19/22	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	BMA	F	3	2	-	1/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	BMA	H	3	2	-	1/2/19/22	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	BMA	I	3	2	-	0/2/19/22	0/1/1/1
3	NAG	J	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	BMA	K	3	2	-	2/2/19/22	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	BMA	L	3	2	-	2/2/19/22	0/1/1/1
3	NAG	M	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	BMA	N	3	2	-	0/2/19/22	0/1/1/1
2	NAG	O	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
2	BMA	O	3	2	-	2/2/19/22	0/1/1/1
3	NAG	P	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	O5-C1	-2.81	1.39	1.43
2	E	3	BMA	O5-C1	-2.66	1.39	1.43
2	N	1	NAG	O5-C1	-2.55	1.39	1.43
3	J	1	NAG	O5-C1	-2.35	1.39	1.43
2	N	3	BMA	O5-C1	-2.30	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2	NAG	O5-C1	-2.22	1.40	1.43
3	J	1	NAG	O5-C5	-2.06	1.39	1.43

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	C1-O5-C5	6.84	121.36	112.19
3	J	1	NAG	C1-O5-C5	4.87	118.72	112.19
2	N	1	NAG	O5-C1-C2	-4.60	104.17	111.29
2	N	3	BMA	C1-O5-C5	4.56	118.30	112.19
3	M	1	NAG	O6-C6-C5	-4.12	97.30	111.33
3	J	1	NAG	O5-C5-C6	-4.04	99.80	107.66
2	N	1	NAG	C1-O5-C5	3.86	117.36	112.19
2	N	3	BMA	O2-C2-C1	-3.79	100.55	109.22
2	N	3	BMA	O5-C1-C2	-3.67	102.04	110.79
2	E	1	NAG	O5-C5-C6	-3.57	100.71	107.66
3	P	1	NAG	C1-C2-N2	-3.44	105.01	110.43
3	J	2	NAG	C3-C4-C5	-3.44	103.99	110.23
2	F	3	BMA	C1-O5-C5	-3.21	107.89	112.19
2	L	1	NAG	C1-O5-C5	3.21	116.48	112.19
3	M	1	NAG	C1-C2-N2	-3.17	105.43	110.43
3	J	2	NAG	O5-C1-C2	-3.10	106.50	111.29
2	E	3	BMA	O4-C4-C3	-3.10	103.08	110.38
2	N	2	NAG	O6-C6-C5	-2.97	101.20	111.33
2	N	1	NAG	C6-C5-C4	-2.95	105.78	113.02
2	N	2	NAG	O5-C1-C2	-2.93	106.76	111.29
3	M	2	NAG	C1-C2-N2	-2.92	105.83	110.43
3	M	1	NAG	C1-O5-C5	2.81	115.95	112.19
3	G	2	NAG	O5-C1-C2	-2.80	106.95	111.29
3	J	1	NAG	C1-C2-N2	-2.77	106.06	110.43
2	I	2	NAG	O5-C1-C2	-2.77	107.01	111.29
2	E	2	NAG	O7-C7-C8	-2.74	117.17	122.05
2	F	3	BMA	O5-C5-C6	2.74	113.00	107.66
2	H	1	NAG	C1-O5-C5	2.64	115.73	112.19
2	K	3	BMA	C3-C4-C5	2.63	115.00	110.23
2	H	1	NAG	O6-C6-C5	-2.61	102.44	111.33
2	I	1	NAG	O5-C1-C2	-2.59	107.28	111.29
3	M	2	NAG	C1-O5-C5	2.57	115.63	112.19
2	E	3	BMA	C1-O5-C5	2.53	115.58	112.19
2	I	1	NAG	O4-C4-C3	-2.53	104.41	110.38
2	I	2	NAG	O7-C7-N2	2.52	126.43	121.98
2	O	1	NAG	O5-C1-C2	-2.52	107.40	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	1	NAG	O5-C1-C2	-2.51	107.41	111.29
2	K	2	NAG	O5-C1-C2	-2.46	107.48	111.29
2	H	2	NAG	C1-C2-N2	2.46	114.30	110.43
2	K	1	NAG	O6-C6-C5	-2.41	103.13	111.33
2	N	2	NAG	C3-C4-C5	-2.41	105.87	110.23
3	G	2	NAG	C1-O5-C5	2.40	115.40	112.19
3	M	1	NAG	O5-C5-C4	2.38	116.62	110.83
2	K	1	NAG	O5-C1-C2	-2.38	107.62	111.29
2	K	1	NAG	C1-O5-C5	2.37	115.36	112.19
2	N	3	BMA	O5-C5-C6	2.33	112.20	107.66
2	L	3	BMA	C2-C3-C4	-2.33	106.77	110.86
2	H	1	NAG	O5-C1-C2	-2.31	107.71	111.29
3	G	2	NAG	O7-C7-C8	-2.31	117.95	122.05
2	O	3	BMA	O5-C5-C6	2.28	112.11	107.66
2	N	3	BMA	O6-C6-C5	2.27	119.07	111.33
2	I	1	NAG	C1-O5-C5	2.27	115.23	112.19
2	I	1	NAG	C2-N2-C7	2.26	125.93	122.90
2	I	1	NAG	O7-C7-N2	2.26	125.98	121.98
2	H	1	NAG	C6-C5-C4	-2.24	107.51	113.02
2	F	1	NAG	O4-C4-C3	-2.24	105.09	110.38
2	E	1	NAG	C6-C5-C4	-2.24	107.52	113.02
2	F	1	NAG	O5-C1-C2	-2.24	107.83	111.29
3	M	2	NAG	O4-C4-C5	2.23	114.82	109.32
3	G	1	NAG	C1-O5-C5	-2.23	109.20	112.19
2	E	3	BMA	O6-C6-C5	2.20	118.83	111.33
2	I	3	BMA	O2-C2-C1	-2.17	104.25	109.22
2	N	2	NAG	C6-C5-C4	-2.16	107.72	113.02
3	G	2	NAG	O4-C4-C5	2.13	114.56	109.32
3	J	2	NAG	O7-C7-C8	-2.12	118.27	122.05
2	E	2	NAG	O5-C1-C2	-2.12	108.01	111.29
2	E	3	BMA	C6-C5-C4	2.12	118.22	113.02
2	L	1	NAG	O7-C7-C8	-2.12	118.29	122.05
2	E	1	NAG	O6-C6-C5	-2.11	104.15	111.33
2	I	2	NAG	C8-C7-N2	-2.10	112.64	116.12
2	H	2	NAG	C2-N2-C7	-2.07	120.13	122.90
2	N	3	BMA	O3-C3-C4	2.06	115.24	110.38
3	M	1	NAG	C6-C5-C4	-2.06	107.96	113.02
2	N	1	NAG	O6-C6-C5	-2.05	104.34	111.33
2	L	1	NAG	O5-C1-C2	-2.05	108.11	111.29
2	K	3	BMA	O3-C3-C4	2.05	115.21	110.38
3	J	2	NAG	O4-C4-C5	2.04	114.35	109.32
2	K	2	NAG	C1-C2-N2	2.04	113.64	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	BMA	O3-C3-C2	2.03	114.20	110.05
2	F	1	NAG	O7-C7-C8	-2.03	118.44	122.05
3	P	2	NAG	C2-N2-C7	2.01	125.60	122.90
2	K	1	NAG	C6-C5-C4	-2.01	108.08	113.02
2	H	2	NAG	C1-O5-C5	-2.00	109.50	112.19

There are no chirality outliers.

All (26) torsion outliers are listed below:

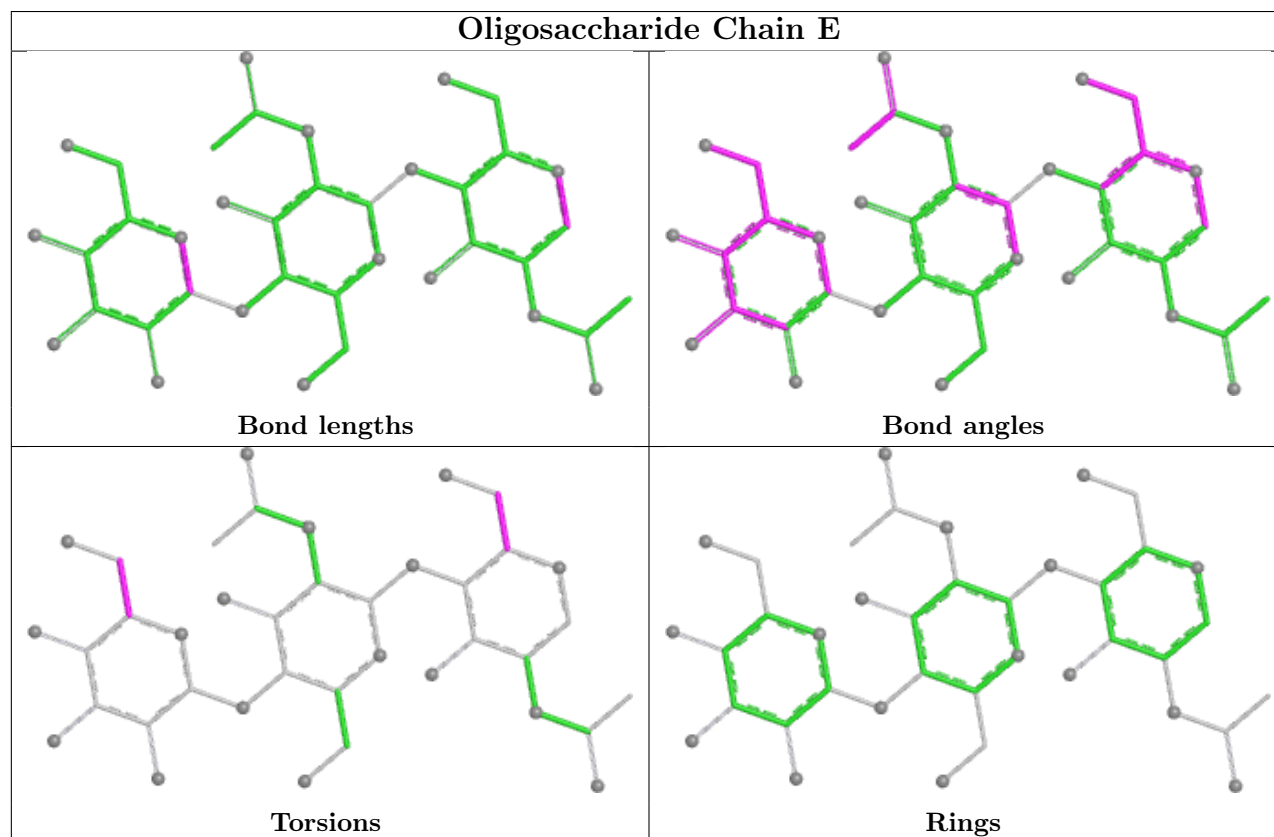
Mol	Chain	Res	Type	Atoms
2	O	3	BMA	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	K	3	BMA	O5-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	O	3	BMA	C4-C5-C6-O6
2	K	3	BMA	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	H	3	BMA	O5-C5-C6-O6
2	L	3	BMA	C4-C5-C6-O6
2	F	3	BMA	C4-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	L	3	BMA	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6

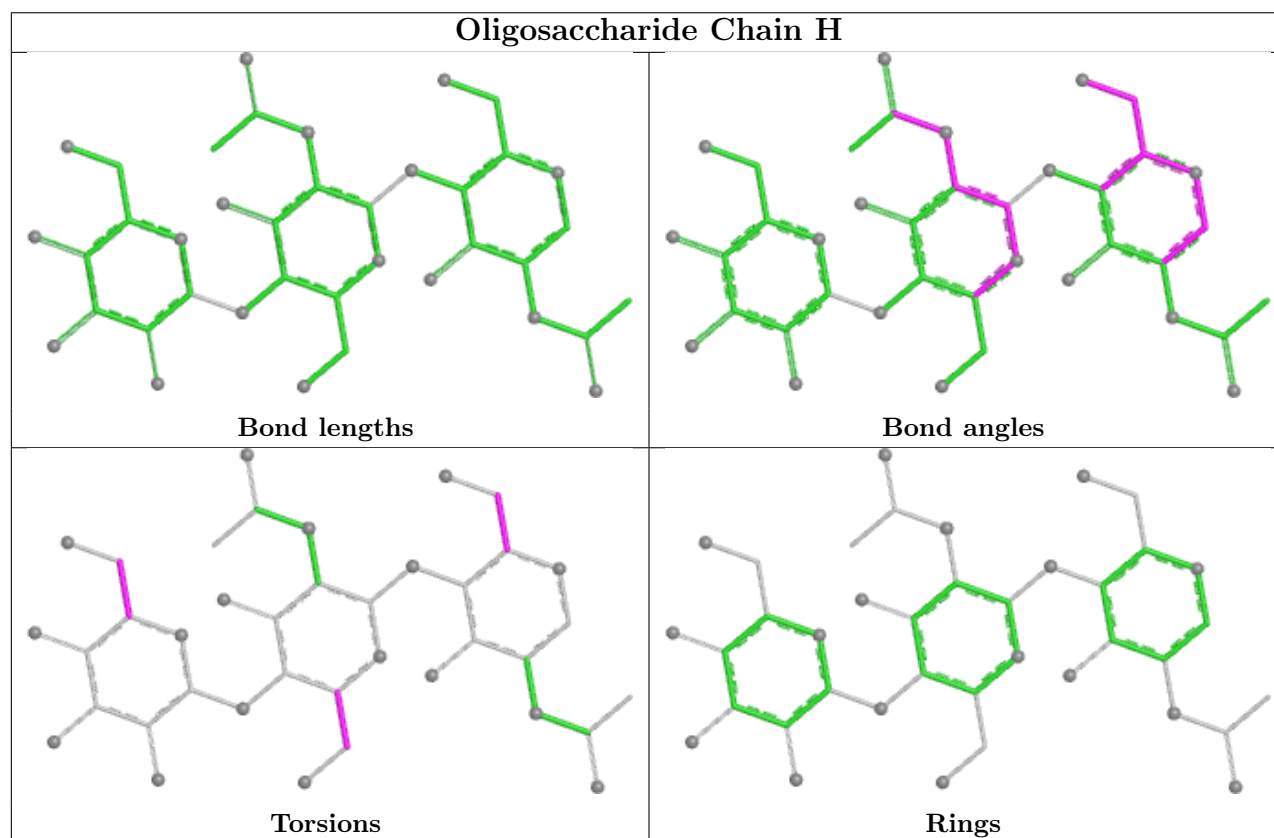
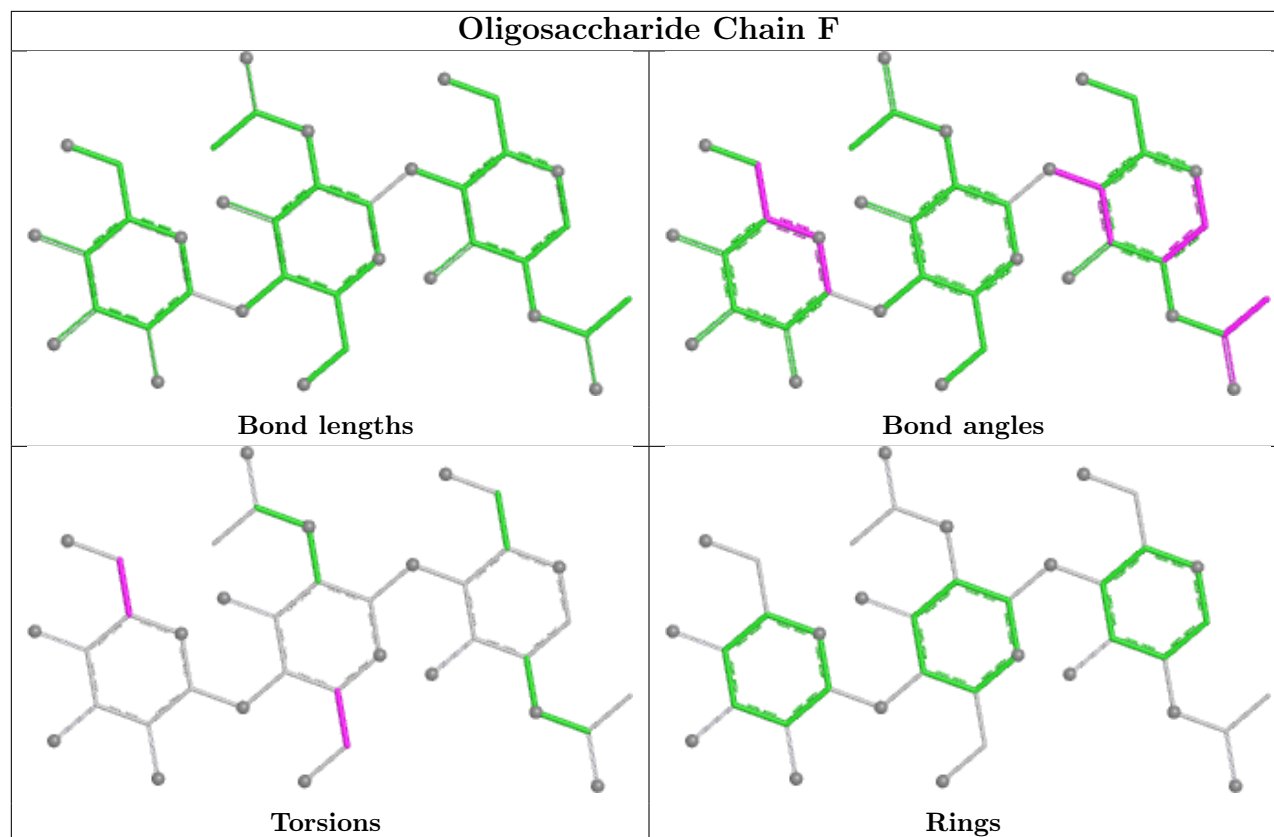
There are no ring outliers.

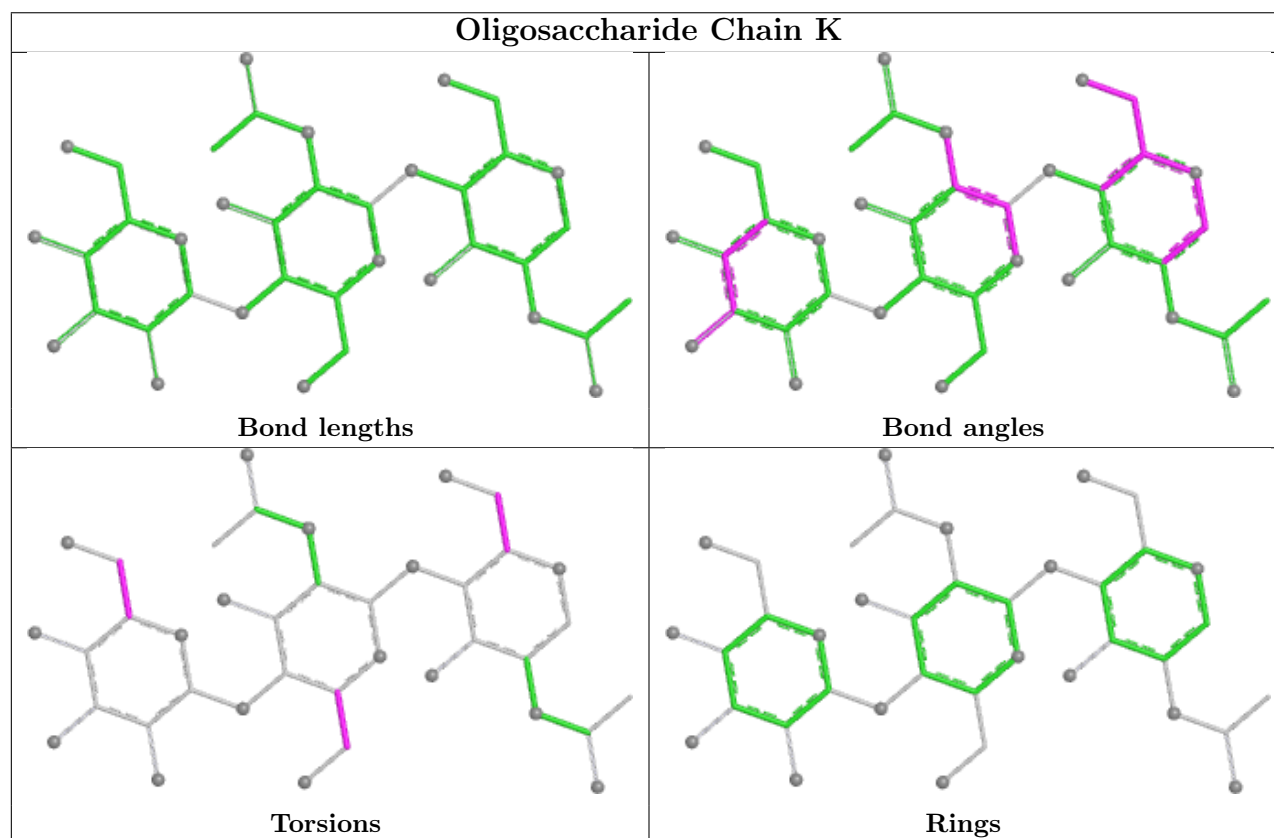
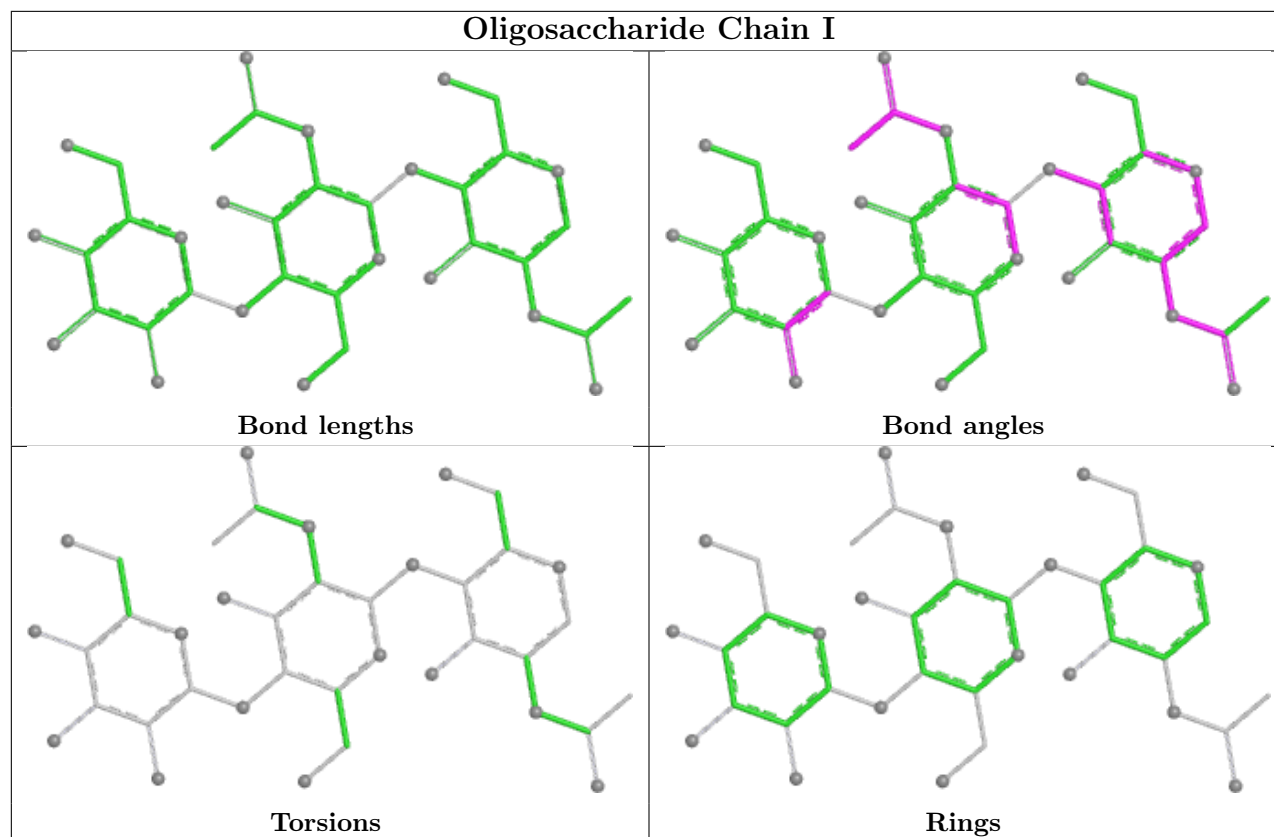
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	2	0
2	N	1	NAG	2	0

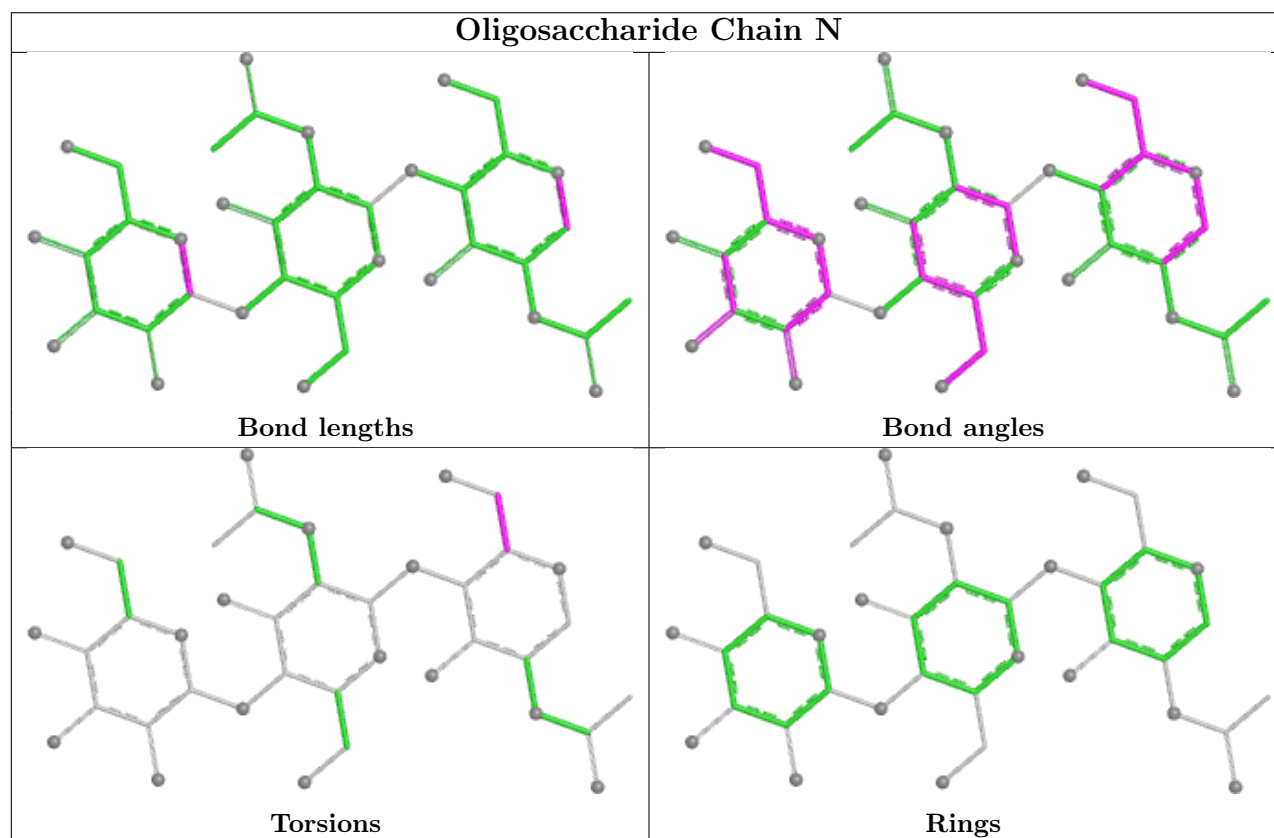
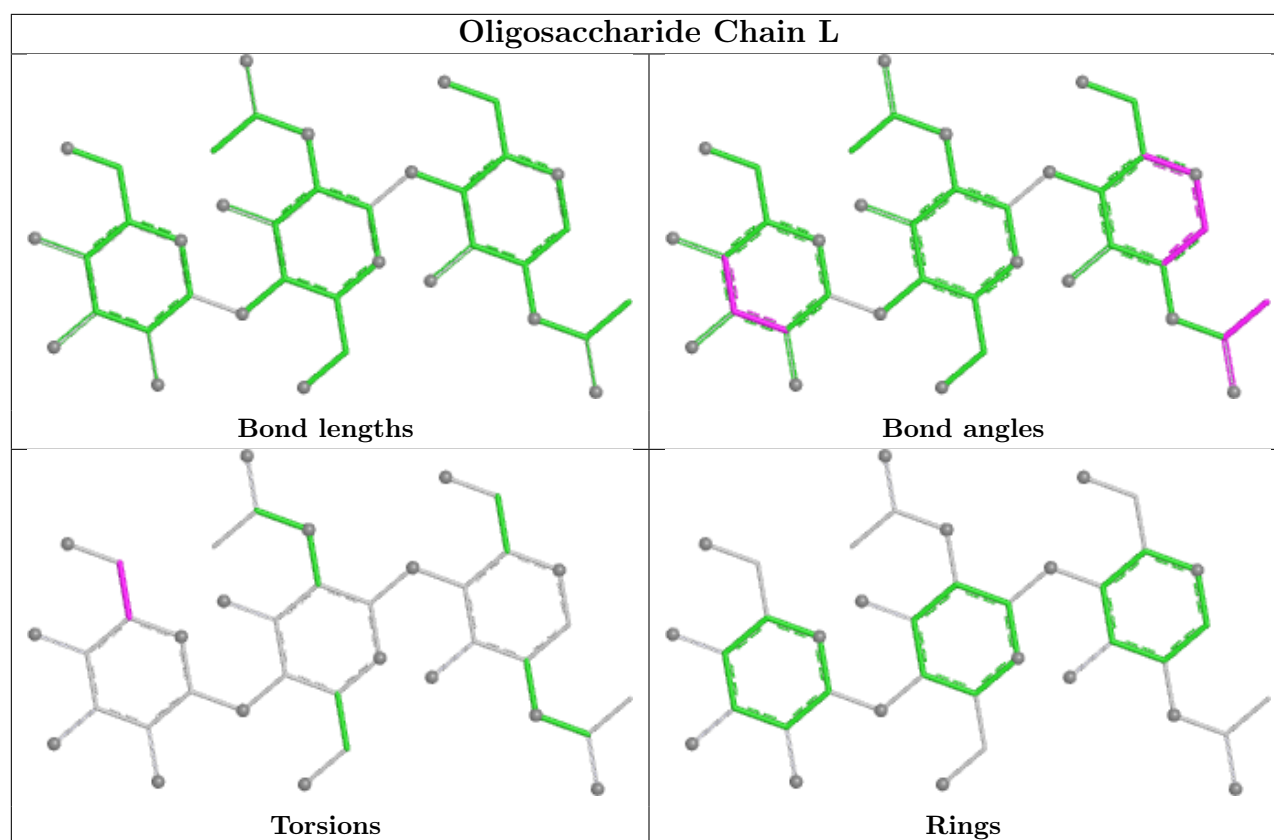
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

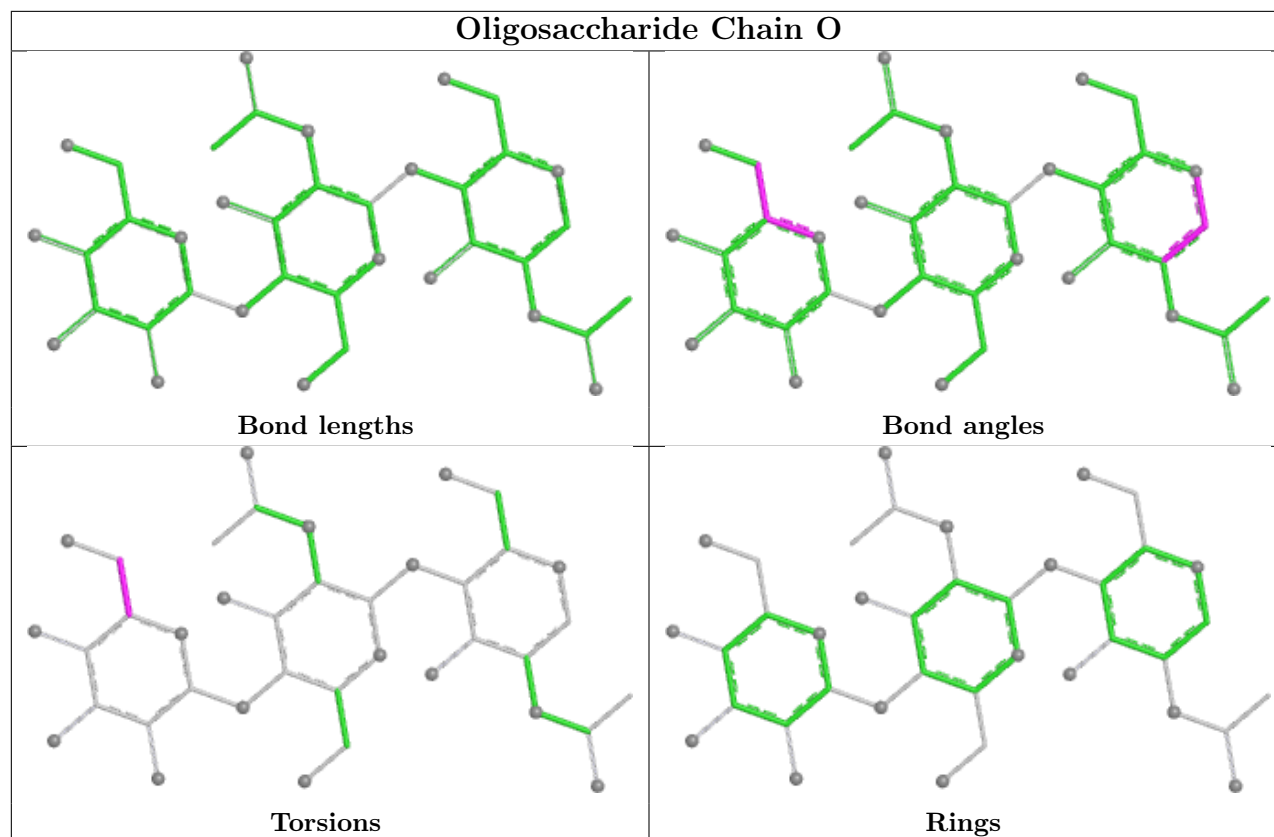


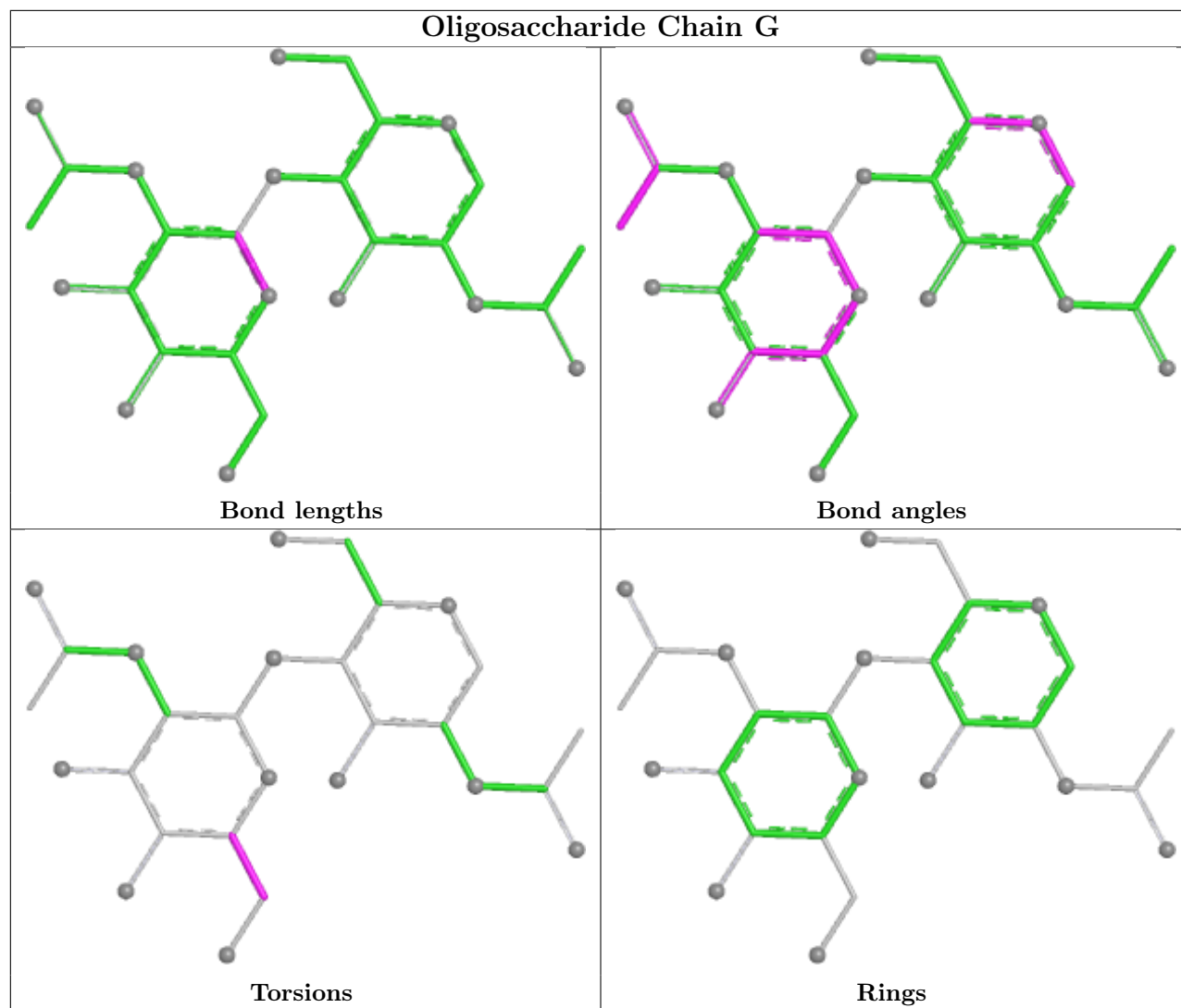


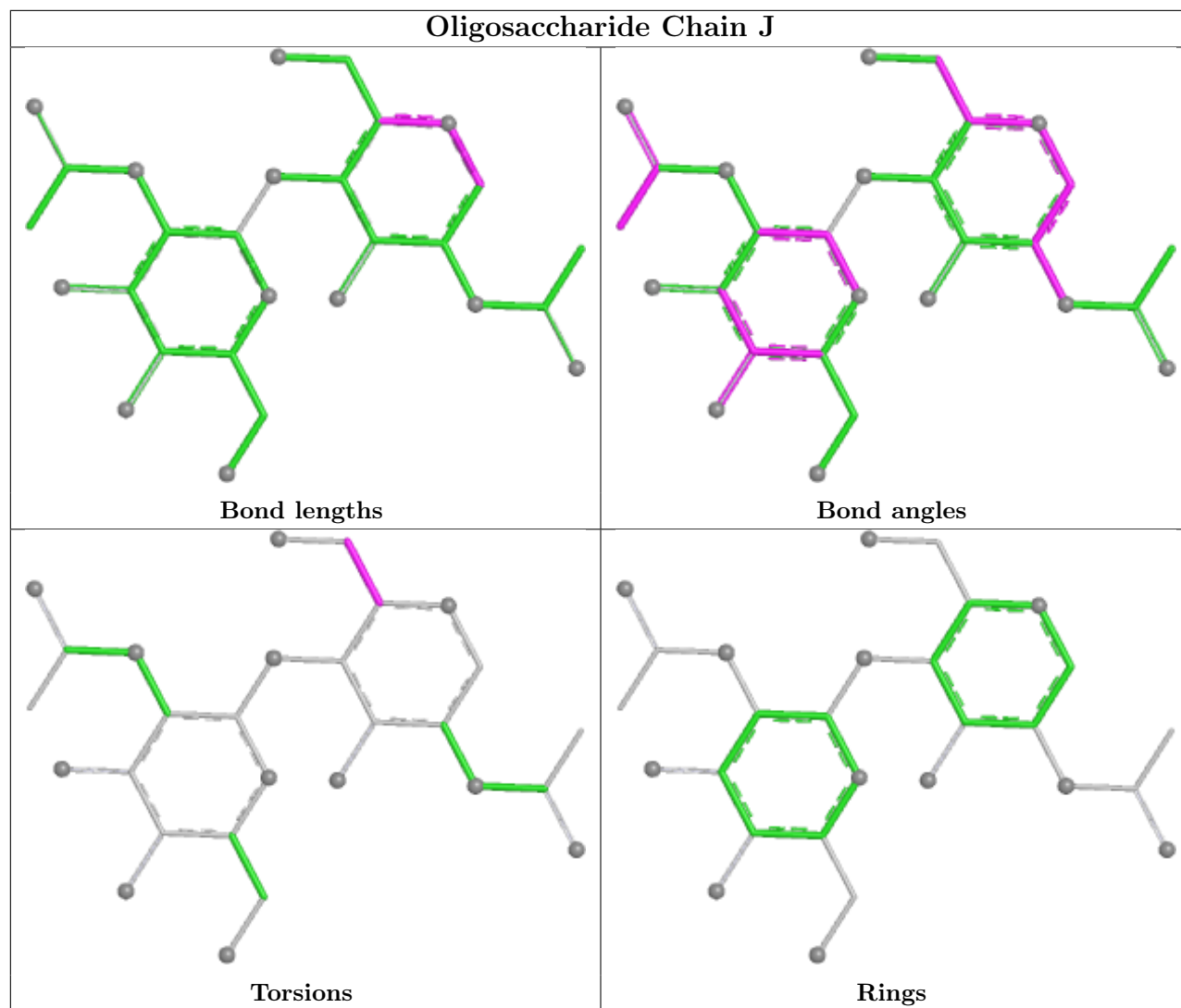


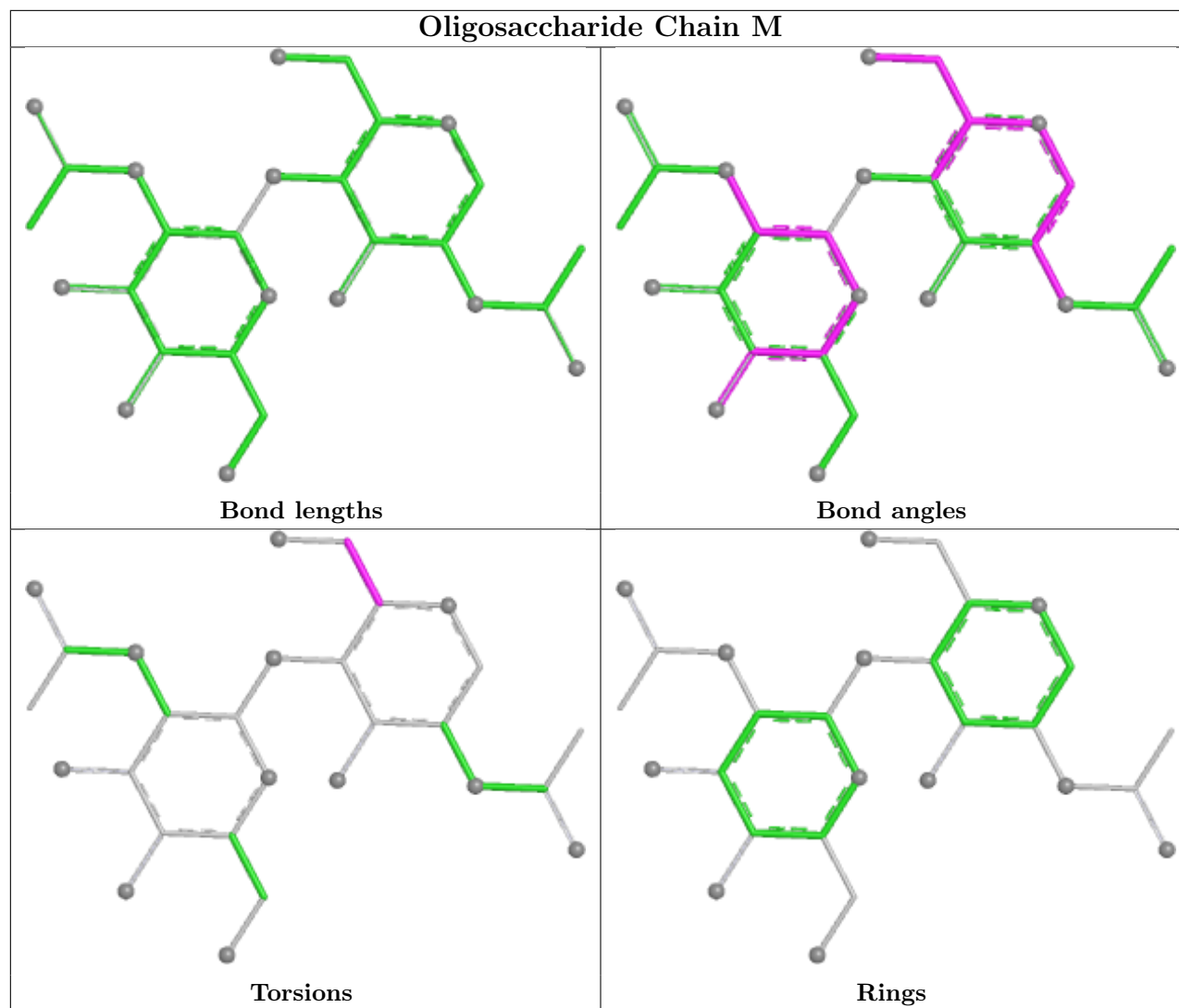


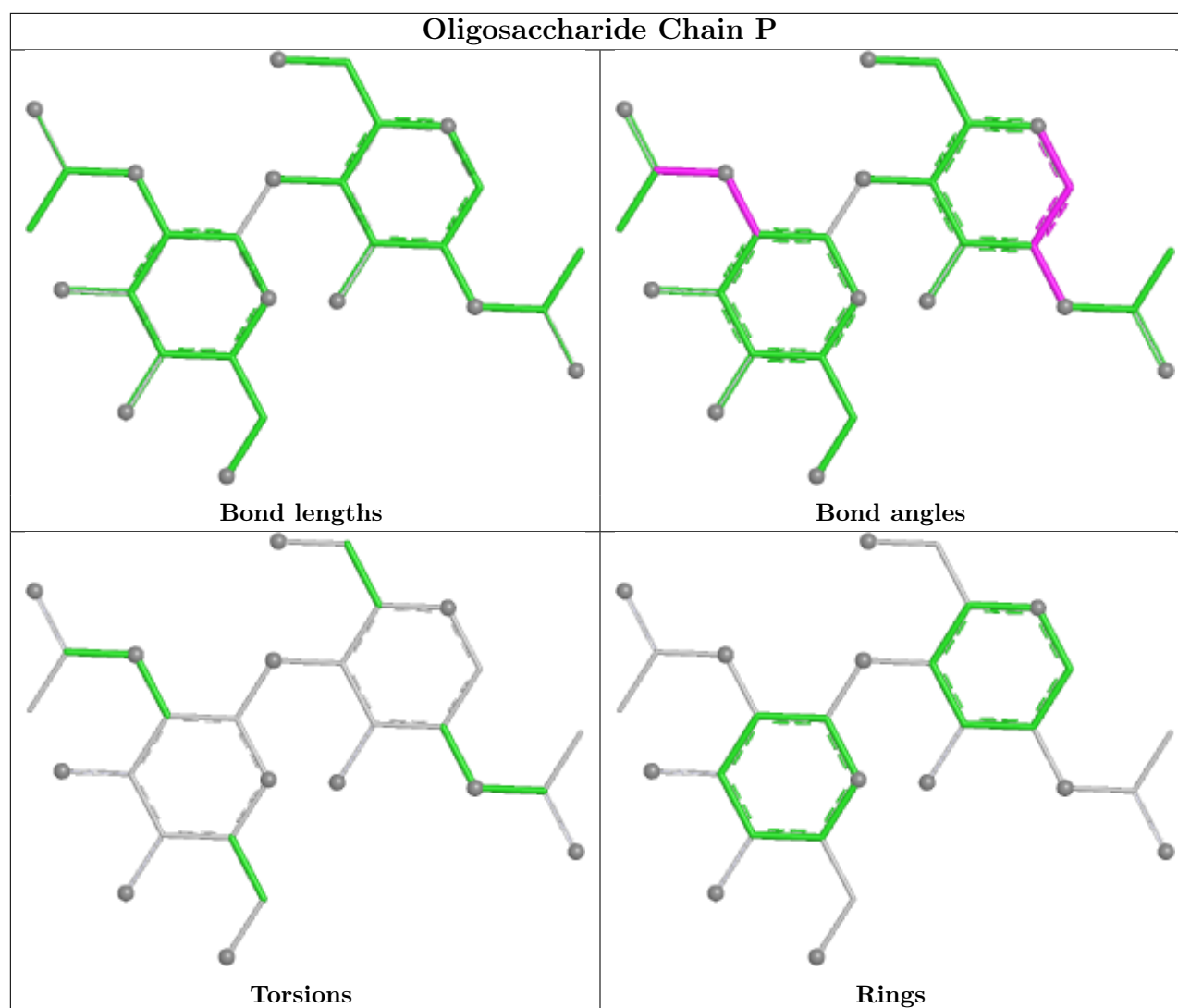












## 5.6 Ligand geometry [i](#)

26 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	$\# Z  > 2$
6	UCG	A	915	-	46,52,52	1.36	5 (10%)	61,82,82	2.32	21 (34%)
5	NAG	B	911	1	14,14,15	0.30	0	17,19,21	0.56	0
5	NAG	B	912	1	14,14,15	0.52	0	17,19,21	1.58	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	B	913	1	14,14,15	0.58	0	17,19,21	1.27	1 (5%)
5	NAG	D	914	1	14,14,15	0.52	0	17,19,21	2.20	4 (23%)
4	URI	B	901	-	18,18,18	1.39	4 (22%)	26,26,26	1.72	5 (19%)
5	NAG	A	911	1	14,14,15	0.29	0	17,19,21	0.56	0
5	NAG	C	912	1	14,14,15	0.80	0	17,19,21	1.25	1 (5%)
6	UCG	C	901	-	46,52,52	1.36	5 (10%)	61,82,82	2.10	15 (24%)
5	NAG	A	913	1	14,14,15	0.59	0	17,19,21	1.24	2 (11%)
5	NAG	C	913	1	14,14,15	0.57	0	17,19,21	1.42	3 (17%)
5	NAG	D	912	1	14,14,15	0.63	0	17,19,21	1.31	1 (5%)
4	URI	A	901	-	18,18,18	1.26	4 (22%)	26,26,26	1.77	5 (19%)
5	NAG	A	912	1	14,14,15	0.28	0	17,19,21	0.56	0
5	NAG	C	914	1	14,14,15	0.50	0	17,19,21	1.65	2 (11%)
5	NAG	D	913	1	14,14,15	0.28	0	17,19,21	0.56	0
5	NAG	A	914	1	14,14,15	0.70	0	17,19,21	1.31	2 (11%)
5	NAG	B	908	1	14,14,15	0.64	0	17,19,21	0.64	0
5	NAG	B	914	1	14,14,15	0.30	0	17,19,21	0.56	0
4	URI	C	902	-	18,18,18	1.55	4 (22%)	26,26,26	2.19	9 (34%)
4	URI	D	901	-	18,18,18	1.42	3 (16%)	26,26,26	2.02	7 (26%)
5	NAG	A	908	1	14,14,15	0.29	0	17,19,21	0.56	0
5	NAG	D	909	1	14,14,15	0.78	0	17,19,21	2.54	5 (29%)
6	UCG	D	902	-	46,52,52	1.43	5 (10%)	61,82,82	2.31	21 (34%)
5	NAG	C	909	1	14,14,15	0.54	0	17,19,21	1.19	1 (5%)
6	UCG	B	915	-	46,52,52	1.35	5 (10%)	61,82,82	2.13	20 (32%)

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
6	UCG	A	915	-	-	5/21/67/67	0/6/6/6
5	NAG	B	911	1	-	2/6/23/26	0/1/1/1
5	NAG	B	912	1	-	2/6/23/26	0/1/1/1
5	NAG	B	913	1	-	0/6/23/26	0/1/1/1
5	NAG	D	914	1	-	0/6/23/26	0/1/1/1
4	URI	B	901	-	-	4/6/22/22	0/2/2/2
5	NAG	A	911	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	912	1	-	2/6/23/26	0/1/1/1
6	UCG	C	901	-	-	5/21/67/67	0/6/6/6
5	NAG	A	913	1	-	2/6/23/26	0/1/1/1
5	NAG	C	913	1	-	2/6/23/26	0/1/1/1
5	NAG	D	912	1	-	0/6/23/26	0/1/1/1
4	URI	A	901	-	-	4/6/22/22	0/2/2/2
5	NAG	A	912	1	-	2/6/23/26	0/1/1/1
5	NAG	C	914	1	-	2/6/23/26	0/1/1/1
5	NAG	D	913	1	-	1/6/23/26	0/1/1/1
5	NAG	A	914	1	-	1/6/23/26	0/1/1/1
5	NAG	B	908	1	-	0/6/23/26	0/1/1/1
5	NAG	B	914	1	-	2/6/23/26	0/1/1/1
4	URI	C	902	-	-	5/6/22/22	0/2/2/2
4	URI	D	901	-	-	3/6/22/22	0/2/2/2
5	NAG	A	908	1	-	0/6/23/26	0/1/1/1
5	NAG	D	909	1	-	2/6/23/26	0/1/1/1
6	UCG	D	902	-	-	5/21/67/67	0/6/6/6
5	NAG	C	909	1	-	2/6/23/26	0/1/1/1
6	UCG	B	915	-	-	2/21/67/67	0/6/6/6

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	915	UCG	P2-O16	4.60	1.66	1.50
6	B	915	UCG	P2-O16	4.48	1.66	1.50
6	C	901	UCG	P2-O16	4.36	1.65	1.50
6	D	902	UCG	C9-C11	-4.33	1.38	1.47
6	D	902	UCG	P2-O16	4.31	1.65	1.50
6	B	915	UCG	C9-C11	-4.12	1.39	1.47
6	A	915	UCG	C9-C11	-3.81	1.39	1.47
6	C	901	UCG	C9-C11	-3.66	1.40	1.47
4	C	902	URI	C4-N3	-3.40	1.32	1.38
6	D	902	UCG	C8-N	2.72	1.42	1.38
4	C	902	URI	C2-N1	2.69	1.42	1.38
4	D	901	URI	C5-C4	-2.68	1.37	1.43
4	B	901	URI	C2-N1	2.60	1.42	1.38
4	C	902	URI	C5-C4	-2.60	1.38	1.43
4	D	901	URI	C4-N3	-2.59	1.34	1.38
6	D	902	UCG	P2-O17	2.59	1.67	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	915	UCG	C8-N	2.57	1.42	1.38
6	C	901	UCG	C8-N	2.56	1.42	1.38
4	A	901	URI	O2-C2	2.50	1.27	1.23
4	B	901	URI	C4-N3	-2.50	1.34	1.38
6	A	915	UCG	C8-N	2.42	1.42	1.38
6	C	901	UCG	P2-O17	2.40	1.66	1.55
6	A	915	UCG	C6-C5	2.39	1.40	1.35
4	C	902	URI	C2-N3	-2.35	1.33	1.38
4	A	901	URI	C5-C4	-2.29	1.38	1.43
6	B	915	UCG	P2-O17	2.28	1.65	1.55
4	B	901	URI	O2-C2	2.27	1.27	1.23
6	D	902	UCG	C7-N1	-2.17	1.34	1.38
6	A	915	UCG	C15-C16	2.13	1.57	1.53
6	B	915	UCG	C6-C5	2.12	1.40	1.35
4	A	901	URI	C4-N3	-2.10	1.35	1.38
4	A	901	URI	C2-N1	2.08	1.41	1.38
4	D	901	URI	C6-C5	2.08	1.39	1.35
4	B	901	URI	C5-C4	-2.07	1.39	1.43
6	C	901	UCG	C5-C7	-2.01	1.39	1.43

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	909	NAG	C1-O5-C5	8.10	123.04	112.19
6	D	902	UCG	O12-P2-O16	-7.90	94.91	115.76
6	C	901	UCG	O12-P2-O16	-7.66	95.53	115.76
5	D	914	NAG	C1-O5-C5	6.72	121.19	112.19
6	B	915	UCG	O12-P2-O16	-6.00	99.91	115.76
6	D	902	UCG	C7-N1-C8	-5.98	119.19	126.61
6	A	915	UCG	C17-O10-C14	-5.82	104.60	109.92
6	A	915	UCG	O12-P2-O16	-5.73	100.62	115.76
6	A	915	UCG	C7-N1-C8	-5.43	119.88	126.61
6	D	902	UCG	N1-C8-N	5.40	121.92	114.89
6	A	915	UCG	N1-C8-N	5.31	121.80	114.89
6	C	901	UCG	O13-P2-O16	-5.29	101.78	115.76
4	D	901	URI	C4-N3-C2	-5.16	120.21	126.61
6	B	915	UCG	C7-N1-C8	-5.05	120.34	126.61
6	C	901	UCG	C7-N1-C8	-5.03	120.36	126.61
6	B	915	UCG	N1-C8-N	4.97	121.37	114.89
6	A	915	UCG	O5-C8-N	-4.82	116.53	122.80
4	C	902	URI	C1'-N1-C2	4.68	126.00	117.59
6	A	915	UCG	O12-C15-C16	4.57	123.61	104.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	901	URI	C5-C4-N3	4.40	120.96	114.80
6	C	901	UCG	N1-C8-N	4.34	120.54	114.89
6	C	901	UCG	O13-C16-C15	4.26	122.29	104.34
4	A	901	URI	C5-C4-N3	4.25	120.76	114.80
6	C	901	UCG	O12-C15-C16	4.21	122.07	104.34
4	C	902	URI	C4-N3-C2	-4.21	121.39	126.61
4	A	901	URI	C4-N3-C2	-4.20	121.40	126.61
4	A	901	URI	O4-C4-C5	-4.17	117.97	125.16
5	C	914	NAG	C1-O5-C5	4.14	117.73	112.19
6	D	902	UCG	O12-C15-C16	4.14	121.76	104.34
6	B	915	UCG	O12-C15-C16	4.13	121.74	104.34
6	B	915	UCG	O10-C17-C16	4.12	113.60	104.92
4	C	902	URI	O4-C4-C5	-4.02	118.23	125.16
4	B	901	URI	C5-C4-N3	3.94	120.32	114.80
6	B	915	UCG	O13-P2-O16	-3.92	105.41	115.76
6	D	902	UCG	O13-C16-C15	3.89	120.73	104.34
4	C	902	URI	C5-C4-N3	3.88	120.24	114.80
6	C	901	UCG	C5-C7-N1	3.85	120.20	114.80
4	C	902	URI	N3-C2-N1	3.83	119.88	114.89
6	D	902	UCG	O10-C17-C16	3.82	112.97	104.92
6	D	902	UCG	C5-C7-N1	3.81	120.14	114.80
4	D	901	URI	N3-C2-N1	3.76	119.79	114.89
4	B	901	URI	C4-N3-C2	-3.62	122.12	126.61
5	D	912	NAG	O5-C1-C2	-3.61	105.70	111.29
4	D	901	URI	O4-C4-C5	-3.56	119.03	125.16
6	B	915	UCG	O13-C16-C15	3.49	119.05	104.34
6	A	915	UCG	O10-C17-C16	3.45	112.20	104.92
6	A	915	UCG	O17-P2-O16	-3.44	98.78	109.89
4	B	901	URI	O4-C4-C5	-3.44	119.23	125.16
6	B	915	UCG	C5-C7-N1	3.44	119.61	114.80
6	B	915	UCG	C13-N5-C9	3.43	108.39	102.55
5	D	914	NAG	C4-C3-C2	-3.42	106.00	111.02
6	A	915	UCG	C5-C7-N1	3.38	119.53	114.80
6	D	902	UCG	O13-P2-O16	-3.35	106.93	115.76
6	D	902	UCG	O4-C7-C5	-3.31	119.46	125.16
5	B	913	NAG	C3-C4-C5	3.29	116.19	110.23
5	C	912	NAG	C1-O5-C5	3.19	116.46	112.19
6	A	915	UCG	O4-C7-C5	-3.15	119.74	125.16
4	B	901	URI	C1'-N1-C2	3.14	123.23	117.59
6	A	915	UCG	O13-C16-C15	3.12	117.49	104.34
6	A	915	UCG	C15-C16-C17	-3.03	96.75	103.78
6	D	902	UCG	O17-P2-O16	-3.02	100.15	109.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	902	UCG	C9-C11-N3	3.01	119.81	114.07
6	D	902	UCG	C12-N3-C11	-3.00	119.61	125.11
6	A	915	UCG	C12-N3-C11	-2.93	119.75	125.11
6	B	915	UCG	C17-O10-C14	-2.93	107.25	109.92
6	C	901	UCG	O10-C17-C16	2.88	110.99	104.92
6	A	915	UCG	O10-C14-C15	-2.86	101.72	106.61
6	B	915	UCG	C9-C11-N3	2.81	119.44	114.07
5	B	912	NAG	O5-C5-C6	2.79	113.10	107.66
4	B	901	URI	N3-C2-N1	2.77	118.50	114.89
5	C	913	NAG	C2-N2-C7	-2.75	119.21	122.90
5	D	909	NAG	C3-C4-C5	2.74	115.21	110.23
6	A	915	UCG	C9-C11-N3	2.74	119.30	114.07
5	C	914	NAG	O5-C1-C2	-2.72	107.08	111.29
6	B	915	UCG	C2-C1-C	2.72	105.87	99.89
6	B	915	UCG	O4-C7-C5	-2.69	120.52	125.16
6	D	902	UCG	C-N-C8	2.66	122.37	117.59
5	B	912	NAG	C1-C2-N2	2.66	114.62	110.43
6	C	901	UCG	C13-N5-C9	2.65	107.06	102.55
5	B	912	NAG	O7-C7-N2	2.62	126.61	121.98
6	C	901	UCG	O4-C7-C5	-2.58	120.72	125.16
6	A	915	UCG	C6-N-C8	-2.53	117.92	121.00
4	A	901	URI	C1'-N1-C2	2.53	122.13	117.59
6	C	901	UCG	C9-C11-N3	2.51	118.87	114.07
6	D	902	UCG	C13-N5-C9	2.50	106.80	102.55
6	B	915	UCG	O17-P2-O16	-2.48	101.88	109.89
4	D	901	URI	O3'-C3'-C2'	-2.48	103.88	111.82
6	B	915	UCG	C15-C16-C17	-2.47	98.05	103.78
5	D	909	NAG	O5-C1-C2	2.47	115.11	111.29
5	C	909	NAG	C2-N2-C7	-2.46	119.61	122.90
6	D	902	UCG	C17-O10-C14	-2.45	107.68	109.92
5	A	913	NAG	C1-O5-C5	2.44	115.46	112.19
5	A	914	NAG	C3-C4-C5	2.43	114.64	110.23
5	A	914	NAG	C1-O5-C5	2.43	115.45	112.19
5	D	909	NAG	O3-C3-C4	-2.43	104.64	110.38
6	B	915	UCG	C6-N-C8	-2.40	118.08	121.00
6	C	901	UCG	C12-N3-C11	-2.39	120.73	125.11
5	C	913	NAG	O5-C1-C2	-2.38	107.61	111.29
4	A	901	URI	N3-C2-N1	2.36	117.97	114.89
4	C	902	URI	C1'-N1-C6	-2.35	115.76	120.78
6	D	902	UCG	C6-N-C8	-2.35	118.14	121.00
5	D	914	NAG	C3-C4-C5	-2.34	105.99	110.23
6	D	902	UCG	C2-C1-C	2.33	105.01	99.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	915	UCG	C13-N5-C9	2.30	106.47	102.55
4	C	902	URI	C6-N1-C2	-2.29	118.20	121.00
6	D	902	UCG	O5-C8-N	-2.29	119.81	122.80
6	D	902	UCG	O9-C11-C9	-2.28	119.80	124.32
6	A	915	UCG	C2-C1-C	2.24	104.82	99.89
6	B	915	UCG	O5-C8-N	-2.24	119.88	122.80
4	D	901	URI	C1'-N1-C2	2.22	121.59	117.59
6	D	902	UCG	O10-C17-C18	-2.22	102.22	109.33
6	B	915	UCG	C12-N3-C11	-2.21	121.07	125.11
4	D	901	URI	O2'-C2'-C3'	-2.19	104.80	111.82
4	C	902	URI	O2-C2-N3	-2.18	117.48	121.49
6	B	915	UCG	O9-C11-C9	-2.15	120.05	124.32
5	A	913	NAG	C1-C2-N2	2.15	113.81	110.43
6	A	915	UCG	O13-P2-O16	-2.13	110.14	115.76
4	C	902	URI	O2'-C2'-C3'	-2.12	105.02	111.82
6	A	915	UCG	O7-P-O6	2.11	115.73	107.80
5	D	914	NAG	C2-N2-C7	-2.09	120.11	122.90
6	A	915	UCG	O10-C17-C18	-2.08	102.69	109.33
5	C	913	NAG	C4-C3-C2	2.06	114.04	111.02
6	D	902	UCG	O15-P1-O14	2.06	122.01	112.44
6	C	901	UCG	O15-P1-O14	2.03	121.91	112.44
5	D	909	NAG	C6-C5-C4	-2.02	108.06	113.02
5	B	912	NAG	O5-C1-C2	-2.01	108.18	111.29
6	C	901	UCG	O7-P-O6	2.01	115.33	107.80
6	C	901	UCG	C2-C1-C	2.00	104.30	99.89
6	B	915	UCG	O-C-N	2.00	112.89	108.36

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	915	UCG	C4-O1-P-O6
6	A	915	UCG	C4-O1-P-O7
6	A	915	UCG	C4-O1-P-O8
6	C	901	UCG	C4-O1-P-O6
6	C	901	UCG	C4-O1-P-O7
6	D	902	UCG	C18-O11-P1-O3
6	D	902	UCG	C18-O11-P1-O15
6	D	902	UCG	C18-O11-P1-O14
4	C	902	URI	O4'-C4'-C5'-O5'
5	C	914	NAG	O5-C5-C6-O6
5	C	913	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	D	909	NAG	O5-C5-C6-O6
5	C	914	NAG	C4-C5-C6-O6
5	B	912	NAG	O5-C5-C6-O6
5	D	909	NAG	C4-C5-C6-O6
5	C	913	NAG	C4-C5-C6-O6
5	A	911	NAG	C8-C7-N2-C2
6	D	902	UCG	C16-C17-C18-O11
6	D	902	UCG	O10-C17-C18-O11
5	A	912	NAG	O5-C5-C6-O6
4	C	902	URI	C3'-C4'-C5'-O5'
5	C	912	NAG	O5-C5-C6-O6
5	A	911	NAG	O7-C7-N2-C2
5	B	911	NAG	C8-C7-N2-C2
6	A	915	UCG	O-C3-C4-O1
6	A	915	UCG	C2-C3-C4-O1
5	B	911	NAG	O7-C7-N2-C2
5	C	912	NAG	C4-C5-C6-O6
5	A	913	NAG	C4-C5-C6-O6
5	B	912	NAG	C4-C5-C6-O6
5	D	913	NAG	O5-C5-C6-O6
6	C	901	UCG	C4-O1-P-O8
5	A	912	NAG	C4-C5-C6-O6
5	B	914	NAG	C8-C7-N2-C2
5	A	914	NAG	C4-C5-C6-O6
5	A	913	NAG	O5-C5-C6-O6
5	B	914	NAG	O7-C7-N2-C2
6	C	901	UCG	C1-C2-O3-P1
4	B	901	URI	O4'-C1'-N1-C6
4	D	901	URI	O4'-C1'-N1-C6
6	B	915	UCG	O-C3-C4-O1
4	A	901	URI	O4'-C1'-N1-C6
4	C	902	URI	O4'-C1'-N1-C6
4	D	901	URI	O4'-C1'-N1-C2
4	A	901	URI	C2'-C1'-N1-C6
4	B	901	URI	O4'-C1'-N1-C2
4	B	901	URI	C2'-C1'-N1-C6
5	C	909	NAG	C4-C5-C6-O6
4	C	902	URI	C2'-C1'-N1-C6
6	C	901	UCG	C3-C2-O3-P1
4	D	901	URI	C2'-C1'-N1-C6
5	C	909	NAG	O5-C5-C6-O6
6	B	915	UCG	C2-C3-C4-O1

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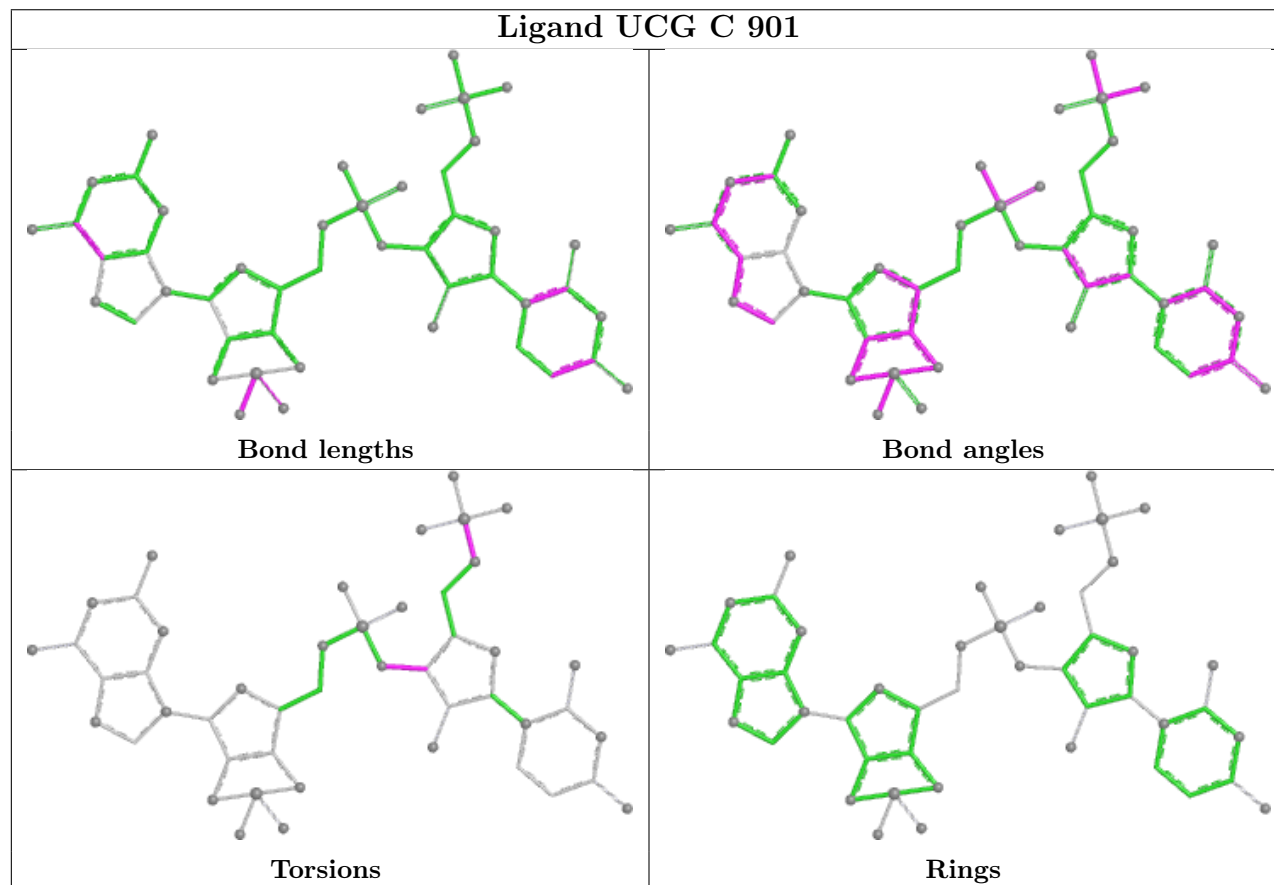
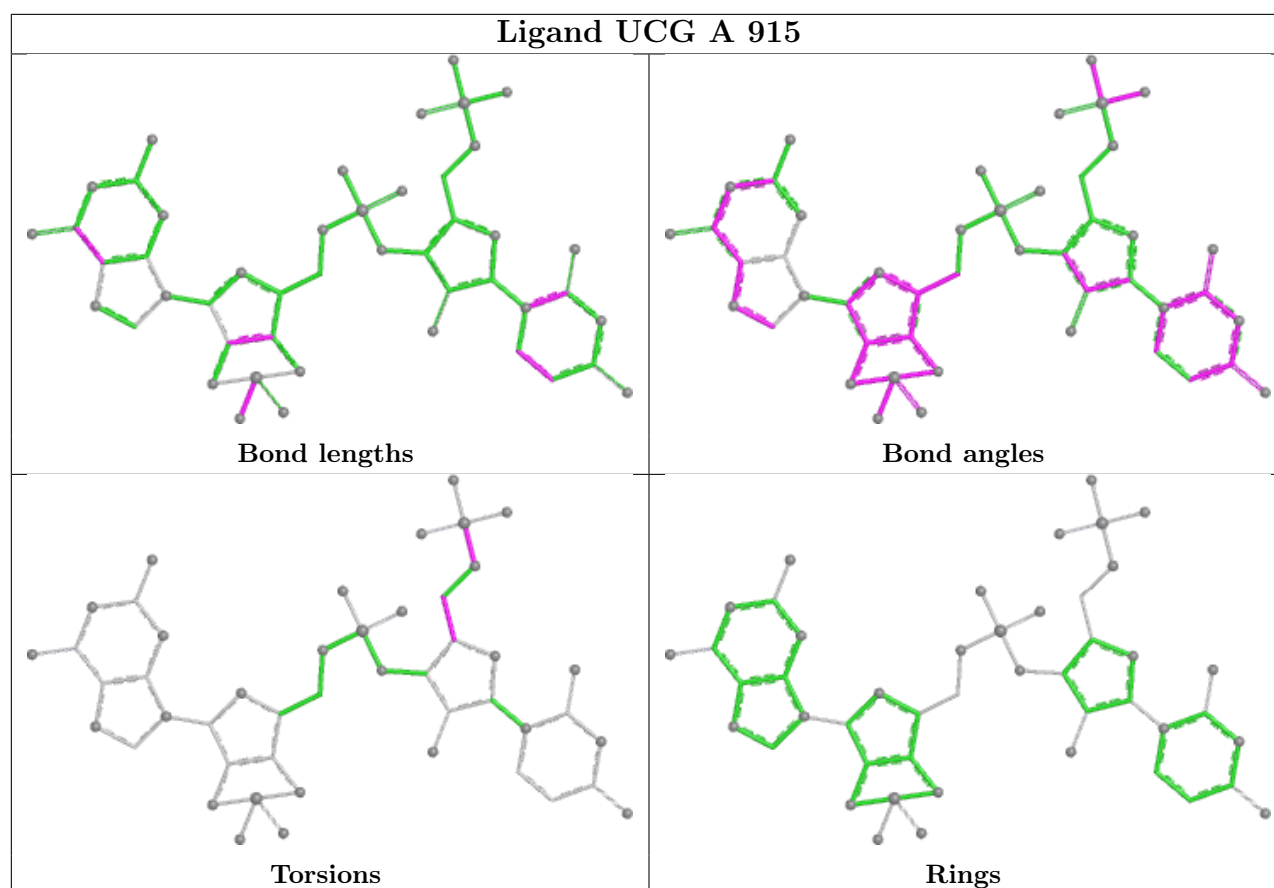
Mol	Chain	Res	Type	Atoms
4	A	901	URI	O4'-C1'-N1-C2
4	C	902	URI	O4'-C1'-N1-C2
5	A	911	NAG	C4-C5-C6-O6
4	A	901	URI	C2'-C1'-N1-C2
4	B	901	URI	C2'-C1'-N1-C2

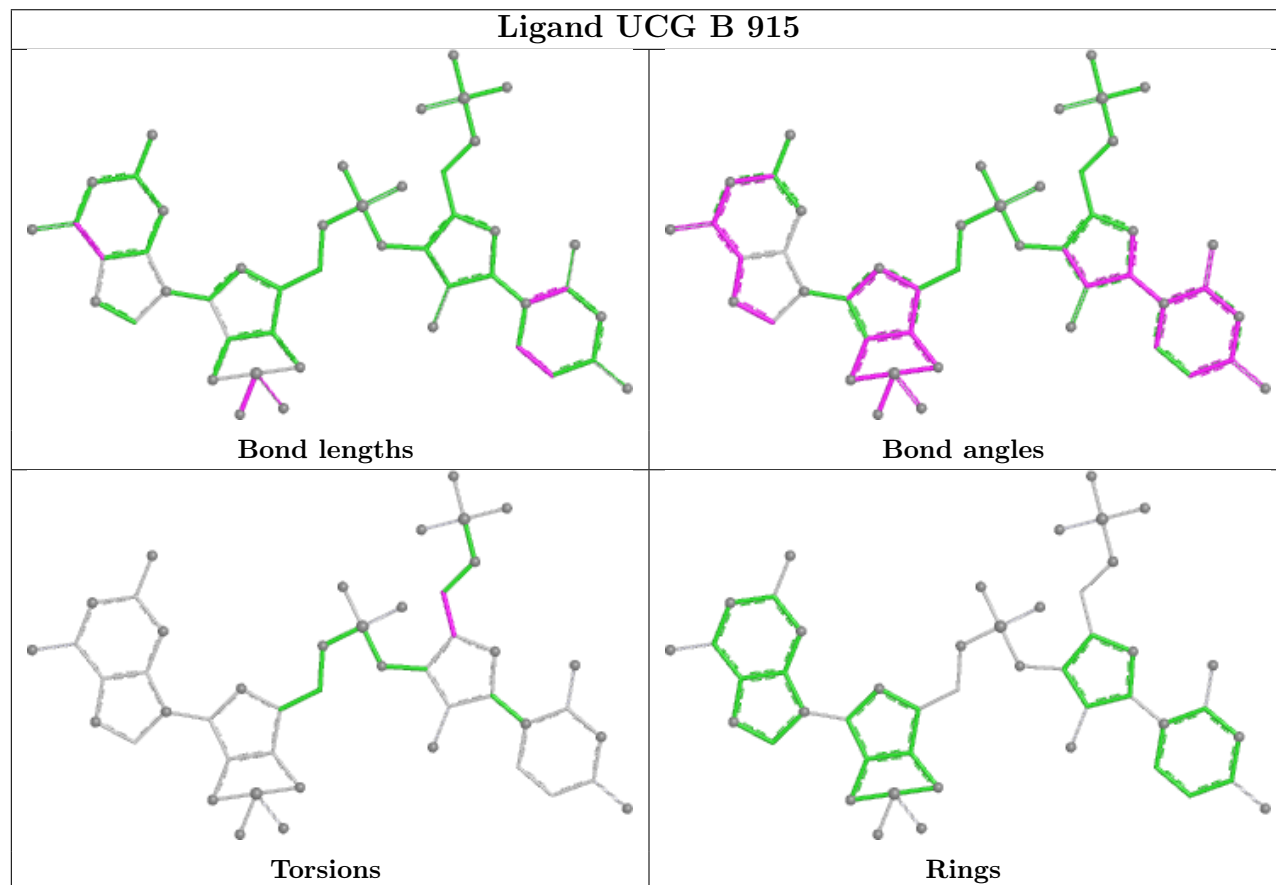
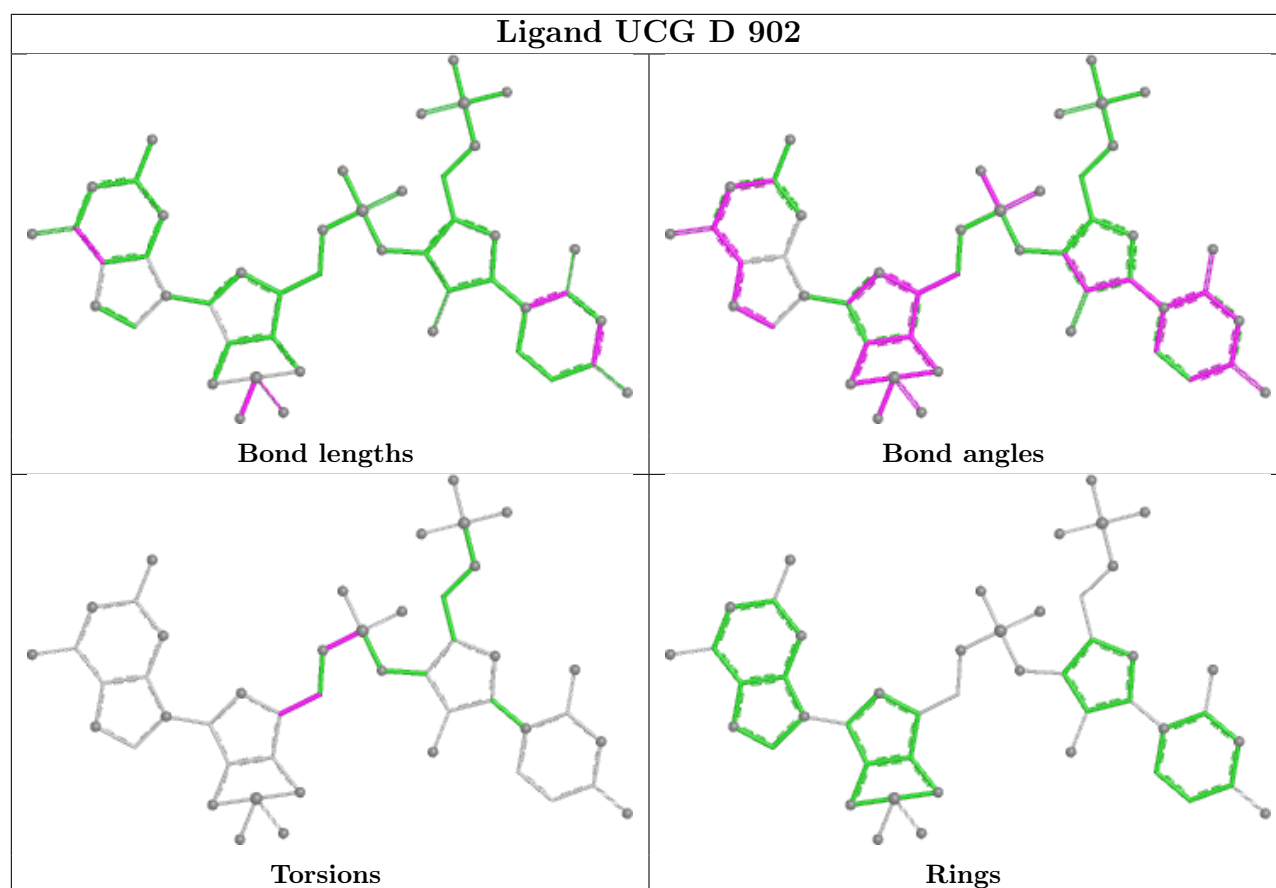
There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	915	UCG	2	0
5	B	911	NAG	1	0
6	C	901	UCG	3	0
5	A	914	NAG	1	0
5	B	914	NAG	1	0
5	D	909	NAG	1	0
6	D	902	UCG	1	0
6	B	915	UCG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	743/811 (91%)	-0.50	5 (0%) 84 81	16, 35, 71, 113	1 (0%)
1	B	737/811 (90%)	-0.28	10 (1%) 73 70	13, 41, 77, 108	1 (0%)
1	C	731/811 (90%)	0.22	55 (7%) 22 20	15, 54, 110, 157	1 (0%)
1	D	743/811 (91%)	-0.09	27 (3%) 46 43	17, 44, 97, 146	1 (0%)
All	All	2954/3244 (91%)	-0.16	97 (3%) 49 46	13, 42, 96, 157	4 (0%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	678	PHE	6.7
1	C	815	VAL	5.6
1	D	100	VAL	4.9
1	A	756	LEU	4.6
1	D	736	SER	4.3
1	C	245	LEU	4.2
1	B	100	VAL	4.1
1	D	791	LEU	3.9
1	B	39	LYS	3.8
1	C	780	ILE	3.7
1	C	806	PRO	3.6
1	D	735	VAL	3.6
1	D	774	PHE	3.5
1	B	65	VAL	3.5
1	C	763	LYS	3.5
1	C	274	ALA	3.4
1	B	732	LEU	3.3
1	C	246	ILE	3.2
1	C	735	VAL	3.2
1	C	729	SER	3.2
1	D	243	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	759	LYS	3.1
1	B	817	LEU	3.1
1	A	678	PHE	3.1
1	C	751	ILE	3.0
1	D	739	LYS	3.0
1	D	815	VAL	3.0
1	D	750	THR	3.0
1	D	751	ILE	3.0
1	C	805	SER	2.9
1	D	783	PHE	2.8
1	C	204	GLU	2.8
1	C	189	LYS	2.8
1	D	780	ILE	2.8
1	A	100	VAL	2.7
1	C	218	PRO	2.7
1	C	121	PHE	2.7
1	C	235	LYS	2.6
1	C	809	GLN	2.6
1	B	168	ARG	2.6
1	C	243	LYS	2.6
1	C	236	TYR	2.6
1	C	60	THR	2.6
1	B	113	GLY	2.6
1	C	807	GLY	2.6
1	C	219	LYS	2.6
1	C	124	LEU	2.5
1	C	801	VAL	2.5
1	C	63	LYS	2.5
1	C	814	ILE	2.5
1	D	170	ILE	2.5
1	D	814	ILE	2.5
1	C	55	GLN	2.5
1	D	809	GLN	2.5
1	C	732	LEU	2.5
1	C	306	TRP	2.5
1	C	458	ASP	2.5
1	D	64	TYR	2.5
1	C	778	CYS	2.4
1	D	726	HIS	2.4
1	C	750	THR	2.4
1	C	122	LEU	2.4
1	C	791	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	116	ILE	2.4
1	B	64	TYR	2.4
1	D	794	LYS	2.4
1	C	188	GLU	2.4
1	C	192	ILE	2.4
1	D	761	THR	2.4
1	D	748	LEU	2.3
1	C	799	VAL	2.3
1	B	121	PHE	2.3
1	C	190	THR	2.3
1	D	702	PHE	2.3
1	C	776	CYS	2.3
1	C	220	LEU	2.3
1	C	244	GLY	2.2
1	C	83	PHE	2.2
1	D	807	GLY	2.2
1	C	731	PHE	2.2
1	B	170	ILE	2.2
1	C	140	ILE	2.2
1	C	166	ILE	2.2
1	C	195	GLY	2.2
1	C	733	SER	2.2
1	C	64	TYR	2.1
1	D	786	TRP	2.1
1	C	224	LEU	2.1
1	D	758	THR	2.1
1	C	138	PRO	2.1
1	C	172	LEU	2.1
1	C	33	TYR	2.1
1	A	732	LEU	2.0
1	D	87	GLN	2.0
1	C	275	SER	2.0
1	C	282	ALA	2.0
1	A	757	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

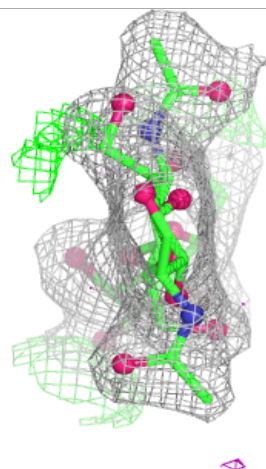
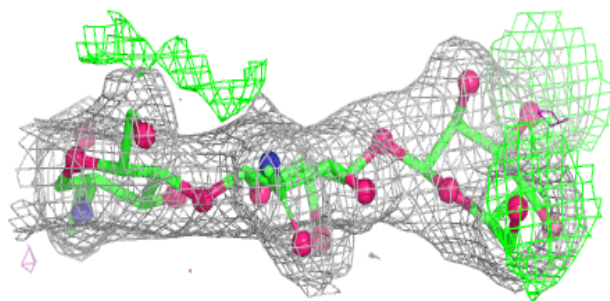
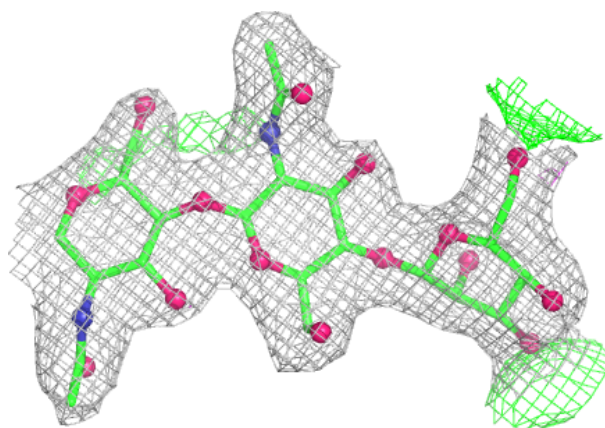
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	BMA	H	3	11/12	0.69	0.16	44,50,54,55	0
2	BMA	E	3	11/12	0.81	0.09	34,37,43,45	0
2	BMA	K	3	11/12	0.81	0.11	52,57,59,61	0
2	BMA	N	3	11/12	0.85	0.11	40,48,51,56	0
2	BMA	F	3	11/12	0.88	0.09	41,43,50,51	0
2	BMA	O	3	11/12	0.88	0.09	50,57,63,68	0
2	BMA	L	3	11/12	0.89	0.09	43,50,57,59	0
3	NAG	P	2	14/15	0.90	0.09	36,46,52,52	0
3	NAG	M	2	14/15	0.91	0.08	33,40,46,51	0
2	BMA	I	3	11/12	0.91	0.07	40,45,54,54	0
2	NAG	K	2	14/15	0.93	0.08	46,49,52,53	0
3	NAG	J	2	14/15	0.93	0.08	32,37,41,44	0
2	NAG	L	2	14/15	0.94	0.07	28,32,38,39	0
2	NAG	O	2	14/15	0.94	0.07	39,42,48,50	0
2	NAG	K	1	14/15	0.94	0.09	39,44,49,50	0
2	NAG	H	1	14/15	0.95	0.07	23,26,31,45	0
2	NAG	F	2	14/15	0.95	0.06	23,27,35,36	0
3	NAG	G	2	14/15	0.95	0.06	27,33,40,43	0
2	NAG	N	1	14/15	0.95	0.07	17,23,29,38	0
3	NAG	M	1	14/15	0.95	0.07	22,28,36,42	0
2	NAG	N	2	14/15	0.95	0.07	27,32,33,41	0
2	NAG	E	2	14/15	0.95	0.07	23,27,32,36	0
2	NAG	H	2	14/15	0.96	0.06	29,35,42,48	0
2	NAG	F	1	14/15	0.96	0.05	18,25,27,28	0
2	NAG	I	2	14/15	0.96	0.07	22,27,31,34	0
2	NAG	L	1	14/15	0.96	0.06	19,23,25,26	0
2	NAG	O	1	14/15	0.96	0.06	29,33,35,36	0
2	NAG	E	1	14/15	0.96	0.06	22,24,28,31	0
2	NAG	I	1	14/15	0.97	0.05	23,25,27,27	0
3	NAG	P	1	14/15	0.97	0.06	24,31,38,38	0
3	NAG	J	1	14/15	0.97	0.06	19,23,28,35	0
3	NAG	G	1	14/15	0.98	0.04	17,20,25,25	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.

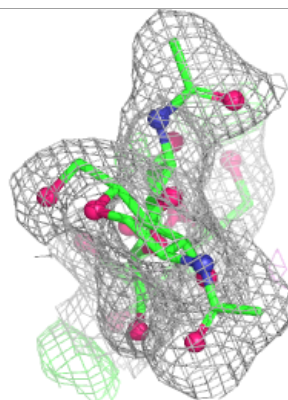
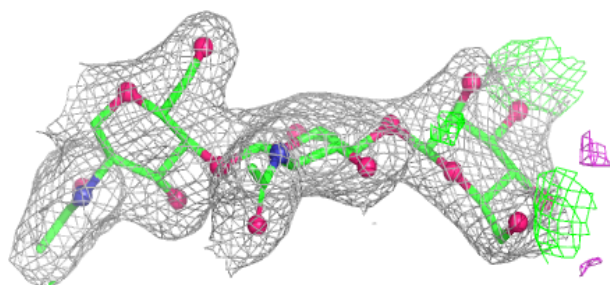
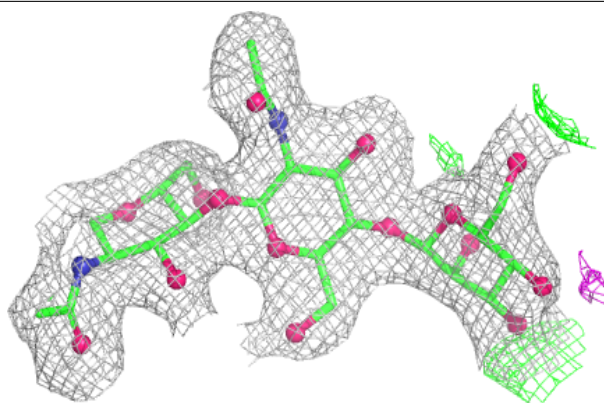
**Electron density around Chain E:**

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

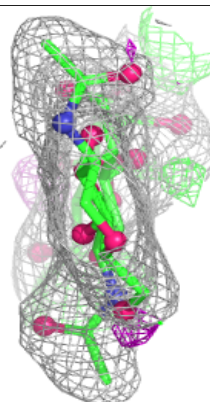
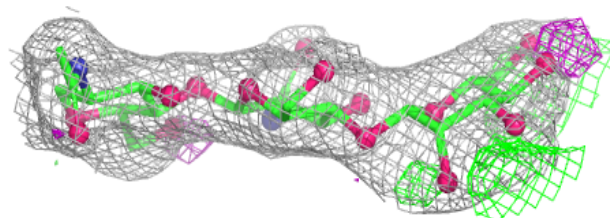
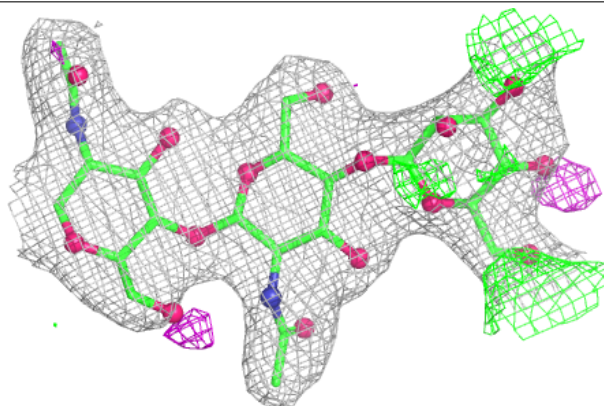


**Electron density around Chain F:**

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

**Electron density around Chain H:**

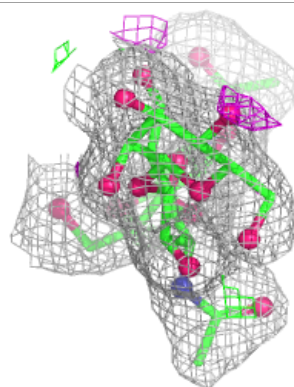
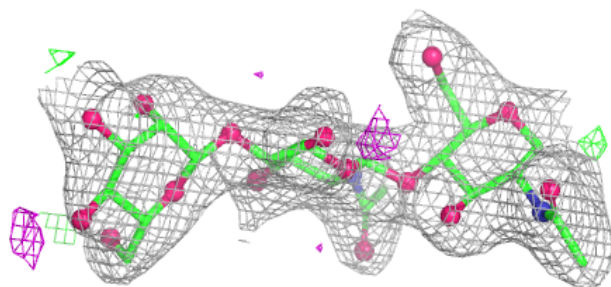
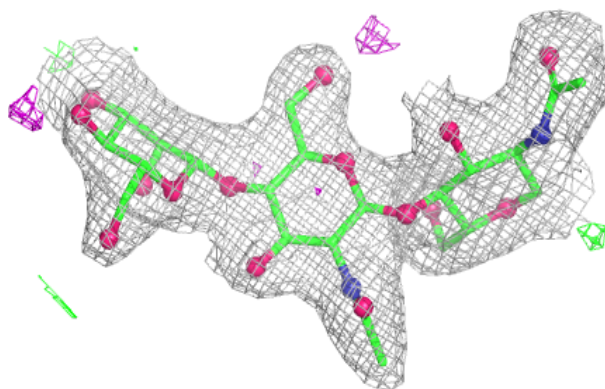
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



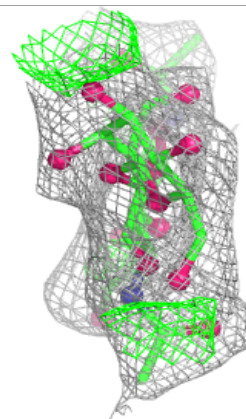
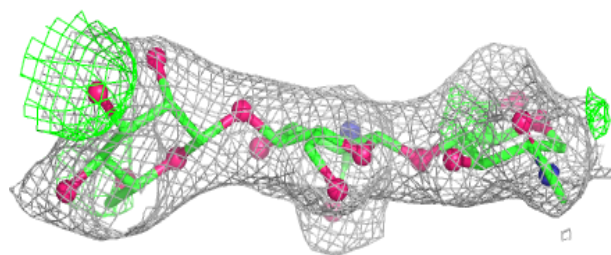
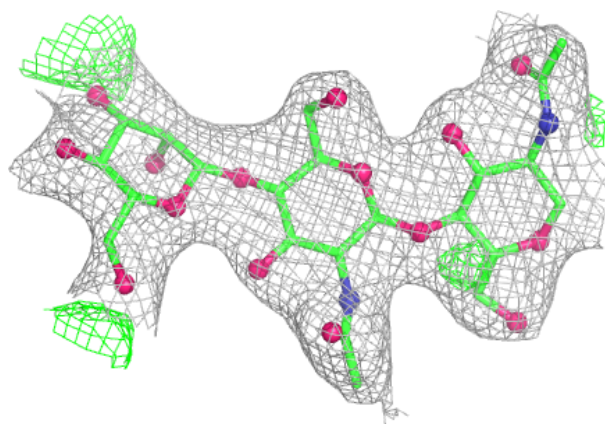


**Electron density around Chain I:**

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

**Electron density around Chain K:**

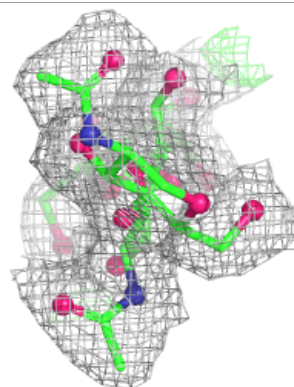
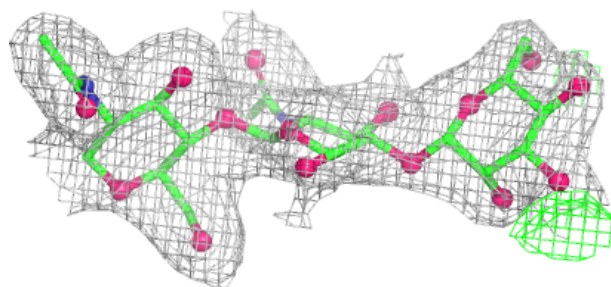
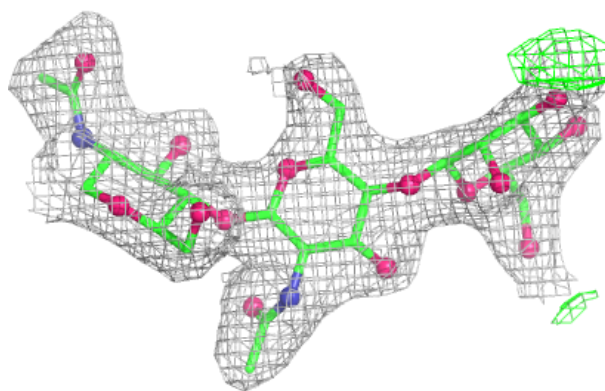
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



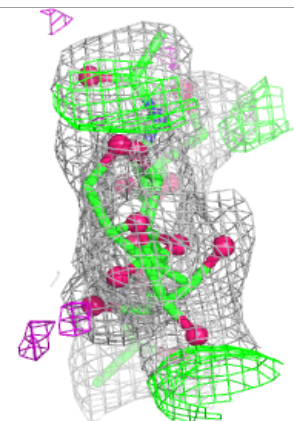
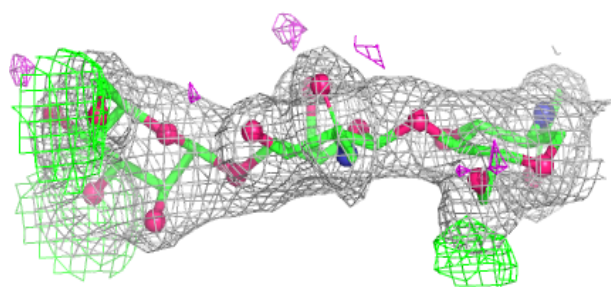
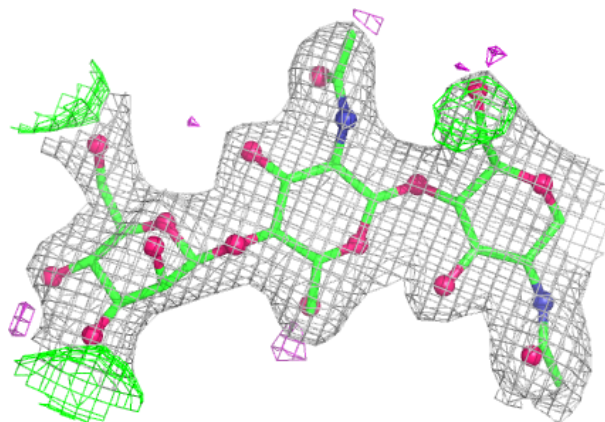


**Electron density around Chain L:**

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

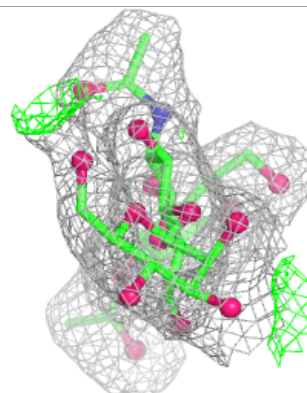
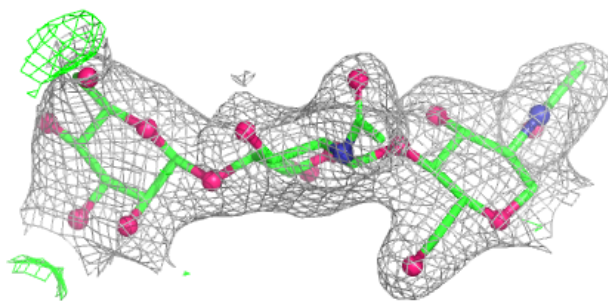
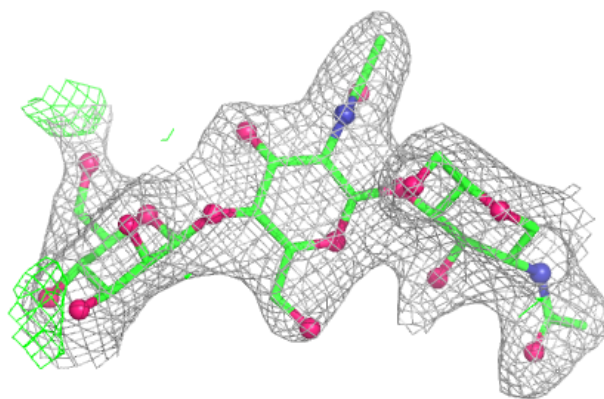
**Electron density around Chain N:**

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



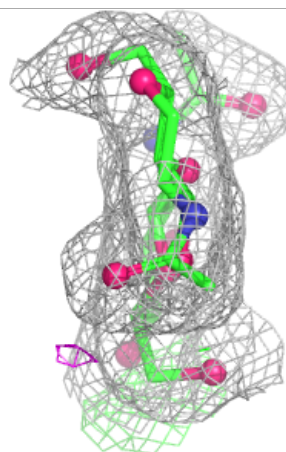
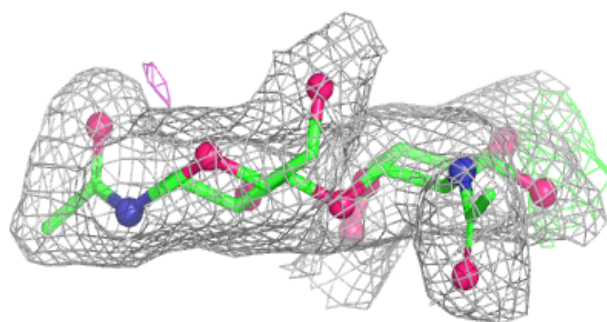
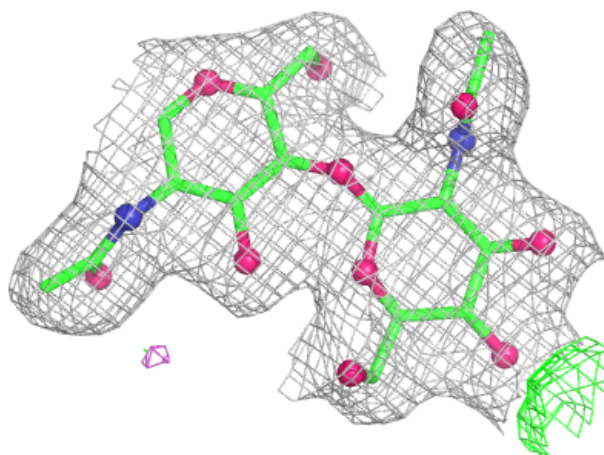
**Electron density around Chain O:**

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



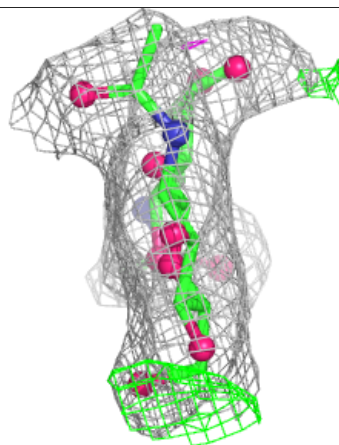
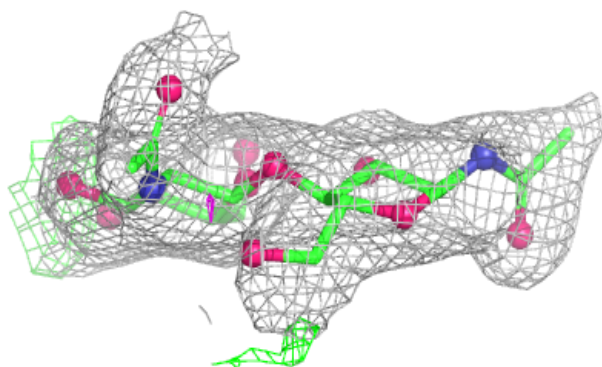
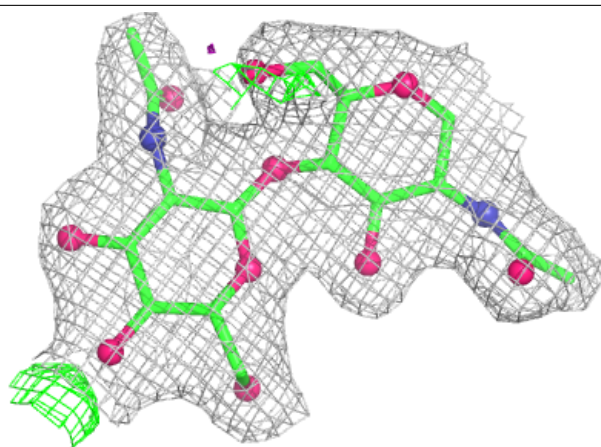
**Electron density around Chain G:**

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



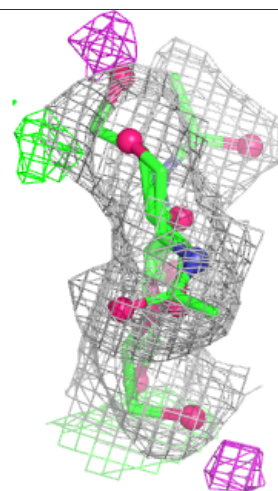
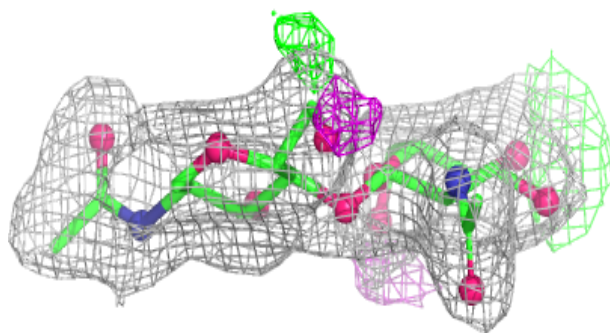
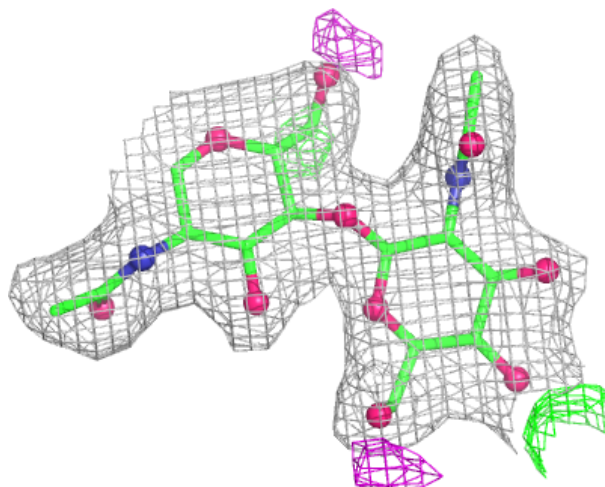
**Electron density around Chain J:**

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

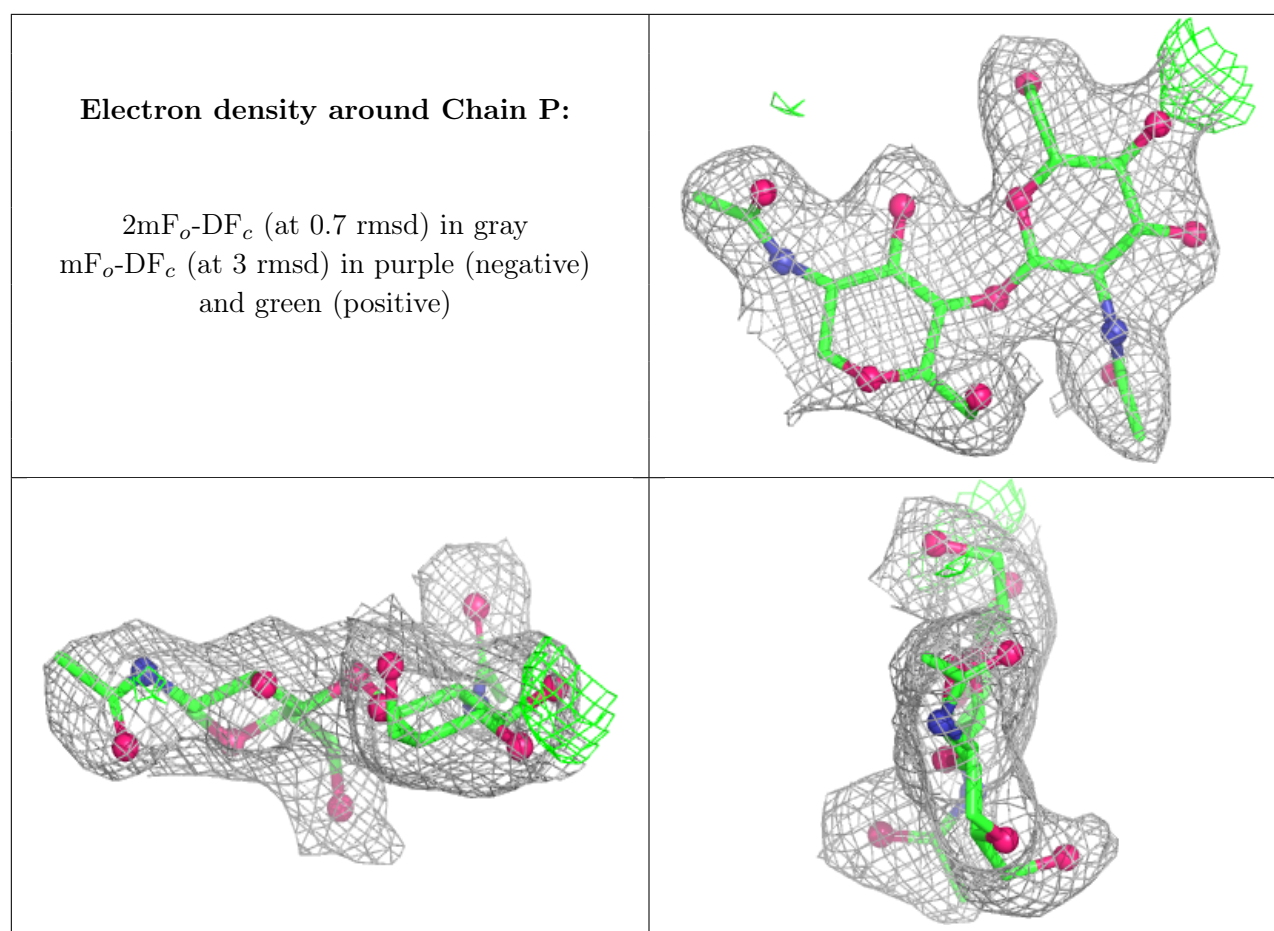


**Electron density around Chain M:**

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







## 6.4 Ligands [i](#)

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

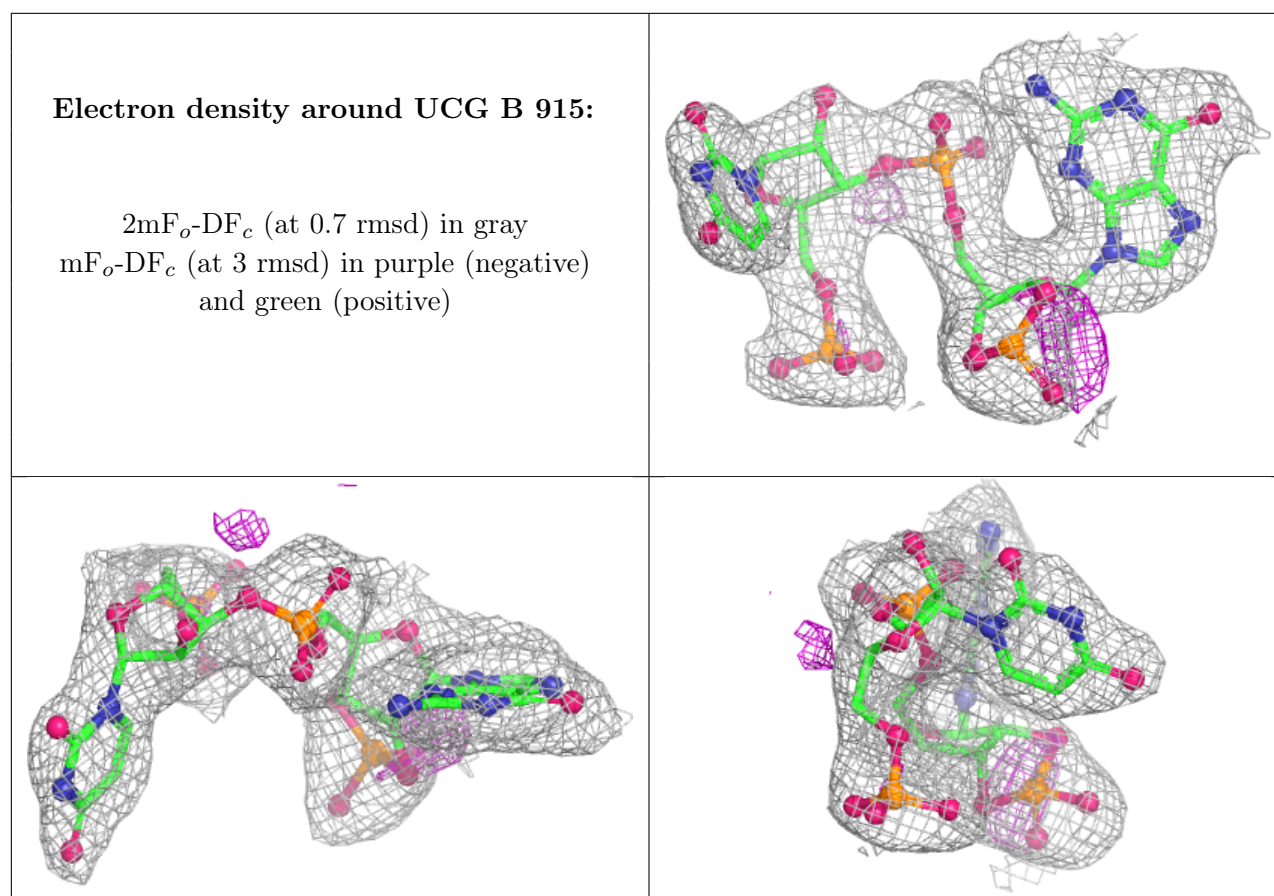
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	D	913	14/15	0.71	0.16	62,72,76,80	0
5	NAG	B	911	14/15	0.72	0.17	50,61,76,77	0
5	NAG	A	912	14/15	0.72	0.18	64,73,80,83	0
5	NAG	A	913	14/15	0.79	0.12	54,65,69,69	0
5	NAG	B	914	14/15	0.79	0.13	53,60,69,71	0
5	NAG	C	909	14/15	0.79	0.15	62,71,82,85	0
5	NAG	B	908	14/15	0.79	0.13	71,83,94,111	0
5	NAG	A	911	14/15	0.82	0.12	46,52,56,60	0
5	NAG	C	914	14/15	0.86	0.12	52,60,68,68	0
5	NAG	D	912	14/15	0.89	0.08	54,62,64,66	0
5	NAG	B	912	14/15	0.89	0.09	40,45,51,56	0
5	NAG	C	913	14/15	0.90	0.09	38,57,68,76	0

*Continued on next page...*

*Continued from previous page...*

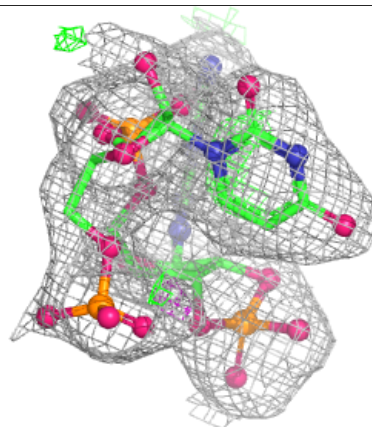
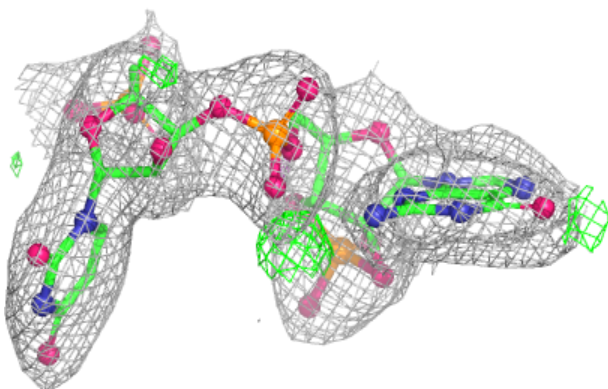
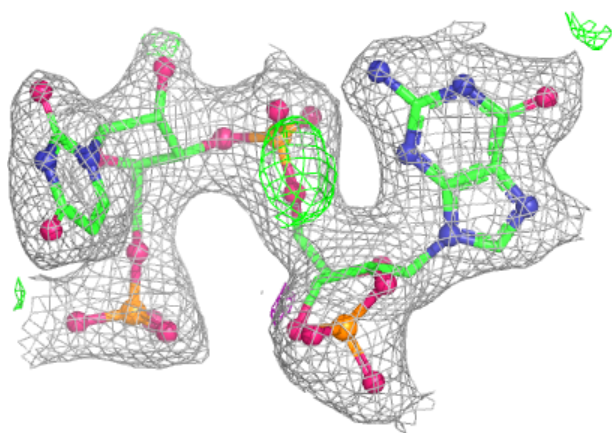
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	D	914	14/15	0.90	0.10	59,69,79,79	0
5	NAG	A	914	14/15	0.91	0.07	38,49,54,57	0
5	NAG	A	908	14/15	0.91	0.08	32,38,46,52	0
5	NAG	D	909	14/15	0.91	0.09	37,41,47,51	0
5	NAG	B	913	14/15	0.92	0.09	46,53,59,61	0
5	NAG	C	912	14/15	0.92	0.10	44,50,78,87	0
4	URI	C	902	17/17	0.94	0.08	26,35,45,48	0
6	UCG	B	915	47/47	0.94	0.08	36,49,83,96	0
6	UCG	C	901	47/47	0.94	0.08	40,48,83,106	0
4	URI	A	901	17/17	0.95	0.06	21,28,34,36	0
6	UCG	D	902	47/47	0.95	0.07	21,38,65,81	0
6	UCG	A	915	47/47	0.97	0.07	24,31,70,79	0
4	URI	B	901	17/17	0.97	0.05	23,25,30,35	0
4	URI	D	901	17/17	0.98	0.05	17,23,29,34	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 UCG C 901:**

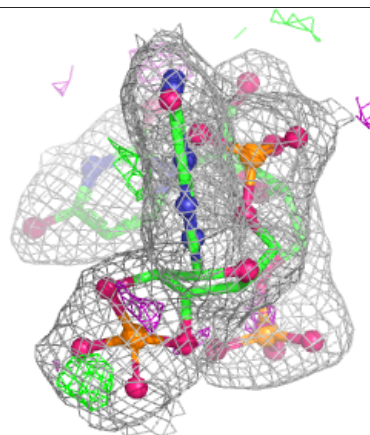
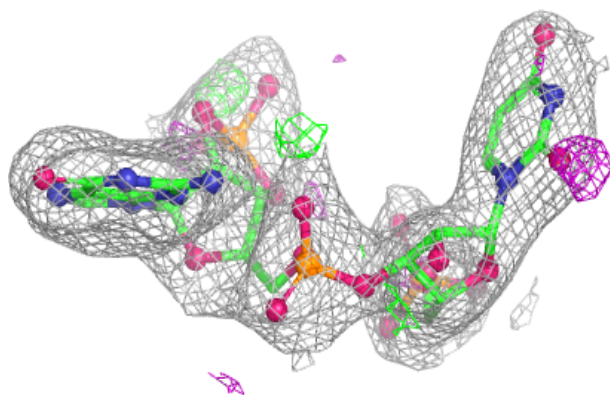
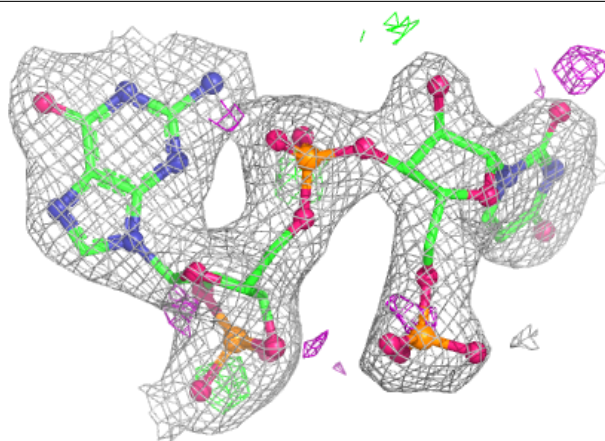
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





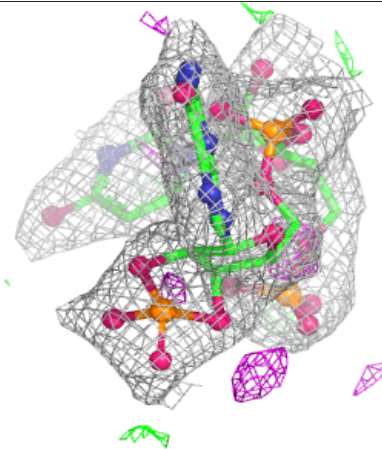
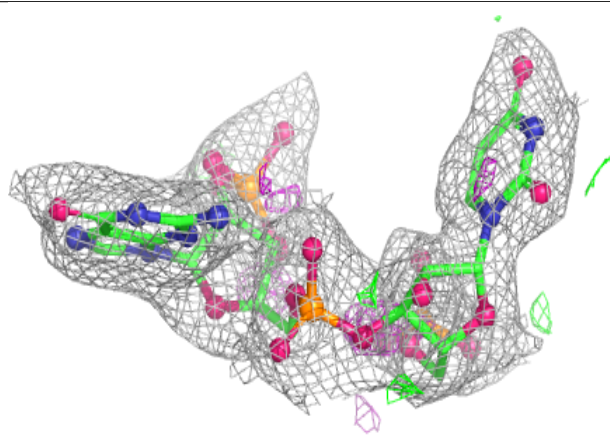
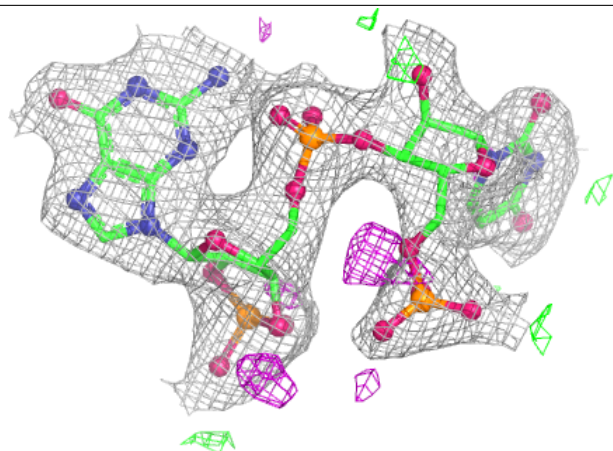
**Electron density around UCG D 902:**

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



**Electron density around UCG A 915:**

$2mF_o-DF_c$  (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.