



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2024 – 08:43 AM EST

PDB ID : 4R09  
Title : Crystal structure of human TLR8 in complex with ORN06S  
Authors : Tanji, H.; Ohto, U.; Shimizu, T.  
Deposited on : 2014-07-30  
Resolution : 2.62 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>.

---

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

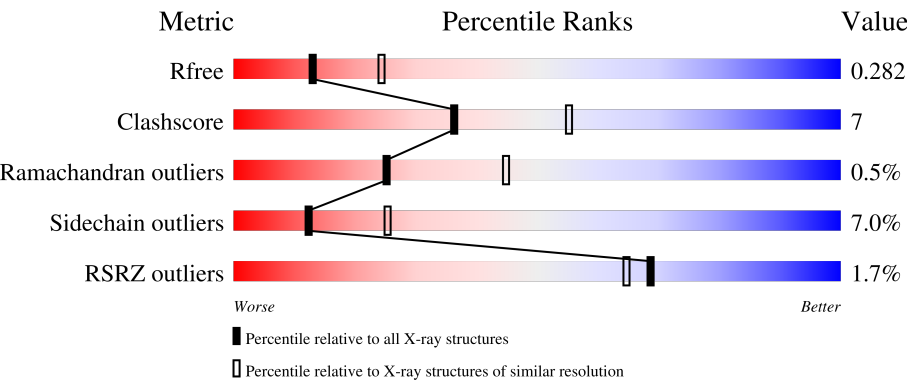
MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : 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 2.62 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.



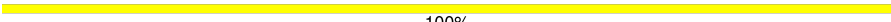
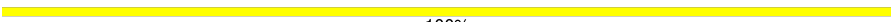

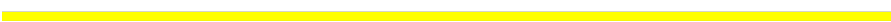






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	164625	4623 (2.64-2.60)
Clashscore	180529	5071 (2.64-2.60)
Ramachandran outliers	177936	5006 (2.64-2.60)
Sidechain outliers	177891	5006 (2.64-2.60)
RSRZ outliers	164620	4622 (2.64-2.60)

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><div>76%15%• 8%</div></div>
1	B	811	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>74%17%• 7%</div></div>
1	C	811	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>70%19%• 8%</div></div>
1	D	811	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>72%19%• 8%</div></div>
2	E	5	<div><div></div><div><div></div><div></div></div><div>60%40%</div></div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	K	5	 100%
3	F	2	 100%
3	G	2	 100%
3	I	2	 100%
3	J	2	 50% 50%
3	M	2	 100%
3	O	2	 100%
4	H	3	 33% 33% 33%
4	L	3	 100%
4	N	3	 100%

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 24895 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	749	Total	C	N	O	S	0	0	0
			6033	3862	1022	1130	19			
1	B	752	Total	C	N	O	S	0	0	0
			6056	3872	1027	1138	19			
1	C	746	Total	C	N	O	S	0	0	0
			6008	3845	1019	1125	19			
1	D	746	Total	C	N	O	S	0	0	0
			6009	3844	1020	1126	19			

There are 40 discrepancies between the modelled and reference sequences:

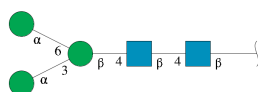
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ARG	-	expression tag	UNP Q9NR97
A	23	SER	-	expression tag	UNP Q9NR97
A	24	PRO	-	expression tag	UNP Q9NR97
A	25	TRP	-	expression tag	UNP Q9NR97
A	828	GLU	-	expression tag	UNP Q9NR97
A	829	PHE	-	expression tag	UNP Q9NR97
A	830	LEU	-	expression tag	UNP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

*Continued on next page...*

Continued from previous page...

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 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.



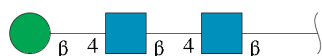
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	K	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



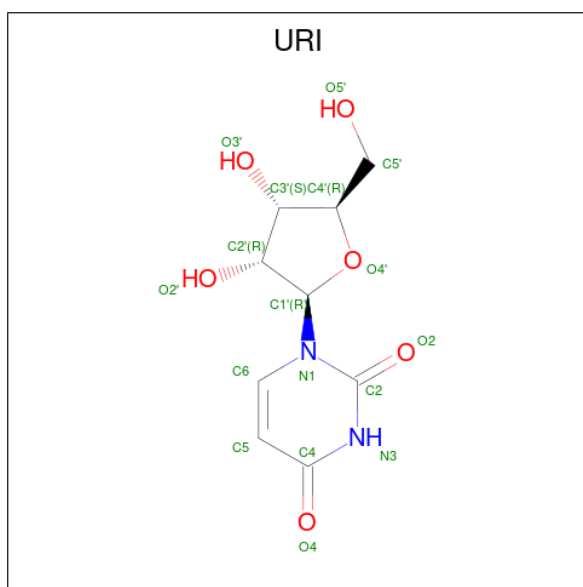
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	O	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.



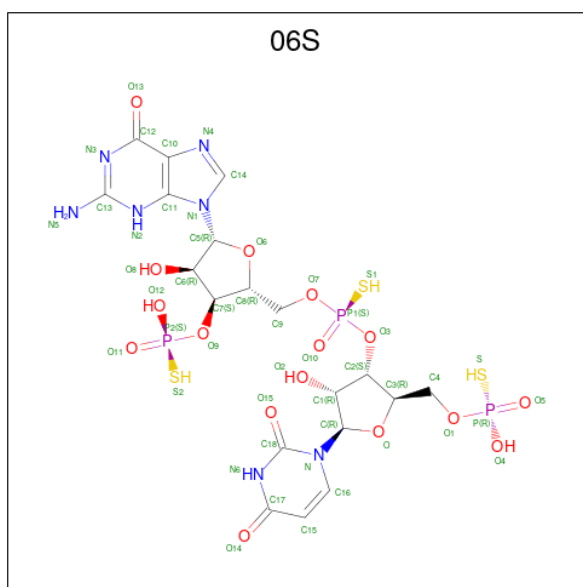
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	L	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is URIDINE (three-letter code: URI) (formula: C<sub>9</sub>H<sub>12</sub>N<sub>2</sub>O<sub>6</sub>).



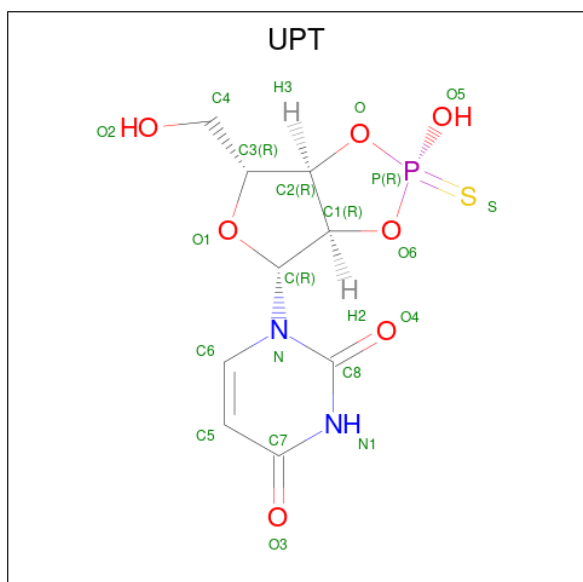
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			17	9	2	6		
5	B	1	Total	C	N	O	0	0
			17	9	2	6		
5	D	1	Total	C	N	O	0	0
			17	9	2	6		
5	D	1	Total	C	N	O	0	0
			17	9	2	6		

- Molecule 6 is O-[(2R,3S,4R,5R)-5-(2-amino-6-oxo-3,6-dihydro-9H-purin-9-yl)-2-({[(S)-{(2R,3S,4R,5R)-5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-4-hydroxy-2-[(thiophosphonooxy)methyl]tetrahydrofuran-3-yl}oxy)(sulfanyl)phosphoryl}oxy)methyl)-4-hydroxytetrahydrofuran-3-yl] dihydrogen (S)-phosphorothioate (three-letter code: 06S) (formula: C<sub>19</sub>H<sub>26</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S<sub>3</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total 48	C 19	N 7	O 16	P 3	S 3	0	0
6	B	1	Total 48	C 19	N 7	O 16	P 3	S 3	0	0
6	C	1	Total 48	C 19	N 7	O 16	P 3	S 3	0	0
6	D	1	Total 48	C 19	N 7	O 16	P 3	S 3	0	0

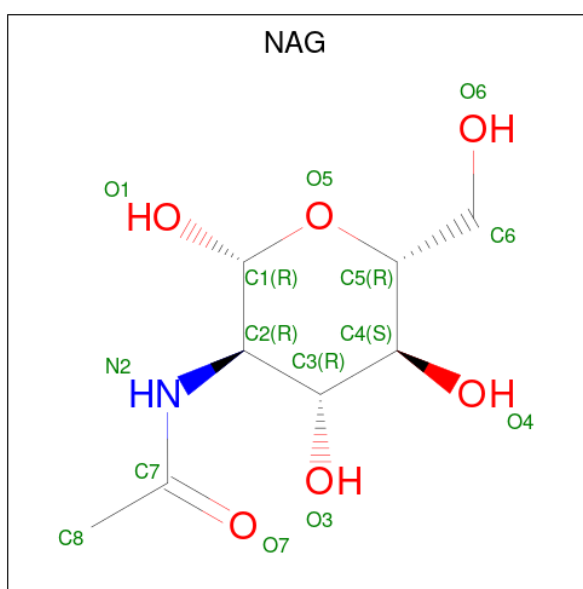
- Molecule 7 is 1-[(2R,3aR,4R,6R,6aR)-2-hydroxy-6-(hydroxymethyl)-2-sulfidotetrahydrofu  
ro[3,4-d][1,3,2]dioxaphosphol-4-yl]pyrimidine-2,4(1H,3H)-dione (three-letter code: UPT)  
(formula: C<sub>9</sub>H<sub>11</sub>N<sub>2</sub>O<sub>7</sub>PS).





Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	S	0	0
			20	9	2	7	1	1		
7	B	1	Total	C	N	O	P	S	0	0
			20	9	2	7	1	1		
7	C	1	Total	C	N	O	P	S	0	0
			20	9	2	7	1	1		
7	D	1	Total	C	N	O	P	S	0	0
			20	9	2	7	1	1		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

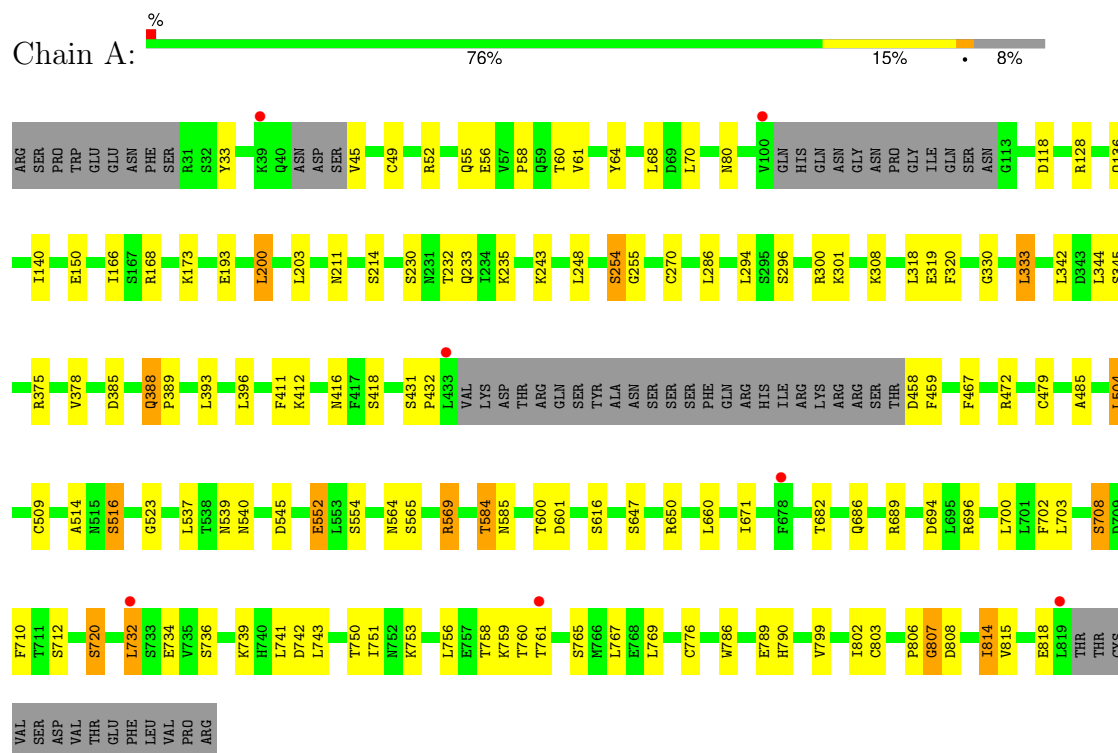


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	D	1	Total	C	N	O	0	0
			14	8	1	5		

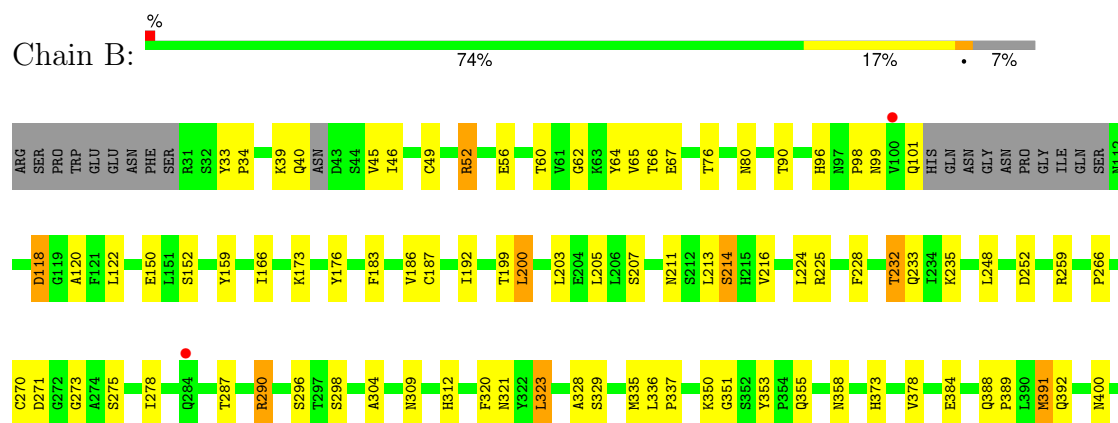
### 3 Residue-property plots [i](#)

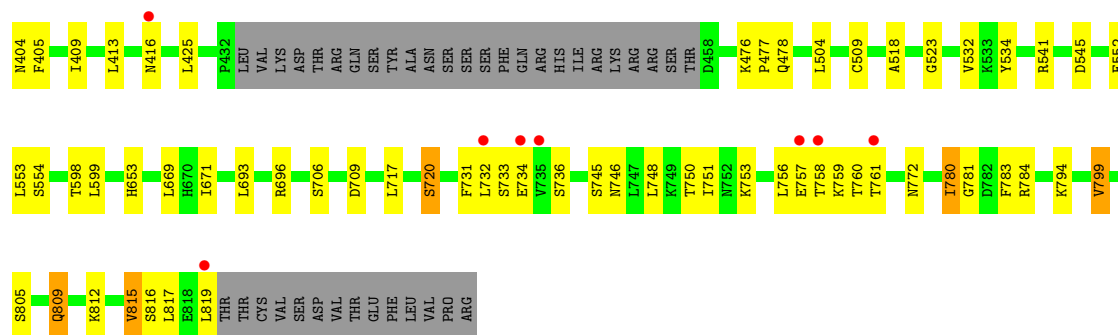
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

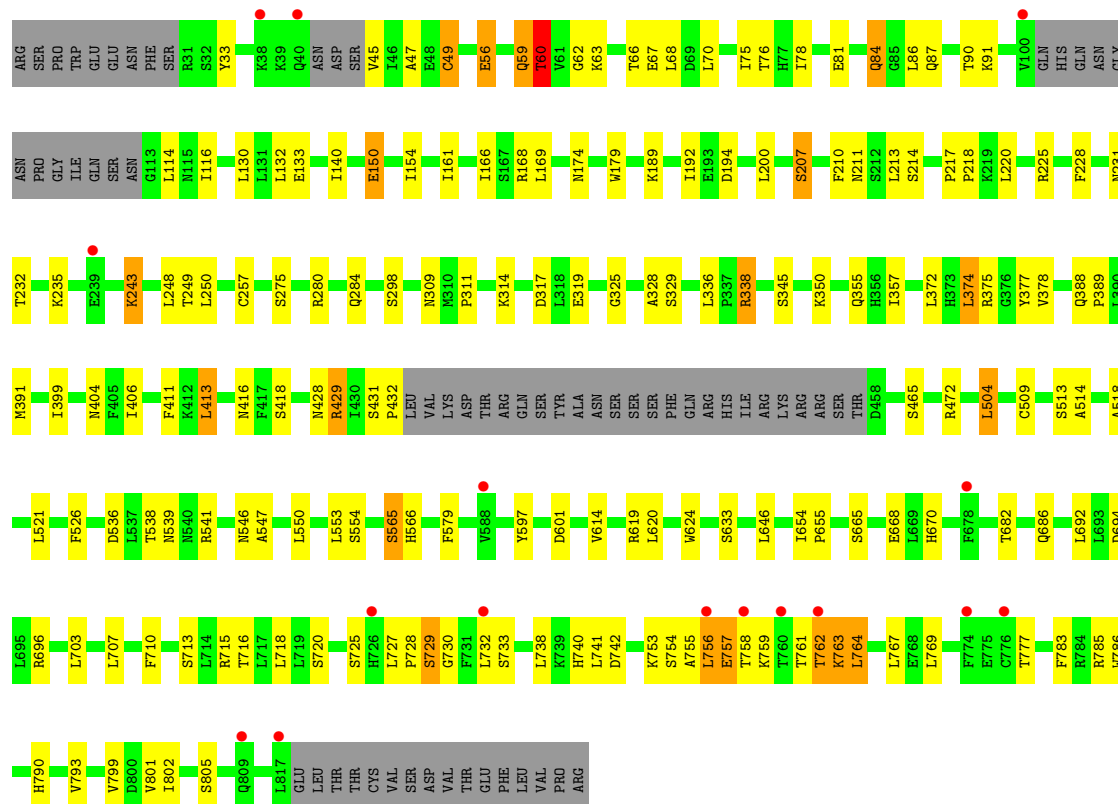


#### • Molecule 1: Toll-like receptor 8





• Molecule 1: Toll-like receptor 8





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

Chain I:  100%

MAG1  
MAG2

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

Chain J:  50% 50%

MAG1  
MAG2

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

Chain M:  100%

MAG1  
MAG2

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

Chain O:  100%

MAG1  
MAG2

- 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% 33% 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 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 N:  100%

MAG1  
MAG2  
BMA3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.68Å 141.34Å 170.04Å 90.00° 89.46° 90.00°	Depositor
Resolution (Å)	31.56 – 2.62 31.56 – 2.62	Depositor EDS
% Data completeness (in resolution range)	98.9 (31.56-2.62) 99.0 (31.56-2.62)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.89 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.216 , 0.285 0.217 , 0.282	Depositor DCC
$R_{free}$ test set	6112 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.7	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 18.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	24895	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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, MAN, UPT, 06S, NAG

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	0.62	0/6157	0.64	0/8350
1	B	0.60	1/6180 (0.0%)	0.62	1/8381 (0.0%)
1	C	0.54	0/6132	0.60	0/8316
1	D	0.52	0/6133	0.58	0/8317
All	All	0.57	1/24602 (0.0%)	0.61	1/33364 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	477	PRO	N-CD	5.19	1.55	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	476	LYS	C-N-CD	5.35	139.63	128.40

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	254	SER	Peptide
1	B	756	LEU	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	6033	0	6023	60	0
1	B	6056	0	6035	78	0
1	C	6008	0	5996	101	0
1	D	6009	0	5993	109	0
2	E	61	0	52	2	0
2	K	61	0	52	0	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	2	0
3	M	28	0	25	0	0
3	O	28	0	25	0	0
4	H	39	0	34	1	0
4	L	39	0	34	0	0
4	N	39	0	34	0	0
5	A	17	0	12	0	0
5	B	17	0	12	0	0
5	D	34	0	24	3	0
6	A	48	0	24	0	0
6	B	48	0	24	0	0
6	C	48	0	24	0	0
6	D	48	0	24	1	0
7	A	20	0	11	0	0
7	B	20	0	11	0	0
7	C	20	0	11	1	0
7	D	20	0	11	4	0
8	A	14	0	13	0	0
8	B	14	0	13	0	0
8	D	14	0	13	0	0
All	All	24895	0	24630	349	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 (349) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:731:PHE:HA	1:D:733:SER:H	1.25	1.00
1:C:429:ARG:NH1	5:D:901:URI:O4	1.95	0.99
1:D:432:PRO:HA	1:D:433:LEU:HB2	1.46	0.95
1:C:764:LEU:HD11	1:C:793:VAL:CG1	1.97	0.94
1:D:742:ASP:OD1	1:D:744:SER:OG	1.86	0.92
1:B:478:GLN:NE2	3:J:2:NAG:O3	2.03	0.90
1:C:764:LEU:HD11	1:C:793:VAL:HG11	1.55	0.89
1:D:730:GLY:O	1:D:733:SER:HB3	1.74	0.88
1:D:70:LEU:O	1:D:93:ASN:O	1.94	0.86
1:D:732:LEU:H	1:D:732:LEU:HD22	1.42	0.84
1:C:755:ALA:HB3	1:C:756:LEU:HA	1.58	0.83
1:A:319:GLU:OE2	1:A:375:ARG:NH2	2.12	0.82
1:A:230:SER:HA	1:A:254:SER:O	1.80	0.81
1:B:192:ILE:HD11	1:B:213:LEU:HD22	1.62	0.81
1:D:375:ARG:NH1	7:D:904:UPT:O5	2.14	0.81
1:C:754:SER:HA	1:C:756:LEU:HA	1.65	0.78
1:D:731:PHE:HA	1:D:733:SER:N	2.00	0.77
1:D:432:PRO:CA	1:D:433:LEU:HB2	2.15	0.76
1:B:759:LYS:O	1:B:760:THR:HG22	1.87	0.74
1:D:732:LEU:N	1:D:732:LEU:HD13	2.03	0.72
1:C:764:LEU:HD11	1:C:793:VAL:HG13	1.70	0.72
1:C:755:ALA:CB	1:C:756:LEU:HA	2.20	0.71
1:D:725:SER:HA	1:D:747:LEU:O	1.91	0.71
1:A:682:THR:HG22	1:A:710:PHE:CZ	2.26	0.70
1:C:764:LEU:CD1	1:C:793:VAL:HG13	2.23	0.69
1:C:84:GLN:O	1:C:87:GLN:NE2	2.26	0.68
1:A:720:SER:OG	1:A:742:ASP:OD2	2.11	0.68
1:C:754:SER:HA	1:C:756:LEU:CA	2.24	0.68
1:C:59:GLN:HA	1:C:59:GLN:HE21	1.58	0.68
1:B:816:SER:O	1:B:817:LEU:HD13	1.95	0.67
1:C:33:TYR:O	1:C:60:THR:HB	1.95	0.66
1:C:317:ASP:OD1	1:C:319:GLU:OE1	2.13	0.66
1:A:33:TYR:O	1:A:60:THR:OG1	2.12	0.66
1:C:411:PHE:HB3	1:C:504:LEU:HD13	1.78	0.66
1:D:732:LEU:C	1:D:735:VAL:HG22	2.16	0.66
1:C:192:ILE:HD11	1:C:213:LEU:HD22	1.78	0.66
1:C:764:LEU:HD21	1:C:793:VAL:HG21	1.78	0.65
1:D:731:PHE:O	1:D:755:ALA:O	2.15	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:PHE:HB3	1:A:504:LEU:CD1	2.27	0.65
1:C:429:ARG:NH2	1:D:518:ALA:O	2.31	0.64
1:B:214:SER:HA	1:B:233:GLN:O	1.99	0.63
1:B:757:GLU:HA	1:B:758:THR:OG1	1.99	0.62
1:C:783:PHE:O	1:C:786:TRP:HB3	1.99	0.62
1:D:806:PRO:N	1:D:807:GLY:HA2	2.15	0.62
1:D:411:PHE:HB3	1:D:504:LEU:HD13	1.81	0.62
1:A:211:ASN:O	1:A:232:THR:HA	2.01	0.61
1:B:52:ARG:HG2	1:B:799:VAL:HG11	1.82	0.61
1:B:809:GLN:HE21	1:B:809:GLN:HA	1.65	0.61
1:C:536:ASP:OD1	1:C:538:THR:HG23	2.00	0.61
1:B:66:THR:HG22	1:B:90:THR:HG22	1.81	0.61
1:C:799:VAL:O	1:C:802:ILE:HD11	1.99	0.61
1:B:478:GLN:HE21	3:J:2:NAG:HO3	1.43	0.61
1:D:692:LEU:HD23	1:D:693:LEU:N	2.16	0.61
1:D:779:ASP:O	1:D:780:ILE:HB	2.00	0.60
1:D:732:LEU:O	1:D:735:VAL:HG22	2.02	0.60
1:C:764:LEU:HG	1:C:764:LEU:O	2.02	0.59
1:A:516:SER:O	1:A:516:SER:OG	2.17	0.59
1:A:758:THR:OG1	1:A:760:THR:O	2.21	0.59
1:D:732:LEU:CB	1:D:735:VAL:HG21	2.33	0.59
1:B:391:MET:HG2	1:B:416:ASN:HB3	1.85	0.58
1:C:311:PRO:O	1:C:338:ARG:HD2	2.03	0.58
1:D:86:LEU:HD13	1:D:89:LEU:HD12	1.85	0.58
1:C:716:THR:HG23	1:C:740:HIS:HB3	1.84	0.58
1:D:732:LEU:H	1:D:732:LEU:HD13	1.68	0.58
1:B:118:ASP:N	1:B:118:ASP:OD1	2.37	0.57
1:D:775:GLU:HG3	1:D:805:SER:O	2.04	0.57
1:B:733:SER:OG	1:B:758:THR:N	2.29	0.57
1:C:755:ALA:CB	1:C:756:LEU:CA	2.82	0.57
1:D:732:LEU:H	1:D:732:LEU:CD2	2.10	0.57
1:A:708:SER:OG	1:A:734:GLU:HG3	2.05	0.57
1:C:764:LEU:HG	1:C:793:VAL:HG22	1.87	0.56
1:C:47:ALA:HB3	1:C:68:LEU:HD13	1.87	0.56
1:C:375:ARG:NH1	7:C:902:UPT:O5	2.38	0.56
1:B:52:ARG:CG	1:B:799:VAL:HG21	2.35	0.56
1:B:287:THR:HA	1:B:309:ASN:O	2.06	0.56
1:C:526:PHE:HB3	1:C:553:LEU:HD21	1.87	0.56
1:A:52:ARG:CG	1:A:799:VAL:HG21	2.36	0.56
1:B:60:THR:HG22	1:B:60:THR:O	2.06	0.56
1:D:708:SER:CB	1:D:734:GLU:HB2	2.36	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:LEU:C	1:B:205:LEU:HD23	2.27	0.55
1:C:764:LEU:CD1	1:C:767:LEU:HB2	2.37	0.55
1:D:758:THR:HG22	1:D:762:THR:HG21	1.88	0.55
1:C:753:LYS:HD2	1:C:753:LYS:N	2.22	0.55
1:D:163:LYS:HA	1:D:196:VAL:HG23	1.89	0.55
1:D:669:LEU:HD21	1:D:671:ILE:HD11	1.88	0.55
1:A:255:GLY:CA	1:A:296:SER:O	2.55	0.55
1:D:746:ASN:C	1:D:772:ASN:OD1	2.45	0.55
1:D:291:TYR:HE2	6:D:903:06S:H19	1.55	0.55
1:D:545:ASP:O	1:D:545:ASP:CG	2.43	0.54
1:D:735:VAL:O	1:D:735:VAL:HG23	2.06	0.54
1:A:799:VAL:O	1:A:802:ILE:HD11	2.07	0.54
1:D:297:THR:OG1	1:D:299:LEU:HG	2.08	0.54
1:A:523:GLY:O	1:A:552:GLU:HG3	2.08	0.54
1:D:731:PHE:HB2	1:D:732:LEU:HA	1.90	0.54
1:B:321:ASN:HB2	1:B:323:LEU:CD2	2.38	0.54
1:D:805:SER:N	1:D:806:PRO:CD	2.70	0.54
1:B:750:THR:HG22	1:B:751:ILE:N	2.23	0.53
1:C:620:LEU:HD11	1:C:646:LEU:HD22	1.90	0.53
1:D:83:PHE:O	1:D:86:LEU:HD11	2.09	0.53
1:C:518:ALA:HB2	1:C:541:ARG:HD2	1.89	0.53
1:B:203:LEU:HD23	1:B:224:LEU:HD21	1.90	0.53
1:D:429:ARG:NH2	5:D:902:URI:O4	2.38	0.53
1:A:616:SER:HA	1:A:647:SER:O	2.09	0.53
1:B:545:ASP:CG	1:B:545:ASP:O	2.47	0.53
1:C:670:HIS:HA	1:C:694:ASP:HB3	1.90	0.53
1:D:732:LEU:HD22	1:D:732:LEU:N	2.19	0.53
1:C:718:LEU:HA	1:C:742:ASP:HB3	1.90	0.53
1:D:616:SER:HA	1:D:647:SER:O	2.08	0.53
1:B:731:PHE:O	1:B:732:LEU:HG	2.08	0.53
1:D:52:ARG:HG3	1:D:799:VAL:HG21	1.90	0.53
1:C:275:SER:HA	1:C:298:SER:HB2	1.91	0.52
1:D:328:ALA:HB1	1:D:358:ASN:HD22	1.73	0.52
1:A:388:GLN:N	1:A:389:PRO:CD	2.72	0.52
1:A:214:SER:HA	1:A:233:GLN:O	2.10	0.52
1:D:462:ASP:OD2	1:D:465:SER:OG	2.24	0.52
1:D:670:HIS:HA	1:D:694:ASP:HB3	1.91	0.52
1:C:762:THR:C	1:C:763:LYS:HG3	2.30	0.52
1:C:769:LEU:O	1:C:801:VAL:HG13	2.10	0.52
1:A:565:SER:O	1:A:569:ARG:HG2	2.10	0.52
1:B:748:LEU:H	1:B:772:ASN:HD22	1.58	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:LEU:C	1:C:250:LEU:HD23	2.30	0.52
1:D:49:CYS:HB3	1:D:70:LEU:HD23	1.92	0.52
1:D:803:CYS:HB3	1:D:806:PRO:HG3	1.92	0.52
1:D:382:LEU:HD23	1:D:413:LEU:HD21	1.92	0.52
1:C:357:ILE:HG13	1:C:377:TYR:CZ	2.45	0.51
1:A:467:PHE:HB3	2:E:1:NAG:H81	1.92	0.51
1:B:518:ALA:HA	1:B:541:ARG:O	2.10	0.51
1:D:209:SER:OG	1:D:230:SER:N	2.44	0.51
1:B:66:THR:HG22	1:B:90:THR:CG2	2.40	0.51
1:B:228:PHE:HA	1:B:252:ASP:HB3	1.91	0.51
1:A:52:ARG:HG3	1:A:799:VAL:HG21	1.93	0.51
1:A:255:GLY:HA2	1:A:296:SER:O	2.10	0.51
1:A:750:THR:HG22	1:A:751:ILE:H	1.75	0.51
1:B:235:LYS:HD2	1:B:270:CYS:SG	2.51	0.51
1:C:758:THR:O	1:C:790:HIS:NE2	2.44	0.51
1:D:732:LEU:CB	1:D:735:VAL:CG2	2.89	0.51
1:B:296:SER:HA	1:B:320:PHE:O	2.11	0.50
1:A:330:GLY:HA3	1:A:333:LEU:HD22	1.93	0.50
1:D:732:LEU:HB2	1:D:735:VAL:CG2	2.41	0.50
1:D:779:ASP:O	1:D:780:ILE:CB	2.60	0.50
1:C:799:VAL:O	1:C:799:VAL:HG12	2.12	0.50
1:D:432:PRO:HA	1:D:433:LEU:CB	2.31	0.50
1:C:217:PRO:HG2	1:C:220:LEU:HD21	1.94	0.50
1:C:597:TYR:HB3	1:C:619:ARG:HB2	1.94	0.50
1:B:33:TYR:CD1	1:B:34:PRO:HA	2.46	0.50
1:B:211:ASN:O	1:B:232:THR:HA	2.12	0.49
1:B:809:GLN:HE21	1:B:809:GLN:CA	2.25	0.49
1:A:750:THR:HG22	1:A:751:ILE:N	2.27	0.49
1:D:181:CYS:O	1:D:211:ASN:HA	2.11	0.49
1:A:741:LEU:HD21	1:A:743:LEU:HD11	1.94	0.49
1:B:809:GLN:OE1	1:B:817:LEU:HD12	2.12	0.49
1:D:731:PHE:CB	1:D:732:LEU:HA	2.43	0.49
1:B:746:ASN:HB2	1:B:772:ASN:HD21	1.78	0.49
1:C:56:GLU:HA	1:C:75:ILE:HG12	1.94	0.49
1:C:399:ILE:HG23	1:C:399:ILE:O	2.13	0.49
1:B:96:HIS:O	1:B:99:ASN:HB2	2.13	0.48
1:C:413:LEU:C	1:C:413:LEU:HD12	2.34	0.48
1:D:80:ASN:HA	1:D:120:ALA:O	2.13	0.48
1:B:46:ILE:HG22	1:B:67:GLU:HB2	1.94	0.48
1:B:328:ALA:HB1	1:B:358:ASN:ND2	2.28	0.48
1:C:372:LEU:HG	1:C:374:LEU:HD22	1.96	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:780:ILE:HG12	1:D:781:GLY:H	1.79	0.48
1:C:49:CYS:HB3	1:C:70:LEU:HD23	1.94	0.48
1:A:140:ILE:HD13	1:A:166:ILE:HD11	1.95	0.48
1:C:59:GLN:HE21	1:C:59:GLN:CA	2.26	0.48
1:D:161:ILE:HD12	1:D:177:LEU:HD13	1.95	0.48
1:D:211:ASN:O	1:D:232:THR:HA	2.14	0.48
1:C:207:SER:HA	1:C:228:PHE:HB2	1.96	0.48
1:A:479:CYS:O	1:A:509:CYS:HB2	2.13	0.47
1:C:404:ASN:HB2	1:C:428:ASN:HD21	1.79	0.47
1:B:780:ILE:O	1:B:783:PHE:N	2.43	0.47
1:C:284:GLN:O	1:C:309:ASN:ND2	2.44	0.47
1:C:518:ALA:HA	1:C:541:ARG:O	2.14	0.47
1:B:784:ARG:NH2	1:B:817:LEU:O	2.47	0.47
1:D:540:ASN:O	1:D:564:ASN:HA	2.15	0.47
2:E:1:NAG:O3	2:E:2:NAG:O5	2.27	0.47
1:A:732:LEU:HD12	1:A:732:LEU:O	2.15	0.47
1:B:321:ASN:CB	1:B:323:LEU:CD2	2.92	0.47
1:C:211:ASN:O	1:C:232:THR:HA	2.15	0.47
1:C:325:GLY:O	1:C:328:ALA:HB3	2.13	0.47
1:D:52:ARG:CG	1:D:799:VAL:HG21	2.44	0.47
1:C:411:PHE:HB3	1:C:504:LEU:CD1	2.43	0.47
1:C:565:SER:O	1:C:566:HIS:C	2.53	0.47
1:C:431:SER:HB2	1:C:432:PRO:CD	2.45	0.47
1:D:294:LEU:HB2	1:D:318:LEU:HD23	1.97	0.47
1:C:319:GLU:OE2	1:C:375:ARG:NH2	2.48	0.47
1:A:296:SER:HA	1:A:320:PHE:O	2.15	0.46
1:C:210:PHE:CZ	1:C:231:ASN:ND2	2.82	0.46
1:D:164:GLU:N	1:D:165:GLY:HA3	2.30	0.46
1:D:276:ILE:HG21	1:D:297:THR:HB	1.97	0.46
1:D:732:LEU:CD2	1:D:756:LEU:HA	2.45	0.46
1:A:319:GLU:HG2	1:A:345:SER:HB2	1.97	0.46
1:A:514:ALA:HA	1:A:539:ASN:O	2.15	0.46
1:B:52:ARG:HG3	1:B:799:VAL:HG21	1.97	0.46
1:D:119:GLY:HA2	1:D:143:GLY:HA3	1.97	0.46
1:D:479:CYS:SG	1:D:534:TYR:HB3	2.55	0.46
1:D:278:ILE:HB	1:D:306:TRP:CZ2	2.50	0.46
1:A:540:ASN:O	1:A:564:ASN:HA	2.15	0.46
1:C:218:PRO:HA	1:C:243:LYS:HE3	1.96	0.46
1:A:52:ARG:HG2	1:A:799:VAL:HG21	1.97	0.46
1:A:767:LEU:HD21	1:A:769:LEU:HD11	1.97	0.46
1:D:732:LEU:HB3	1:D:735:VAL:HG21	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:TYR:OH	1:B:405:PHE:O	2.23	0.46
1:C:179:TRP:CE2	1:C:210:PHE:CD1	3.04	0.46
1:D:777:THR:OG1	1:D:778:CYS:N	2.47	0.46
1:C:67:GLU:HG2	1:C:91:LYS:HB3	1.98	0.46
1:D:276:ILE:CG2	1:D:297:THR:HB	2.45	0.46
1:A:294:LEU:HB2	1:A:318:LEU:HD23	1.98	0.45
1:A:818:GLU:OE1	1:A:818:GLU:HA	2.16	0.45
1:B:413:LEU:HD12	1:B:413:LEU:C	2.36	0.45
1:D:620:LEU:HD23	1:D:623:LEU:HD12	1.98	0.45
1:C:257:CYS:O	1:C:298:SER:OG	2.21	0.45
1:C:374:LEU:N	1:C:374:LEU:CD2	2.79	0.45
1:D:320:PHE:CZ	7:D:904:UPT:C8	3.00	0.45
1:B:478:GLN:OE1	1:B:478:GLN:N	2.45	0.45
1:D:166:ILE:HG22	1:D:200:LEU:HD21	1.98	0.45
1:D:805:SER:N	1:D:806:PRO:HD2	2.31	0.45
1:B:290:ARG:HH11	1:B:290:ARG:CG	2.29	0.45
1:D:424:TYR:CZ	1:D:426:SER:HB3	2.52	0.45
1:B:384:GLU:HA	1:B:413:LEU:CB	2.47	0.45
1:C:357:ILE:HG13	1:C:377:TYR:CE1	2.52	0.45
1:D:479:CYS:HA	1:D:534:TYR:CD2	2.52	0.45
1:A:411:PHE:HB3	1:A:504:LEU:HD13	1.99	0.45
1:A:584:THR:HG22	1:A:585:ASN:ND2	2.31	0.45
1:B:98:PRO:O	1:B:99:ASN:C	2.55	0.45
1:C:150:GLU:HG2	1:C:174:ASN:HB2	1.99	0.45
1:B:693:LEU:HD23	1:B:717:LEU:CD1	2.48	0.44
1:C:728:PRO:HA	1:C:729:SER:HB2	1.99	0.44
1:D:225:ARG:CZ	1:D:247:ASN:HB3	2.47	0.44
1:D:600:THR:O	1:D:602:LYS:N	2.48	0.44
1:D:777:THR:HG23	1:D:779:ASP:CB	2.46	0.44
1:A:660:LEU:HD22	1:A:686:GLN:HG3	1.99	0.44
1:B:373:HIS:HA	1:B:400:ASN:HB3	1.99	0.44
1:C:130:LEU:HD21	1:C:132:LEU:HD11	1.99	0.44
1:B:409:ILE:CD1	1:B:425:LEU:HD22	2.46	0.44
1:D:501:PHE:O	1:D:504:LEU:HB2	2.18	0.44
1:A:58:PRO:HG2	1:A:61:VAL:CG2	2.47	0.44
1:A:393:LEU:HD12	1:A:396:LEU:HD22	1.99	0.44
1:C:715:ARG:C	1:C:738:LEU:HD12	2.38	0.44
1:A:330:GLY:HA3	1:A:333:LEU:CD2	2.48	0.44
1:A:694:ASP:OD2	1:A:696:ARG:NH2	2.45	0.44
1:C:319:GLU:HG2	1:C:345:SER:HB2	1.99	0.44
1:B:152:SER:HA	1:B:176:TYR:HB2	1.99	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:ILE:HA	1:C:169:LEU:HD13	1.99	0.44
1:A:235:LYS:HD3	1:A:270:CYS:SG	2.58	0.43
1:B:598:THR:O	1:B:599:LEU:HD23	2.18	0.43
1:C:733:SER:HB3	1:C:757:GLU:HB2	2.00	0.43
1:D:703:LEU:CD2	1:D:724:ILE:HG21	2.48	0.43
1:D:732:LEU:HD22	1:D:756:LEU:HA	1.99	0.43
1:A:545:ASP:CG	1:A:545:ASP:O	2.57	0.43
1:B:62:GLY:O	1:B:65:VAL:HG23	2.18	0.43
1:C:547:ALA:O	1:C:579:PHE:HB3	2.18	0.43
1:D:571:ALA:HB2	1:D:597:TYR:OH	2.17	0.43
1:A:802:ILE:HG22	1:A:803:CYS:O	2.17	0.43
1:C:741:LEU:HD23	1:C:767:LEU:CD1	2.48	0.43
1:A:760:THR:HG22	1:A:761:THR:O	2.19	0.43
1:C:391:MET:SD	1:C:416:ASN:HB3	2.58	0.43
1:C:707:LEU:O	1:C:710:PHE:N	2.45	0.43
1:B:166:ILE:CG2	1:B:200:LEU:HD21	2.48	0.43
1:C:696:ARG:HG2	1:C:720:SER:HB2	2.01	0.43
1:D:303:ASN:HB3	1:D:306:TRP:CD2	2.53	0.43
1:D:359:ILE:HG23	1:D:363:PHE:CD1	2.54	0.43
1:D:746:ASN:HB3	1:D:747:LEU:H	1.75	0.43
1:B:270:CYS:O	1:B:273:GLY:HA2	2.19	0.43
1:B:669:LEU:HD21	1:B:671:ILE:HD11	2.00	0.43
1:B:809:GLN:HA	1:B:809:GLN:NE2	2.31	0.43
1:A:776:CYS:SG	1:A:814:ILE:HG22	2.59	0.43
1:B:275:SER:HA	1:B:298:SER:HB2	1.99	0.43
1:C:668:GLU:HG3	1:C:692:LEU:HD22	2.01	0.43
1:D:71:SER:HA	1:D:97:ASN:HD21	1.83	0.43
1:D:410:ASP:OD1	1:D:412:LYS:HG2	2.19	0.43
1:D:320:PHE:CE1	7:D:904:UPT:N1	2.86	0.43
1:B:207:SER:HA	1:B:228:PHE:HB2	2.01	0.42
1:C:62:GLY:HA3	1:C:63:LYS:HA	1.73	0.42
1:C:546:ASN:OD1	1:C:546:ASN:C	2.57	0.42
1:B:39:LYS:O	1:B:40:GLN:C	2.58	0.42
1:C:513:SER:HA	1:C:538:THR:O	2.19	0.42
1:B:696:ARG:HG2	1:B:720:SER:HB2	2.00	0.42
1:B:706:SER:HB3	1:B:709:ASP:OD2	2.19	0.42
1:C:406:ILE:H	1:C:428:ASN:HD22	1.67	0.42
1:C:521:LEU:HD13	1:C:550:LEU:HD21	2.00	0.42
1:D:144:LEU:HB3	1:D:169:LEU:HD21	2.02	0.42
1:C:763:LYS:HB2	1:C:764:LEU:H	1.67	0.42
1:A:789:GLU:O	1:A:790:HIS:CG	2.72	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:727:LEU:HD22	1:D:731:PHE:CE2	2.55	0.42
1:B:523:GLY:O	1:B:552:GLU:HB3	2.20	0.42
1:C:75:ILE:O	1:C:114:LEU:CD1	2.68	0.42
1:D:586:LEU:HD23	1:D:610:LEU:HD13	2.01	0.42
1:A:600:THR:O	1:A:601:ASP:HB2	2.20	0.42
1:B:304:ALA:O	1:B:335:MET:HG3	2.19	0.42
1:C:728:PRO:HA	1:C:729:SER:CB	2.49	0.42
1:D:144:LEU:HA	1:D:145:PRO:HD3	1.89	0.42
1:D:375:ARG:NH1	7:D:904:UPT:H1	2.16	0.42
1:D:378:VAL:HG11	5:D:902:URI:H1'	2.01	0.42
1:B:388:GLN:N	1:B:389:PRO:CD	2.82	0.42
1:B:518:ALA:HB2	1:B:541:ARG:HD2	2.02	0.42
1:C:729:SER:N	1:C:730:GLY:HA2	2.34	0.42
1:C:732:LEU:HD11	1:C:755:ALA:HB2	2.02	0.42
1:B:259:ARG:NH1	1:B:321:ASN:O	2.50	0.42
1:A:68:LEU:HD21	1:A:70:LEU:HD11	2.02	0.41
1:A:485:ALA:HA	1:A:509:CYS:O	2.20	0.41
1:C:428:ASN:HB3	1:C:429:ARG:H	1.77	0.41
1:D:134:ASP:HA	1:D:155:GLN:O	2.21	0.41
1:B:336:LEU:N	1:B:337:PRO:CD	2.83	0.41
1:D:732:LEU:N	1:D:732:LEU:CD1	2.73	0.41
1:A:200:LEU:HB3	1:A:203:LEU:HB2	2.03	0.41
1:C:225:ARG:O	1:C:249:THR:N	2.47	0.41
1:C:654:ILE:O	1:C:655:PRO:C	2.58	0.41
1:A:319:GLU:HA	1:A:345:SER:O	2.21	0.41
1:B:183:PHE:HB3	1:B:266:PRO:HG2	2.02	0.41
1:C:78:ILE:HB	1:C:116:ILE:HG12	2.02	0.41
1:C:624:TRP:HB3	1:C:655:PRO:HG2	2.02	0.41
1:D:740:HIS:C	1:D:740:HIS:CD2	2.93	0.41
1:B:80:ASN:HA	1:B:120:ALA:O	2.21	0.41
1:C:388:GLN:N	1:C:389:PRO:CD	2.84	0.41
1:C:514:ALA:HA	1:C:539:ASN:O	2.21	0.41
1:D:692:LEU:HD23	1:D:692:LEU:C	2.41	0.41
1:D:703:LEU:HD21	1:D:724:ILE:HD13	2.03	0.41
1:A:431:SER:HB2	1:A:432:PRO:CD	2.50	0.41
1:B:186:VAL:O	1:B:186:VAL:HG12	2.21	0.41
1:B:290:ARG:HE	1:B:312:HIS:HB3	1.85	0.41
1:B:350:LYS:HA	1:B:351:GLY:HA2	1.79	0.41
1:D:144:LEU:CB	1:D:169:LEU:HD21	2.51	0.41
1:D:426:SER:HA	1:D:489:SER:O	2.21	0.41
1:D:736:SER:O	1:D:763:LYS:HG3	2.20	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:2:NAG:HO3	4:H:2:NAG:C7	2.34	0.41
1:B:159:TYR:CE1	1:B:187:CYS:HB2	2.56	0.41
1:D:319:GLU:HG2	1:D:345:SER:HB2	2.02	0.41
1:D:529:ILE:O	1:D:529:ILE:HG13	2.21	0.41
1:A:756:LEU:HD13	1:A:786:TRP:HB2	2.03	0.40
1:C:133:GLU:CG	1:C:154:ILE:HB	2.51	0.40
1:D:715:ARG:O	1:D:738:LEU:HD12	2.21	0.40
1:A:700:LEU:HD23	1:A:700:LEU:HA	1.92	0.40
1:A:806:PRO:O	1:A:807:GLY:C	2.60	0.40
1:B:404:ASN:O	1:B:405:PHE:C	2.59	0.40
1:D:164:GLU:OE1	1:D:165:GLY:HA2	2.21	0.40
1:D:342:LEU:O	1:D:372:LEU:HD12	2.22	0.40
1:A:342:LEU:HD21	1:A:344:LEU:HD11	2.03	0.40
1:B:290:ARG:HH11	1:B:290:ARG:HG3	1.86	0.40
1:C:140:ILE:HD11	1:C:161:ILE:HA	2.03	0.40
1:C:504:LEU:HD12	1:C:504:LEU:HA	1.96	0.40
1:B:329:SER:O	1:B:329:SER:OG	2.36	0.40
1:C:431:SER:HB2	1:C:432:PRO:HD2	2.03	0.40
1:C:682:THR:HA	1:C:710:PHE:CD1	2.57	0.40
1:D:319:GLU:OE2	1:D:375:ARG:NH2	2.53	0.40
1:A:537:LEU:HA	1:A:537:LEU:HD23	1.84	0.40
1:B:532:VAL:HB	1:B:553:LEU:HD22	2.04	0.40
1:B:784:ARG:NH1	1:B:815:VAL:O	2.55	0.40
1:D:784:ARG:NH2	1:D:814:ILE:O	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	741/811 (91%)	672 (91%)	66 (9%)	3 (0%)	30 50

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	744/811 (92%)	671 (90%)	70 (9%)	3 (0%)	30	50
1	C	738/811 (91%)	668 (90%)	65 (9%)	5 (1%)	19	36
1	D	738/811 (91%)	640 (87%)	94 (13%)	4 (0%)	25	45
All	All	2961/3244 (91%)	2651 (90%)	295 (10%)	15 (0%)	25	45

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	780	ILE
1	C	60	THR
1	C	757	GLU
1	D	792	ASN
1	A	807	GLY
1	B	45	VAL
1	C	601	ASP
1	D	481	ALA
1	A	378	VAL
1	A	814	ILE
1	B	378	VAL
1	C	378	VAL
1	D	378	VAL
1	C	84	GLN
1	B	781	GLY

### 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	695/755 (92%)	644 (93%)	51 (7%)	11	24
1	B	698/755 (92%)	655 (94%)	43 (6%)	15	31
1	C	692/755 (92%)	637 (92%)	55 (8%)	10	20
1	D	692/755 (92%)	646 (93%)	46 (7%)	14	28
All	All	2777/3020 (92%)	2582 (93%)	195 (7%)	12	25

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	VAL
1	A	49	CYS
1	A	55	GLN
1	A	56	GLU
1	A	64	TYR
1	A	80	ASN
1	A	118	ASP
1	A	128	ARG
1	A	136	GLN
1	A	150	GLU
1	A	168	ARG
1	A	173	LYS
1	A	193	GLU
1	A	200	LEU
1	A	243	LYS
1	A	248	LEU
1	A	286	LEU
1	A	300	ARG
1	A	301	LYS
1	A	308	LYS
1	A	333	LEU
1	A	385	ASP
1	A	388	GLN
1	A	412	LYS
1	A	416	ASN
1	A	418	SER
1	A	458	ASP
1	A	459	PHE
1	A	472	ARG
1	A	504	LEU
1	A	516	SER
1	A	552	GLU
1	A	554	SER
1	A	569	ARG
1	A	584	THR
1	A	650	ARG
1	A	671	ILE
1	A	689	ARG
1	A	702	PHE
1	A	703	LEU
1	A	708	SER
1	A	712	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	720	SER
1	A	732	LEU
1	A	736	SER
1	A	739	LYS
1	A	753	LYS
1	A	759	LYS
1	A	765	SER
1	A	808	ASP
1	A	815	VAL
1	B	49	CYS
1	B	52	ARG
1	B	56	GLU
1	B	64	TYR
1	B	76	THR
1	B	101	GLN
1	B	118	ASP
1	B	122	LEU
1	B	150	GLU
1	B	173	LYS
1	B	199	THR
1	B	200	LEU
1	B	214	SER
1	B	216	VAL
1	B	225	ARG
1	B	232	THR
1	B	248	LEU
1	B	271	ASP
1	B	278	ILE
1	B	290	ARG
1	B	323	LEU
1	B	355	GLN
1	B	391	MET
1	B	392	GLN
1	B	504	LEU
1	B	509	CYS
1	B	534	TYR
1	B	554	SER
1	B	653	HIS
1	B	720	SER
1	B	734	GLU
1	B	736	SER
1	B	745	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	753	LYS
1	B	761	THR
1	B	780	ILE
1	B	794	LYS
1	B	799	VAL
1	B	805	SER
1	B	809	GLN
1	B	812	LYS
1	B	815	VAL
1	B	819	LEU
1	C	45	VAL
1	C	49	CYS
1	C	56	GLU
1	C	59	GLN
1	C	60	THR
1	C	66	THR
1	C	76	THR
1	C	81	GLU
1	C	86	LEU
1	C	90	THR
1	C	150	GLU
1	C	168	ARG
1	C	189	LYS
1	C	194	ASP
1	C	200	LEU
1	C	207	SER
1	C	214	SER
1	C	235	LYS
1	C	243	LYS
1	C	248	LEU
1	C	280	ARG
1	C	314	LYS
1	C	329	SER
1	C	336	LEU
1	C	338	ARG
1	C	350	LYS
1	C	355	GLN
1	C	374	LEU
1	C	413	LEU
1	C	418	SER
1	C	429	ARG
1	C	465	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	472	ARG
1	C	504	LEU
1	C	509	CYS
1	C	554	SER
1	C	565	SER
1	C	614	VAL
1	C	633	SER
1	C	665	SER
1	C	686	GLN
1	C	703	LEU
1	C	713	SER
1	C	725	SER
1	C	727	LEU
1	C	729	SER
1	C	756	LEU
1	C	759	LYS
1	C	761	THR
1	C	762	THR
1	C	763	LYS
1	C	764	LEU
1	C	777	THR
1	C	785	ARG
1	C	805	SER
1	D	49	CYS
1	D	52	ARG
1	D	63	LYS
1	D	86	LEU
1	D	89	LEU
1	D	94	LEU
1	D	122	LEU
1	D	125	LYS
1	D	149	THR
1	D	164	GLU
1	D	168	ARG
1	D	199	THR
1	D	201	THR
1	D	213	LEU
1	D	240	GLU
1	D	300	ARG
1	D	301	LYS
1	D	307	PHE
1	D	314	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	334	THR
1	D	337	PRO
1	D	370	ARG
1	D	397	SER
1	D	416	ASN
1	D	459	PHE
1	D	502	GLU
1	D	569	ARG
1	D	584	THR
1	D	608	LYS
1	D	625	ASN
1	D	632	ILE
1	D	639	LYS
1	D	657	GLU
1	D	729	SER
1	D	731	PHE
1	D	732	LEU
1	D	739	LYS
1	D	744	SER
1	D	749	LYS
1	D	750	THR
1	D	753	LYS
1	D	756	LEU
1	D	761	THR
1	D	779	ASP
1	D	784	ARG
1	D	805	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	284	GLN
1	A	416	ASN
1	A	585	ASN
1	B	77	HIS
1	B	112	ASN
1	B	135	ASN
1	B	174	ASN
1	B	233	GLN
1	B	284	GLN
1	B	285	ASN
1	B	388	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	395	ASN
1	B	408	GLN
1	B	416	ASN
1	B	772	ASN
1	B	809	GLN
1	C	59	GLN
1	C	202	ASN
1	C	231	ASN
1	C	247	ASN
1	C	285	ASN
1	C	428	ASN
1	C	685	GLN
1	C	686	GLN
1	D	55	GLN
1	D	59	GLN
1	D	247	ASN
1	D	358	ASN
1	D	585	ASN
1	D	593	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

31 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	0.91	0	17,19,21	1.48	4 (23%)
2	NAG	E	2	2	14,14,15	0.70	0	17,19,21	1.59	5 (29%)
2	BMA	E	3	2	11,11,12	1.30	1 (9%)	15,15,17	2.79	5 (33%)
2	MAN	E	4	2	11,11,12	0.86	1 (9%)	15,15,17	1.68	3 (20%)
2	MAN	E	5	2	11,11,12	1.02	1 (9%)	15,15,17	1.86	2 (13%)
3	NAG	F	1	3,1	14,14,15	0.74	0	17,19,21	1.46	5 (29%)
3	NAG	F	2	3	14,14,15	0.63	0	17,19,21	1.39	2 (11%)
3	NAG	G	1	3,1	14,14,15	0.84	0	17,19,21	2.57	6 (35%)
3	NAG	G	2	3	14,14,15	0.88	1 (7%)	17,19,21	2.01	7 (41%)
4	NAG	H	1	4,1	14,14,15	0.97	0	17,19,21	1.68	3 (17%)
4	NAG	H	2	4	14,14,15	0.57	0	17,19,21	1.52	3 (17%)
4	BMA	H	3	4	11,11,12	0.70	0	15,15,17	0.93	0
3	NAG	I	1	3,1	14,14,15	0.50	0	17,19,21	1.32	1 (5%)
3	NAG	I	2	3	14,14,15	0.66	0	17,19,21	1.50	4 (23%)
3	NAG	J	1	3,1	14,14,15	0.60	0	17,19,21	1.41	3 (17%)
3	NAG	J	2	3	14,14,15	1.56	2 (14%)	17,19,21	2.59	11 (64%)
2	NAG	K	1	2,1	14,14,15	0.43	0	17,19,21	1.39	3 (17%)
2	NAG	K	2	2	14,14,15	0.69	0	17,19,21	1.11	1 (5%)
2	BMA	K	3	2	11,11,12	0.66	0	15,15,17	2.53	3 (20%)
2	MAN	K	4	2	11,11,12	1.02	0	15,15,17	1.72	2 (13%)
2	MAN	K	5	2	11,11,12	1.03	0	15,15,17	1.56	1 (6%)
4	NAG	L	1	4,1	14,14,15	0.67	0	17,19,21	1.40	3 (17%)
4	NAG	L	2	4	14,14,15	0.97	1 (7%)	17,19,21	1.15	1 (5%)
4	BMA	L	3	4	11,11,12	0.53	0	15,15,17	1.19	1 (6%)
3	NAG	M	1	3,1	14,14,15	0.55	0	17,19,21	1.79	4 (23%)
3	NAG	M	2	3	14,14,15	0.70	0	17,19,21	1.51	2 (11%)
4	NAG	N	1	4,1	14,14,15	0.63	0	17,19,21	1.32	2 (11%)
4	NAG	N	2	4	14,14,15	0.69	0	17,19,21	1.54	3 (17%)
4	BMA	N	3	4	11,11,12	0.89	0	15,15,17	1.42	4 (26%)
3	NAG	O	1	3,1	14,14,15	0.64	0	17,19,21	1.65	2 (11%)
3	NAG	O	2	3	14,14,15	0.97	1 (7%)	17,19,21	1.45	2 (11%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	2	NAG	C1-C2	-3.67	1.47	1.52
3	J	2	NAG	O5-C1	-3.43	1.37	1.43
4	L	2	NAG	O5-C1	-3.10	1.38	1.43
3	O	2	NAG	O5-C1	-2.81	1.39	1.43
2	E	5	MAN	C2-C3	2.57	1.56	1.52
2	E	3	BMA	O3-C3	2.52	1.49	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2	NAG	O5-C1	-2.38	1.39	1.43
2	E	4	MAN	C4-C3	2.32	1.58	1.52

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	BMA	C1-O5-C5	8.51	123.59	112.19
2	K	3	BMA	C1-O5-C5	8.01	122.92	112.19
3	G	1	NAG	C1-O5-C5	7.65	122.44	112.19
3	M	1	NAG	C1-O5-C5	5.62	119.71	112.19
2	K	5	MAN	C1-C2-C3	5.25	117.29	109.64
3	J	2	NAG	C1-O5-C5	5.10	119.02	112.19
2	E	5	MAN	C1-C2-C3	5.02	116.96	109.64
2	E	4	MAN	O5-C1-C2	-4.81	99.31	110.79
3	O	1	NAG	O5-C1-C2	-4.61	104.16	111.29
2	K	4	MAN	C3-C4-C5	4.53	118.44	110.23
2	E	3	BMA	O3-C3-C2	4.49	119.22	110.05
4	H	1	NAG	O5-C1-C2	-4.23	104.74	111.29
3	G	2	NAG	C1-O5-C5	4.20	117.81	112.19
3	J	1	NAG	O5-C1-C2	-4.04	105.05	111.29
4	H	2	NAG	O5-C1-C2	-3.98	105.14	111.29
3	J	2	NAG	C1-C2-N2	-3.78	104.47	110.43
3	G	1	NAG	O7-C7-C8	-3.71	115.44	122.05
2	K	3	BMA	C3-C4-C5	3.58	116.71	110.23
3	I	1	NAG	C1-C2-N2	-3.56	104.82	110.43
4	N	2	NAG	O4-C4-C3	-3.51	102.09	110.38
3	J	2	NAG	O3-C3-C2	-3.34	102.47	109.40
3	J	2	NAG	O5-C1-C2	3.32	116.42	111.29
2	K	4	MAN	C2-C3-C4	3.27	116.61	110.86
3	G	1	NAG	O5-C5-C6	-3.22	101.41	107.66
4	H	1	NAG	C3-C4-C5	-3.16	104.50	110.23
4	L	1	NAG	C1-C2-N2	-3.10	105.55	110.43
2	E	5	MAN	O3-C3-C2	3.00	116.18	110.05
3	J	2	NAG	O4-C4-C3	3.00	117.45	110.38
4	N	1	NAG	O5-C1-C2	-2.97	106.69	111.29
3	O	2	NAG	C1-O5-C5	2.94	116.13	112.19
2	E	2	NAG	O5-C1-C2	-2.90	106.80	111.29
3	G	2	NAG	O6-C6-C5	-2.88	101.51	111.33
4	H	1	NAG	O5-C5-C6	2.86	113.22	107.66
3	G	2	NAG	O5-C5-C6	-2.85	102.12	107.66
4	L	3	BMA	C3-C4-C5	2.84	115.39	110.23
2	E	2	NAG	C2-N2-C7	2.84	126.71	122.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	NAG	O4-C4-C5	2.84	116.32	109.32
4	N	3	BMA	O5-C5-C6	2.80	113.12	107.66
3	M	2	NAG	O4-C4-C5	2.77	116.15	109.32
3	F	2	NAG	C3-C4-C5	-2.76	105.23	110.23
2	E	2	NAG	O7-C7-C8	-2.76	117.14	122.05
4	H	2	NAG	C1-C2-N2	2.74	114.76	110.43
3	I	2	NAG	C1-O5-C5	2.74	115.86	112.19
3	F	1	NAG	O3-C3-C2	-2.74	103.72	109.40
3	I	2	NAG	C4-C3-C2	-2.67	107.10	111.02
3	J	2	NAG	O5-C5-C6	-2.66	102.48	107.66
4	H	2	NAG	C2-N2-C7	-2.65	119.34	122.90
2	E	1	NAG	O5-C1-C2	-2.63	107.22	111.29
3	G	1	NAG	O5-C5-C4	2.61	117.17	110.83
4	L	2	NAG	C4-C3-C2	2.58	114.81	111.02
2	K	1	NAG	C1-O5-C5	2.58	115.64	112.19
2	K	1	NAG	O5-C1-C2	-2.56	107.33	111.29
2	E	1	NAG	C3-C4-C5	-2.55	105.61	110.23
3	O	1	NAG	C3-C4-C5	-2.53	105.65	110.23
3	F	1	NAG	O7-C7-N2	2.51	126.42	121.98
3	G	2	NAG	O4-C4-C3	2.51	116.29	110.38
4	N	3	BMA	C1-C2-C3	2.48	113.25	109.64
2	K	1	NAG	C6-C5-C4	-2.47	106.94	113.02
3	M	1	NAG	C6-C5-C4	-2.46	106.97	113.02
3	G	1	NAG	C6-C5-C4	-2.46	106.99	113.02
2	K	3	BMA	O5-C5-C4	2.45	116.78	110.83
2	E	4	MAN	C3-C4-C5	2.45	114.67	110.23
4	N	2	NAG	C2-N2-C7	-2.45	119.62	122.90
3	J	2	NAG	O3-C3-C4	-2.44	104.63	110.38
3	G	2	NAG	C1-C2-N2	-2.41	106.63	110.43
4	N	3	BMA	C3-C4-C5	2.39	114.56	110.23
3	M	2	NAG	C4-C3-C2	-2.38	107.54	111.02
3	J	2	NAG	C8-C7-N2	2.35	120.01	116.12
3	M	1	NAG	O7-C7-C8	-2.35	117.88	122.05
4	N	2	NAG	C1-C2-N2	2.34	114.11	110.43
3	J	2	NAG	O6-C6-C5	-2.32	103.45	111.33
3	I	2	NAG	C1-C2-N2	2.28	114.03	110.43
4	L	1	NAG	C1-O5-C5	2.26	115.22	112.19
3	F	1	NAG	C1-O5-C5	2.25	115.19	112.19
2	E	4	MAN	C1-C2-C3	-2.23	106.40	109.64
2	K	2	NAG	O6-C6-C5	-2.21	103.80	111.33
2	E	1	NAG	O7-C7-C8	-2.20	118.14	122.05
2	E	3	BMA	O4-C4-C3	-2.18	105.23	110.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	C2-N2-C7	2.17	125.81	122.90
3	O	2	NAG	O7-C7-N2	2.16	125.81	121.98
3	M	1	NAG	O5-C1-C2	-2.11	108.02	111.29
4	N	3	BMA	O4-C4-C3	-2.11	105.40	110.38
4	L	1	NAG	O7-C7-C8	-2.10	118.31	122.05
3	G	1	NAG	C8-C7-N2	2.10	119.61	116.12
4	N	1	NAG	O5-C5-C6	2.10	111.75	107.66
3	I	2	NAG	C3-C4-C5	-2.10	106.43	110.23
2	E	3	BMA	C3-C4-C5	2.09	114.03	110.23
2	E	1	NAG	C1-O5-C5	2.08	114.98	112.19
3	F	1	NAG	O7-C7-C8	-2.08	118.35	122.05
2	E	2	NAG	O7-C7-N2	2.07	125.64	121.98
3	G	2	NAG	C2-N2-C7	-2.07	120.12	122.90
3	J	2	NAG	O5-C5-C4	2.06	115.85	110.83
3	J	1	NAG	C3-C4-C5	-2.05	106.51	110.23
3	G	2	NAG	O7-C7-C8	-2.04	118.43	122.05
3	J	2	NAG	C2-N2-C7	2.02	125.60	122.90
3	J	1	NAG	O7-C7-C8	-2.01	118.47	122.05
2	E	3	BMA	O5-C5-C4	2.01	115.71	110.83
2	E	2	NAG	C3-C4-C5	-2.01	106.59	110.23

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	5	MAN	O5-C5-C6-O6
2	K	3	BMA	C4-C5-C6-O6
2	K	5	MAN	C4-C5-C6-O6
2	K	4	MAN	O5-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
4	N	3	BMA	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
2	K	3	BMA	O5-C5-C6-O6
2	K	4	MAN	C4-C5-C6-O6
4	N	3	BMA	C4-C5-C6-O6
3	J	2	NAG	C8-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2
3	I	1	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
2	E	4	MAN	O5-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

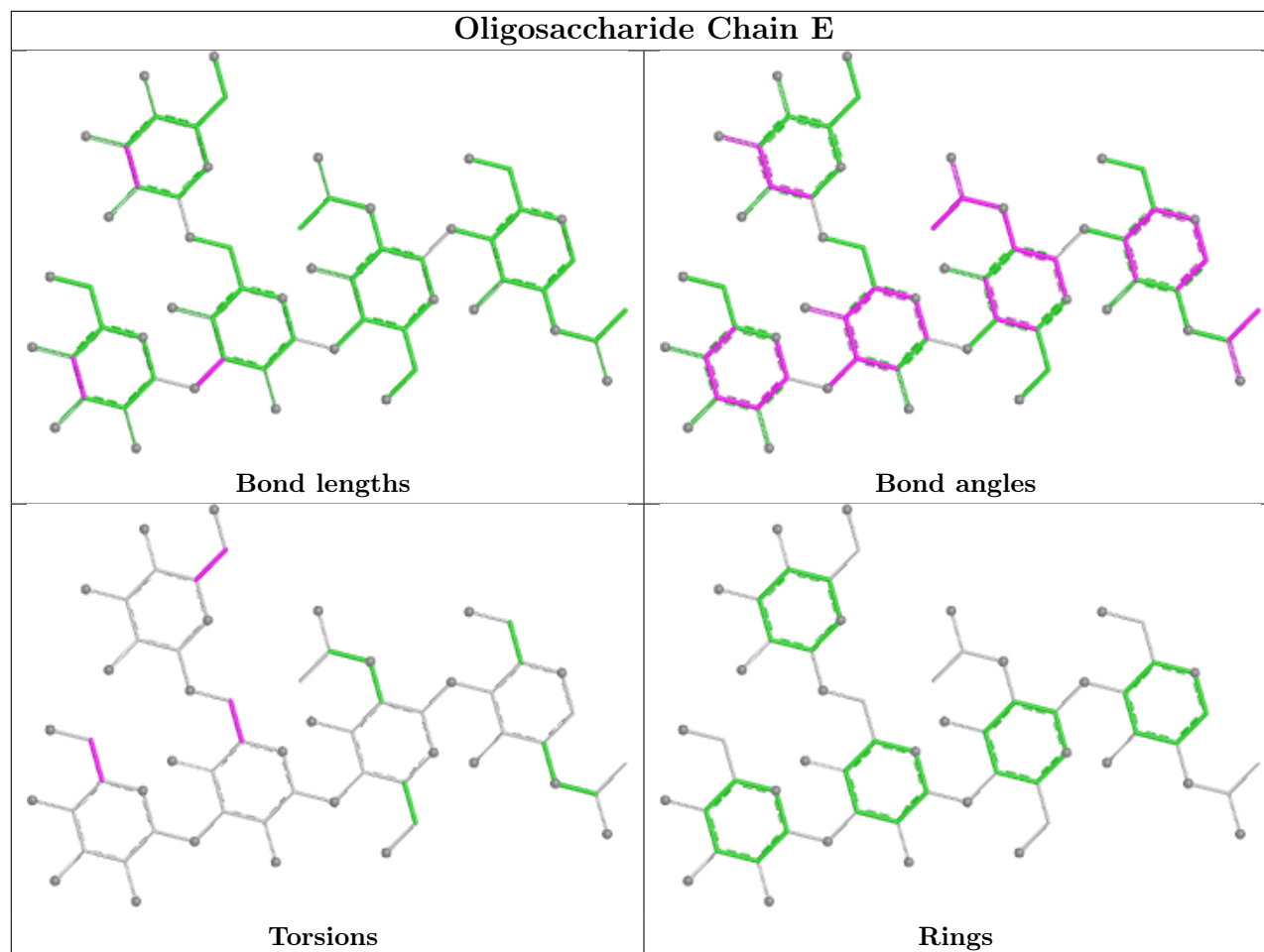
Mol	Chain	Res	Type	Atoms
3	F	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	L	3	BMA	C4-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
2	E	5	MAN	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6

There are no ring outliers.

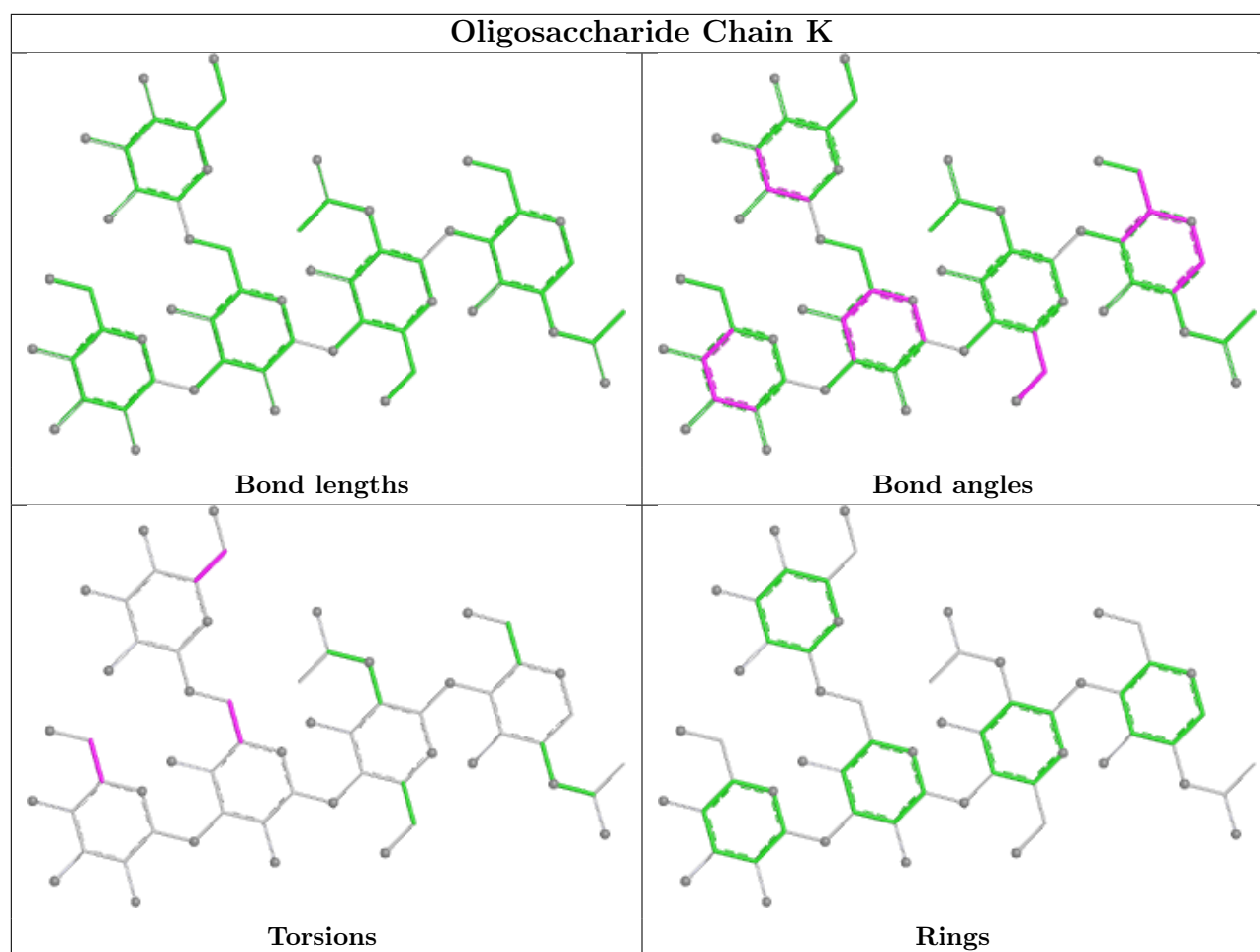
4 monomers are involved in 5 short contacts:

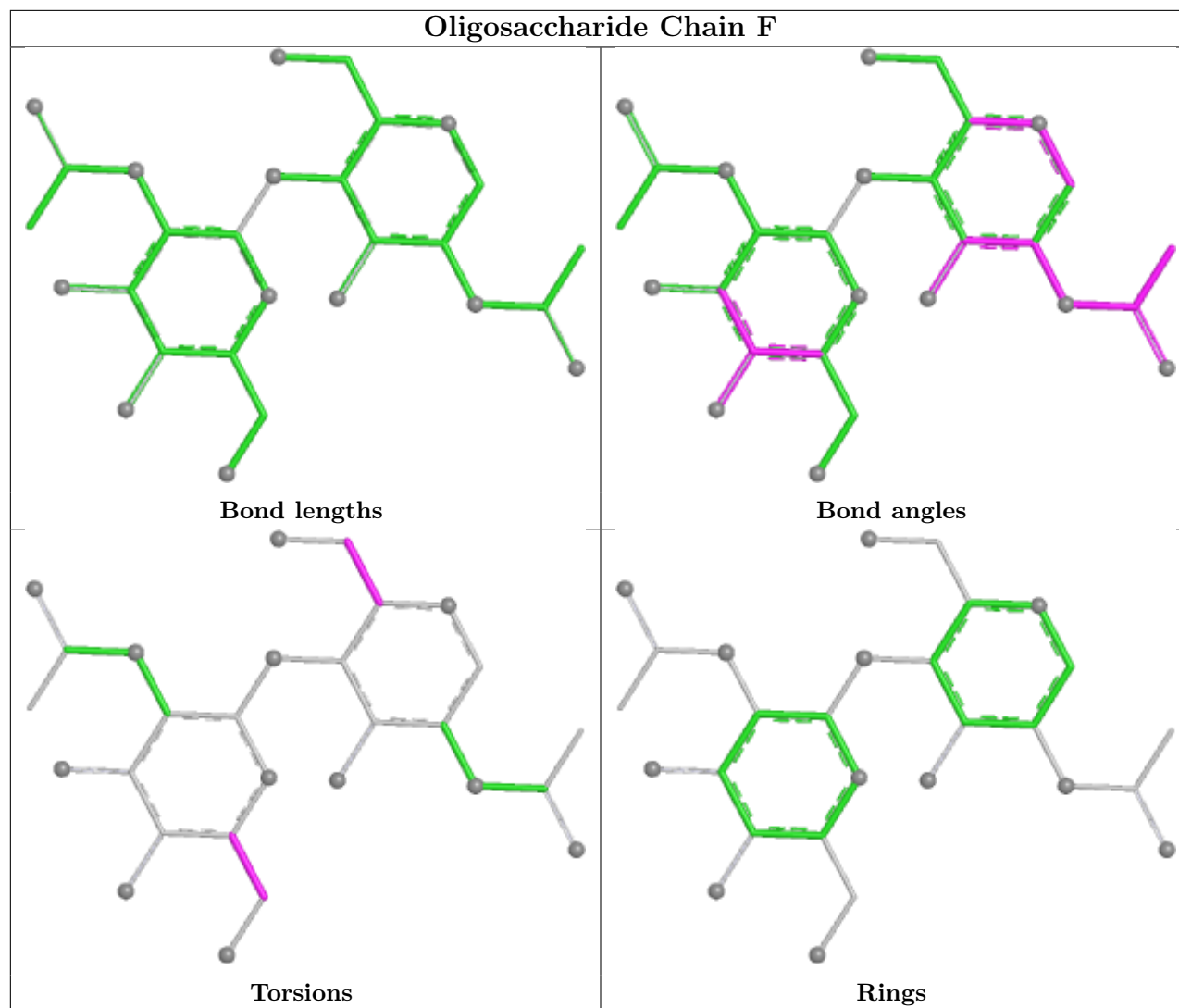
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0
3	J	2	NAG	2	0
4	H	2	NAG	1	0
2	E	1	NAG	2	0

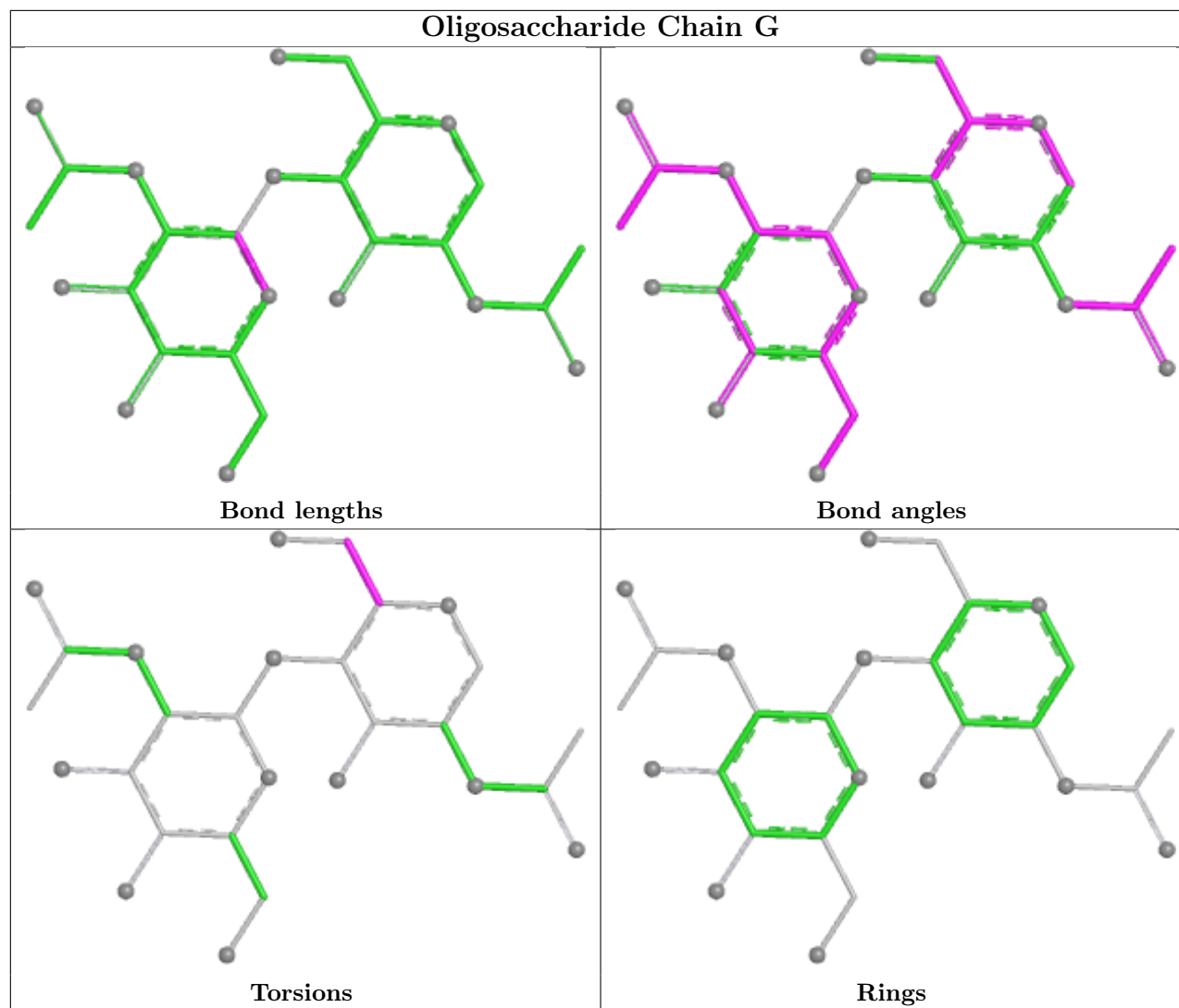
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

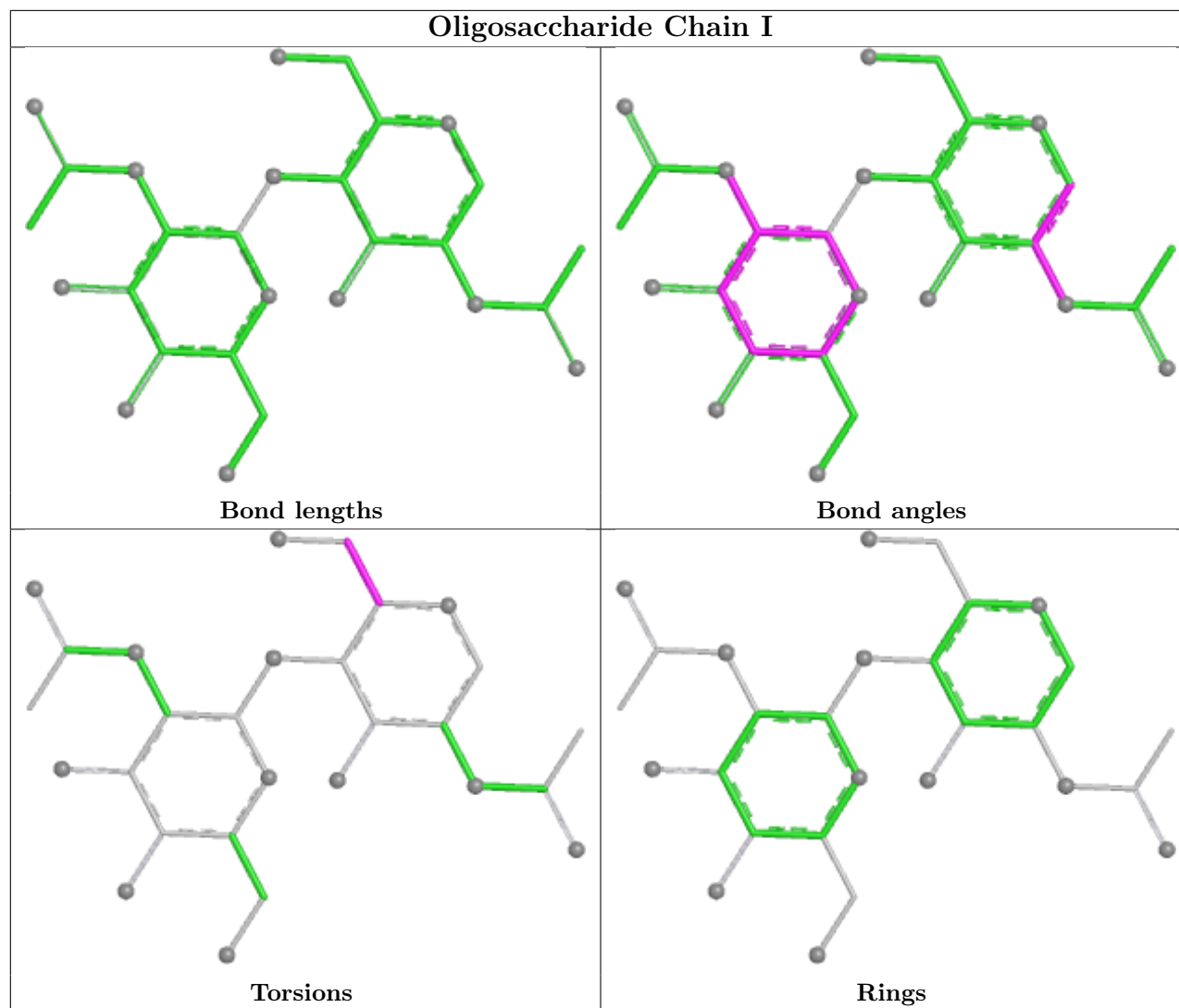


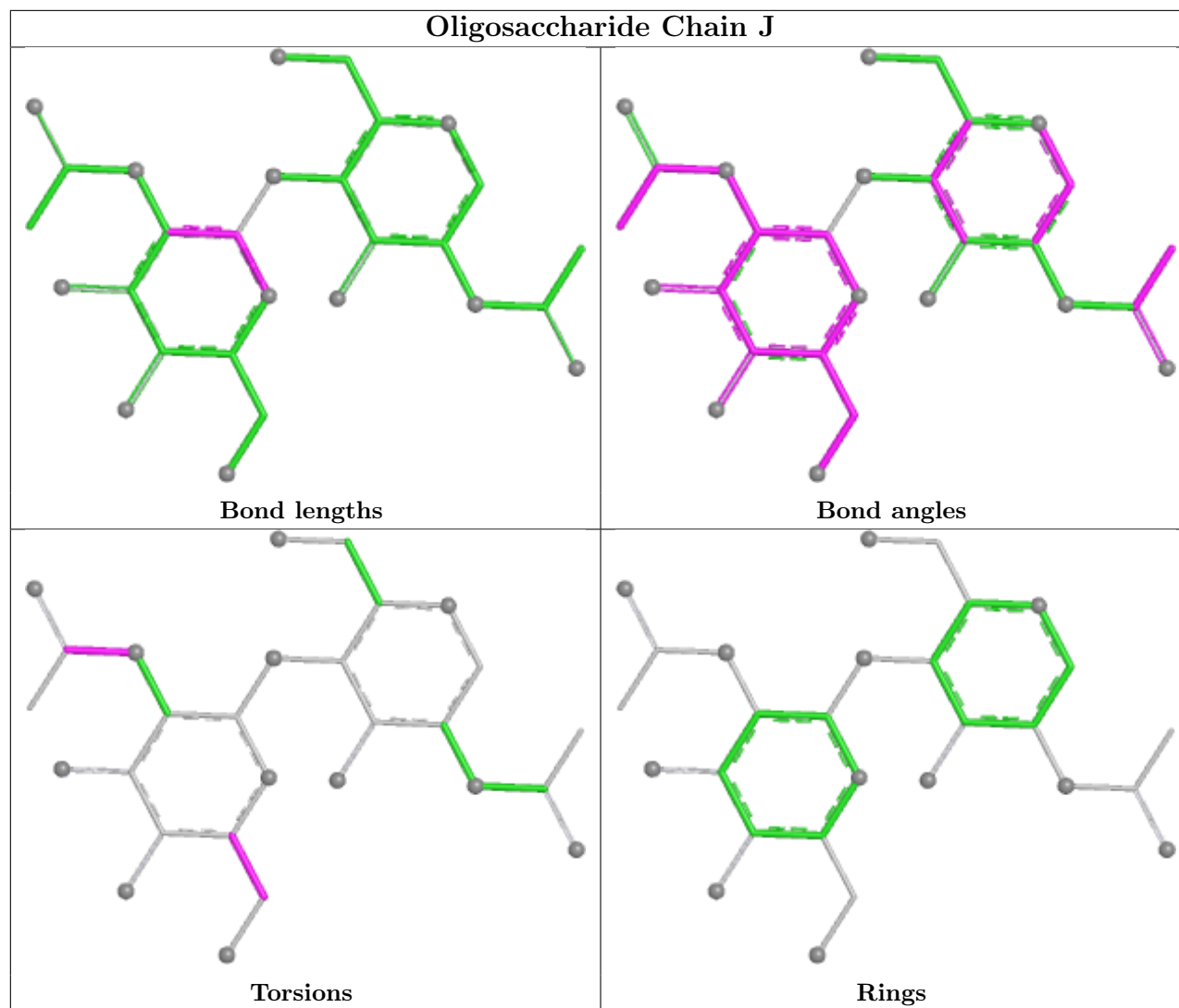


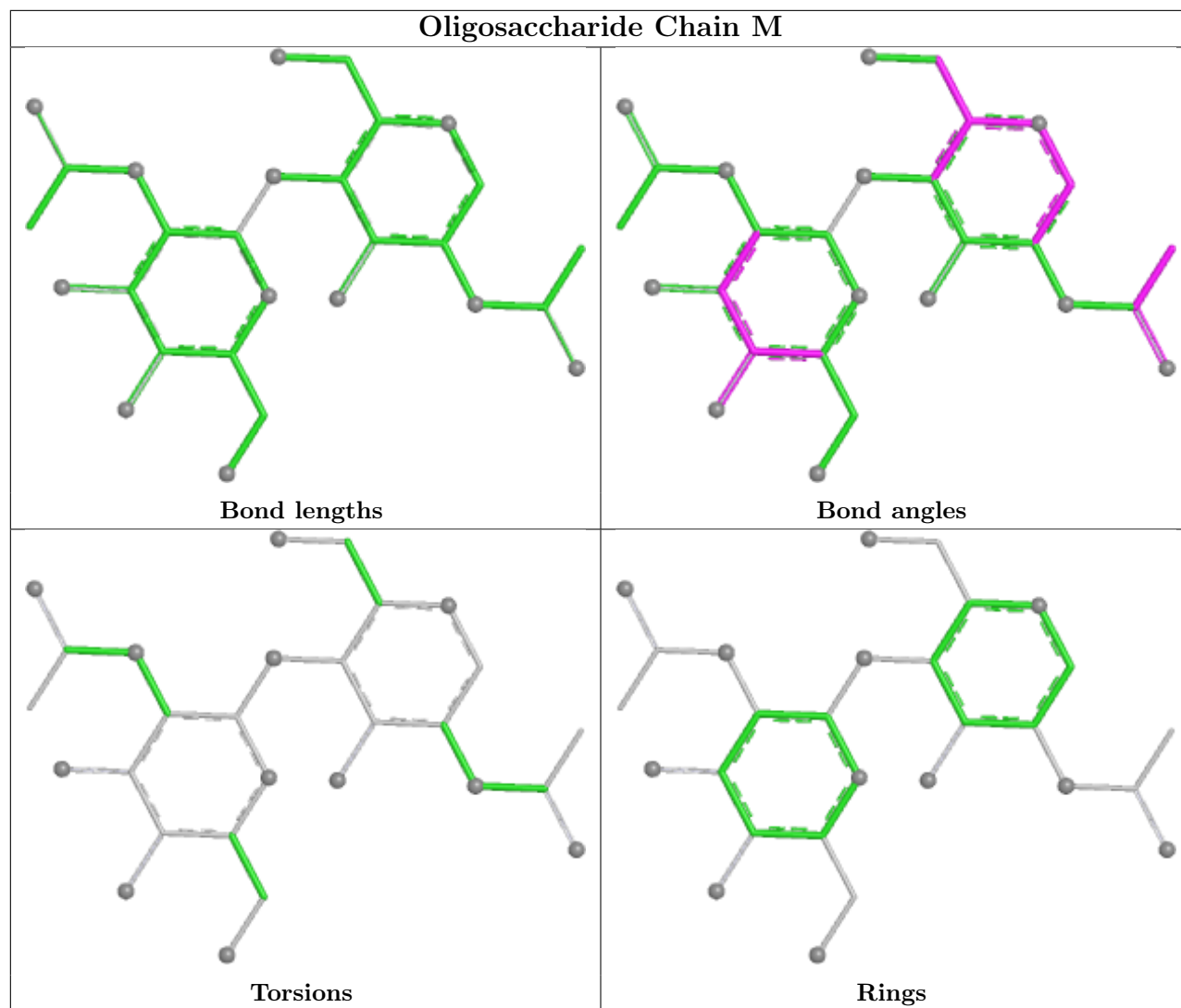


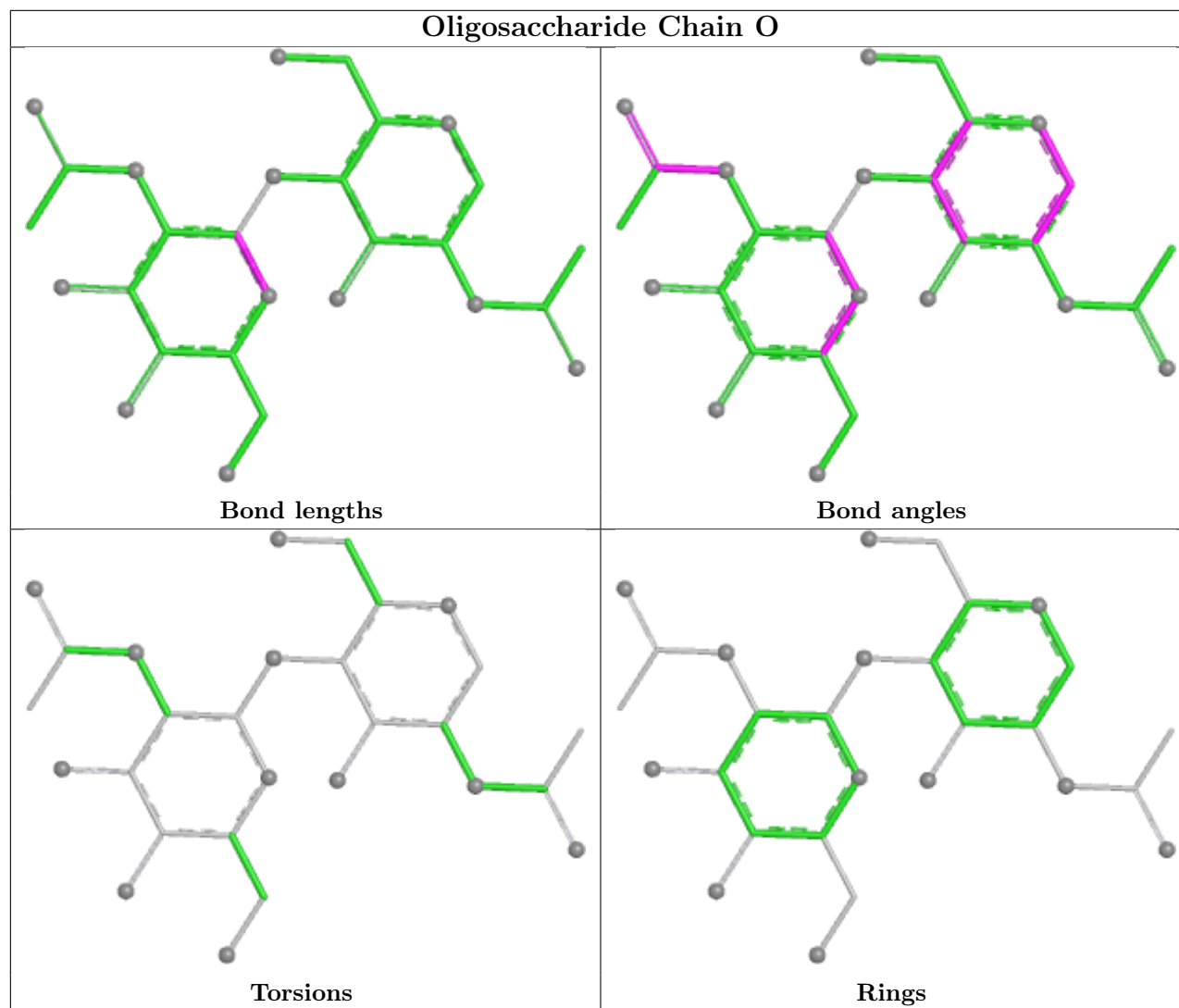


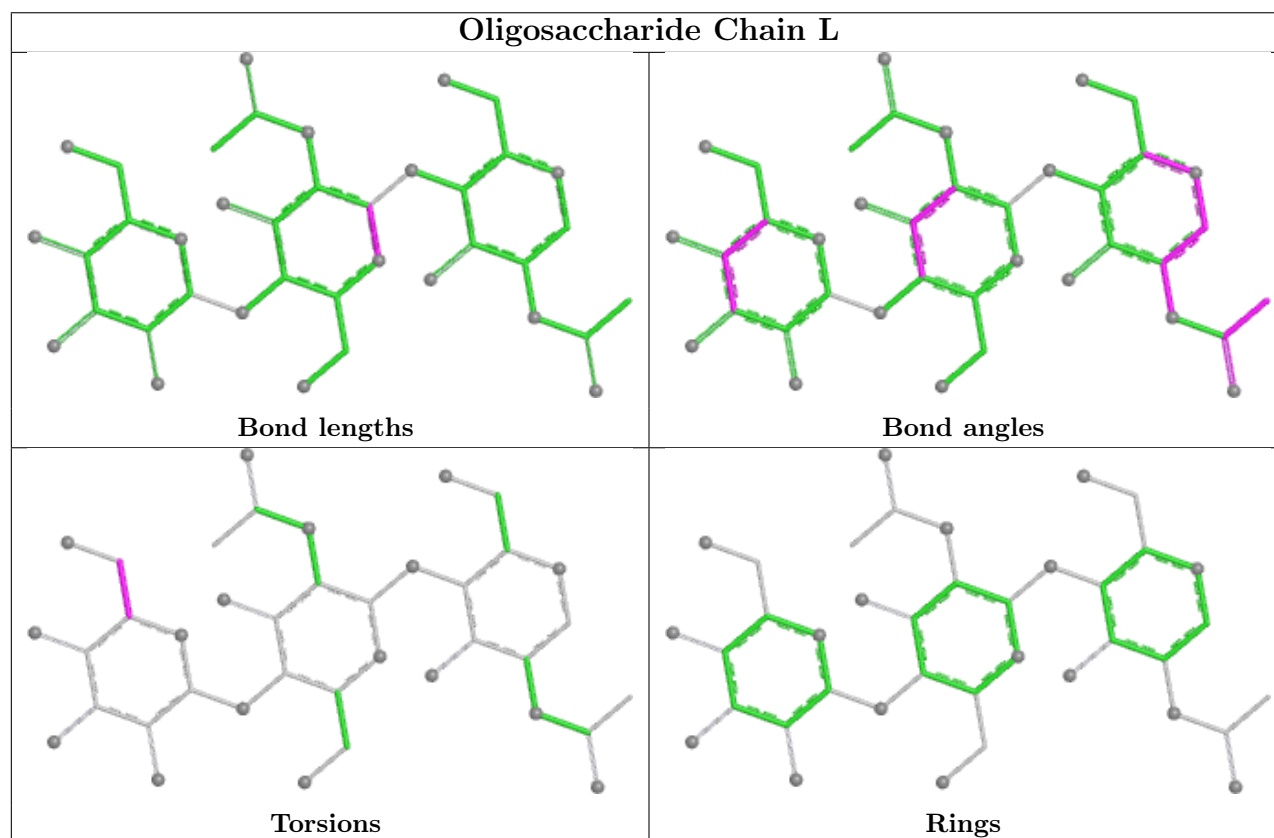
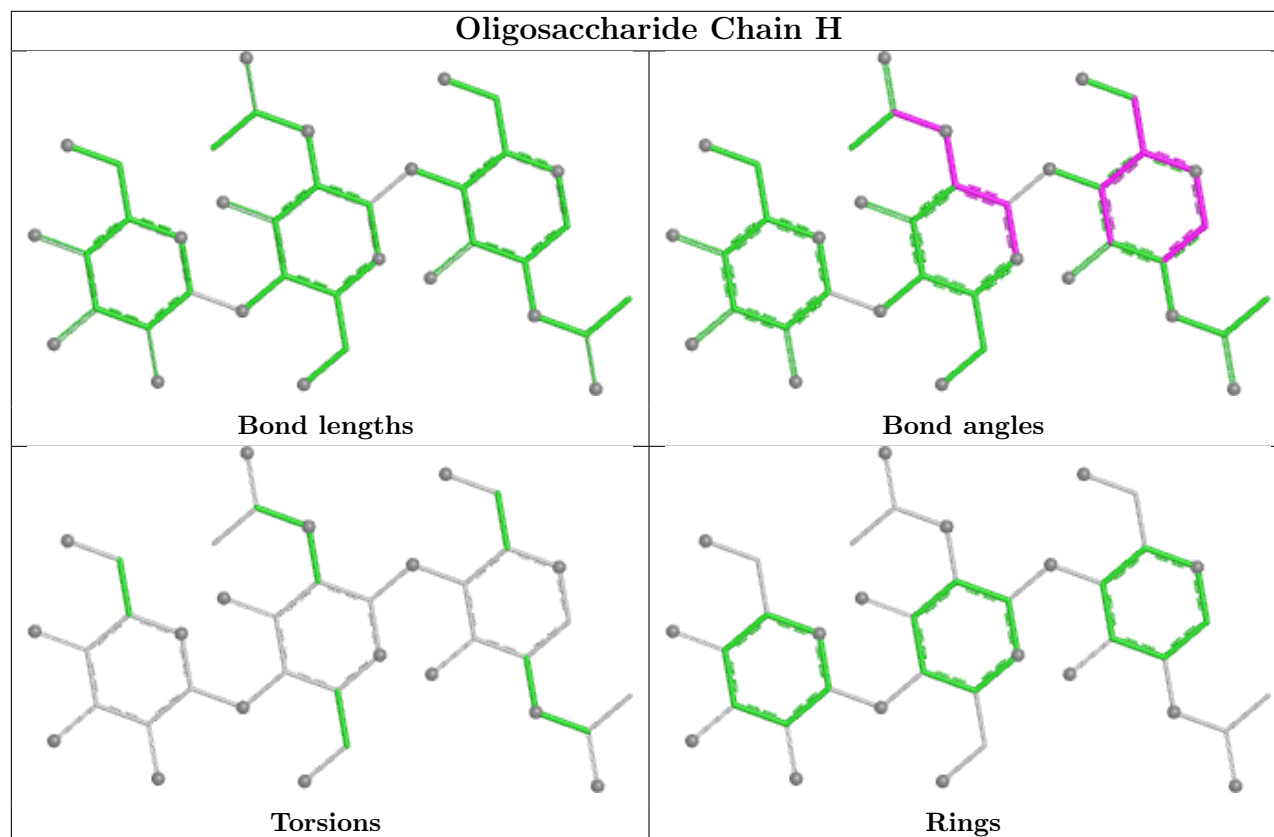




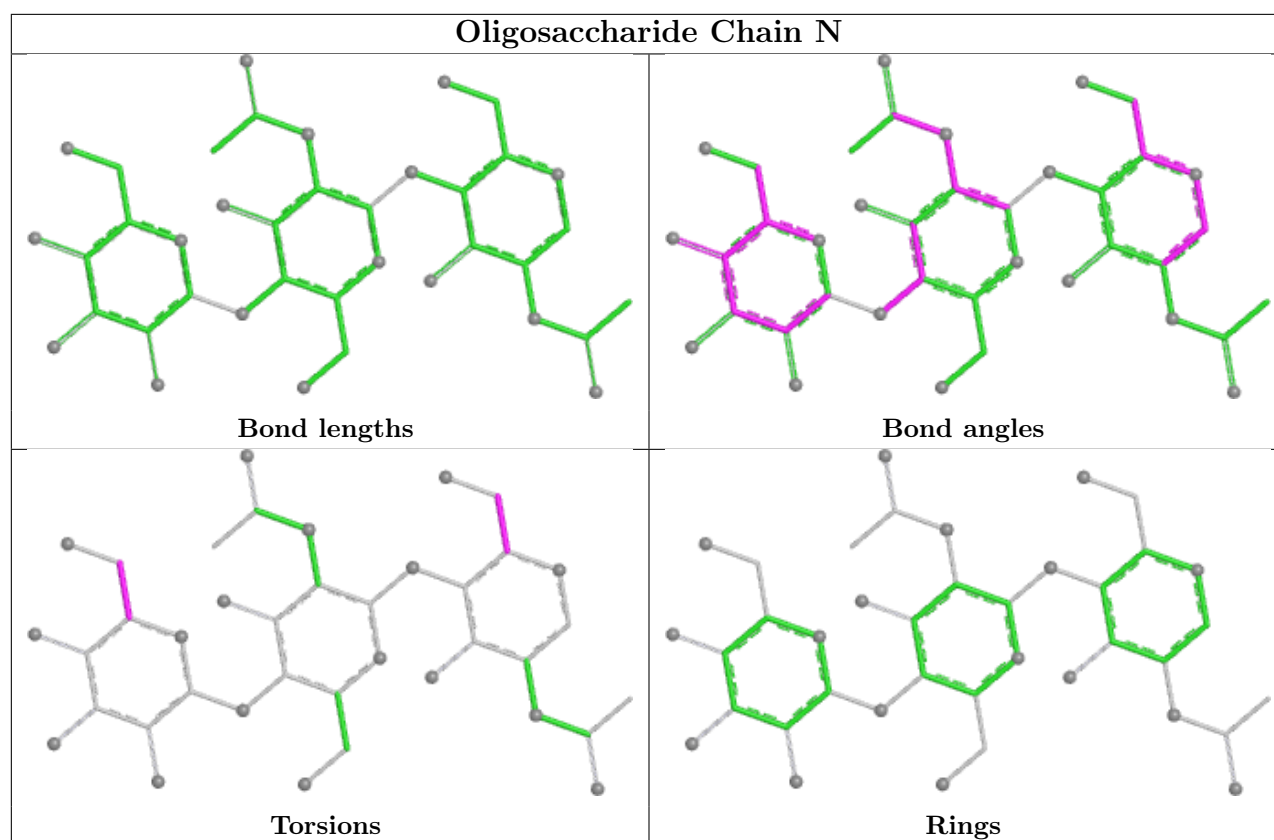












## 5.6 Ligand geometry [i](#)

15 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	06S	C	901	-	40,52,52	1.43	6 (15%)	51,81,81	1.74	9 (17%)
7	UPT	D	904	-	20,22,22	1.35	2 (10%)	25,34,34	2.06	5 (20%)
8	NAG	A	913	1	14,14,15	0.71	0	17,19,21	0.75	0
8	NAG	D	908	1	14,14,15	0.85	0	17,19,21	1.61	3 (17%)
8	NAG	B	911	1	14,14,15	0.66	0	17,19,21	1.20	1 (5%)
5	URI	B	901	-	18,18,18	0.38	0	26,26,26	0.73	0
5	URI	D	901	-	18,18,18	0.44	0	26,26,26	0.79	1 (3%)
7	UPT	B	903	-	20,22,22	1.20	3 (15%)	25,34,34	1.91	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	UPT	C	902	-	20,22,22	1.16	2 (10%)	25,34,34	2.05	5 (20%)
6	06S	D	903	-	40,52,52	1.49	6 (15%)	51,81,81	1.88	13 (25%)
5	URI	D	902	-	18,18,18	0.28	0	26,26,26	0.46	0
5	URI	A	901	-	18,18,18	0.46	0	26,26,26	0.58	1 (3%)
7	UPT	A	903	-	20,22,22	1.44	6 (30%)	25,34,34	2.07	7 (28%)
6	06S	B	902	-	40,52,52	1.43	6 (15%)	51,81,81	1.82	8 (15%)
6	06S	A	902	-	40,52,52	1.56	6 (15%)	51,81,81	1.91	11 (21%)

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	06S	C	901	-	-	5/22/62/62	0/5/5/5
7	UPT	D	904	-	-	0/6/32/32	0/3/3/3
8	NAG	A	913	1	-	0/6/23/26	0/1/1/1
8	NAG	D	908	1	-	1/6/23/26	0/1/1/1
8	NAG	B	911	1	-	0/6/23/26	0/1/1/1
5	URI	B	901	-	-	4/6/22/22	0/2/2/2
5	URI	D	901	-	-	4/6/22/22	0/2/2/2
7	UPT	B	903	-	-	0/6/32/32	0/3/3/3
7	UPT	C	902	-	-	0/6/32/32	0/3/3/3
6	06S	D	903	-	-	7/22/62/62	0/5/5/5
5	URI	D	902	-	-	3/6/22/22	0/2/2/2
5	URI	A	901	-	-	3/6/22/22	0/2/2/2
7	UPT	A	903	-	-	0/6/32/32	0/3/3/3
6	06S	B	902	-	-	6/22/62/62	0/5/5/5
6	06S	A	902	-	-	11/22/62/62	0/5/5/5

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	902	06S	C10-C12	-6.36	1.35	1.47
6	C	901	06S	C10-C12	-4.79	1.38	1.47
6	D	903	06S	C10-C12	-4.54	1.38	1.47
6	B	902	06S	C10-C12	-4.31	1.39	1.47
6	D	903	06S	C18-N	3.93	1.44	1.38
6	D	903	06S	P-O5	2.97	1.53	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	902	06S	P2-O11	2.87	1.52	1.46
7	A	903	UPT	C7-N1	-2.80	1.33	1.38
7	D	904	UPT	C8-N	2.80	1.42	1.38
6	D	903	06S	P2-O11	2.74	1.52	1.46
7	C	902	UPT	C7-N1	-2.58	1.34	1.38
6	B	902	06S	P-O5	2.56	1.52	1.46
7	A	903	UPT	C8-N	2.55	1.42	1.38
6	C	901	06S	P2-O11	2.50	1.52	1.46
6	A	902	06S	P2-O11	2.47	1.52	1.46
6	C	901	06S	C18-N	2.45	1.42	1.38
7	B	903	UPT	C7-N1	-2.44	1.34	1.38
6	A	902	06S	C12-N3	-2.43	1.33	1.38
6	C	901	06S	P-O5	2.42	1.51	1.46
6	D	903	06S	C16-C15	2.41	1.40	1.35
7	D	904	UPT	C7-N1	-2.40	1.34	1.38
6	B	902	06S	P2-O12	-2.27	1.51	1.56
7	A	903	UPT	C6-N	-2.24	1.32	1.38
6	B	902	06S	C18-N	2.22	1.41	1.38
6	C	901	06S	C17-N6	-2.21	1.34	1.38
7	A	903	UPT	C5-C7	-2.17	1.39	1.43
7	A	903	UPT	C8-N1	-2.16	1.34	1.38
7	B	903	UPT	C6-C5	2.14	1.40	1.35
6	A	902	06S	P-O5	2.14	1.51	1.46
6	C	901	06S	C16-C15	2.13	1.40	1.35
6	D	903	06S	P2-O12	-2.11	1.51	1.56
6	A	902	06S	O6-C5	2.08	1.43	1.40
7	C	902	UPT	C6-C5	2.06	1.39	1.35
6	B	902	06S	C12-N3	-2.05	1.34	1.38
7	B	903	UPT	C8-N1	-2.03	1.34	1.38
6	A	902	06S	P2-O12	-2.03	1.51	1.56
7	A	903	UPT	C6-C5	2.00	1.39	1.35

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	902	06S	C17-N6-C18	-5.77	119.45	126.61
6	C	901	06S	O4-P-O5	5.54	121.95	109.86
7	A	903	UPT	C7-N1-C8	-5.49	119.80	126.61
6	B	902	06S	C17-N6-C18	-5.47	119.82	126.61
7	D	904	UPT	C7-N1-C8	-5.39	119.92	126.61
6	D	903	06S	O4-P-O5	5.35	121.52	109.86
7	A	903	UPT	N1-C8-N	5.19	121.65	114.89

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	902	06S	O12-P2-O11	5.06	120.90	109.86
7	B	903	UPT	C7-N1-C8	-5.04	120.35	126.61
6	B	902	06S	N6-C18-N	5.04	121.45	114.89
7	C	902	UPT	C7-N1-C8	-4.93	120.49	126.61
7	D	904	UPT	N1-C8-N	4.91	121.28	114.89
7	C	902	UPT	N1-C8-N	4.87	121.23	114.89
6	A	902	06S	O4-P-O5	4.87	120.48	109.86
6	C	901	06S	C17-N6-C18	-4.80	120.66	126.61
6	C	901	06S	N6-C18-N	4.78	121.12	114.89
6	A	902	06S	C15-C17-N6	4.71	121.40	114.80
6	D	903	06S	N6-C18-N	4.52	120.78	114.89
7	B	903	UPT	N1-C8-N	4.49	120.74	114.89
6	D	903	06S	C17-N6-C18	-4.49	121.04	126.61
7	B	903	UPT	C5-C7-N1	4.29	120.81	114.80
7	C	902	UPT	O4-C8-N	-4.26	117.25	122.80
6	A	902	06S	N6-C18-N	4.15	120.29	114.89
7	D	904	UPT	C5-C7-N1	4.08	120.52	114.80
6	A	902	06S	O12-P2-O11	4.07	118.74	109.86
6	B	902	06S	O4-P-O5	4.04	118.66	109.86
7	A	903	UPT	C5-C7-N1	4.03	120.45	114.80
6	D	903	06S	O12-P2-O11	3.87	118.30	109.86
6	B	902	06S	C15-C17-N6	3.86	120.21	114.80
8	D	908	NAG	C1-O5-C5	3.75	117.21	112.19
6	D	903	06S	C8-O6-C5	-3.62	106.61	109.92
7	C	902	UPT	C5-C7-N1	3.62	119.87	114.80
6	D	903	06S	C15-C17-N6	3.46	119.65	114.80
7	C	902	UPT	O3-C7-C5	-3.33	119.42	125.16
6	C	901	06S	O12-P2-O11	3.33	117.12	109.86
6	A	902	06S	O14-C17-C15	-3.30	119.47	125.16
6	A	902	06S	C8-O6-C5	-3.28	106.92	109.92
7	D	904	UPT	O3-C7-C5	-3.27	119.53	125.16
7	A	903	UPT	O3-C7-C5	-3.26	119.53	125.16
6	C	901	06S	C15-C17-N6	3.21	119.29	114.80
6	D	903	06S	O6-C5-N1	3.03	112.76	108.75
6	B	902	06S	C14-N4-C10	2.95	107.58	102.55
8	D	908	NAG	O5-C5-C6	-2.94	101.94	107.66
6	C	901	06S	C14-N4-C10	2.92	107.53	102.55
8	B	911	NAG	C3-C4-C5	2.78	115.27	110.23
6	D	903	06S	C14-N4-C10	2.71	107.17	102.55
6	D	903	06S	C-N-C18	2.70	122.44	117.59
6	D	903	06S	O15-C18-N6	-2.66	116.59	121.49
7	B	903	UPT	O3-C7-C5	-2.61	120.66	125.16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	903	06S	C16-N-C18	-2.61	117.83	121.00
6	B	902	06S	O14-C17-C15	-2.52	120.82	125.16
6	C	901	06S	O14-C17-C15	-2.50	120.85	125.16
7	B	903	UPT	O4-C8-N	-2.49	119.56	122.80
6	B	902	06S	C8-O6-C5	-2.47	107.66	109.92
7	A	903	UPT	C6-N-C8	-2.42	118.05	121.00
8	D	908	NAG	O4-C4-C5	2.37	115.15	109.32
6	D	903	06S	O14-C17-C15	-2.34	121.13	125.16
6	C	901	06S	C8-O6-C5	-2.32	107.80	109.92
6	A	902	06S	C14-N4-C10	2.31	106.48	102.55
6	A	902	06S	O-C-N	2.22	113.40	108.36
7	D	904	UPT	C-N-C8	2.22	121.57	117.59
6	A	902	06S	O15-C18-N	-2.18	119.96	122.80
6	C	901	06S	C16-N-C18	-2.13	118.40	121.00
7	A	903	UPT	C-N-C8	2.10	121.37	117.59
6	D	903	06S	P1-O3-C2	2.07	128.11	121.80
6	A	902	06S	O9-C7-C6	-2.06	104.29	111.68
5	D	901	URI	O3'-C3'-C2'	-2.04	105.27	111.82
7	A	903	UPT	O4-C8-N	-2.01	120.19	122.80
5	A	901	URI	O3'-C3'-C4'	2.00	116.83	111.08

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	902	06S	C2-C3-C4-O1
6	A	902	06S	O-C3-C4-O1
6	A	902	06S	C4-O1-P-O4
6	B	902	06S	C4-O1-P-O5
6	C	901	06S	C2-O3-P1-O10
6	C	901	06S	C2-C3-C4-O1
6	C	901	06S	O-C3-C4-O1
6	C	901	06S	C4-O1-P-O4
6	D	903	06S	C2-O3-P1-O10
6	D	903	06S	O-C3-C4-O1
6	D	903	06S	C2-C3-C4-O1
5	B	901	URI	O4'-C1'-N1-C2
5	D	902	URI	O4'-C1'-N1-C2
5	D	901	URI	O4'-C4'-C5'-O5'
6	A	902	06S	C3-C2-O3-P1
6	A	902	06S	C1-C2-O3-P1
6	B	902	06S	C3-C2-O3-P1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	B	902	06S	C1-C2-O3-P1
5	D	901	URI	C3'-C4'-C5'-O5'
5	B	901	URI	O4'-C4'-C5'-O5'
5	D	902	URI	O4'-C1'-N1-C6
6	A	902	06S	O6-C8-C9-O7
8	D	908	NAG	O5-C5-C6-O6
6	A	902	06S	C2-O3-P1-O10
6	B	902	06S	C2-O3-P1-O10
5	B	901	URI	O4'-C1'-N1-C6
6	D	903	06S	C9-O7-P1-O3
6	A	902	06S	C7-C8-C9-O7
6	A	902	06S	C4-O1-P-O5
6	C	901	06S	C4-O1-P-O5
5	D	901	URI	O4'-C1'-N1-C6
6	B	902	06S	O-C3-C4-O1
5	D	902	URI	O4'-C4'-C5'-O5'
6	A	902	06S	C8-C7-O9-P2
5	B	901	URI	C3'-C4'-C5'-O5'
5	A	901	URI	O4'-C1'-N1-C6
6	D	903	06S	C1-C2-O3-P1
5	D	901	URI	O4'-C1'-N1-C2
6	D	903	06S	C3-C2-O3-P1
6	D	903	06S	C9-O7-P1-O10
5	A	901	URI	O4'-C1'-N1-C2
6	A	902	06S	C6-C7-O9-P2
6	B	902	06S	C7-O9-P2-O12
5	A	901	URI	C2'-C1'-N1-C2

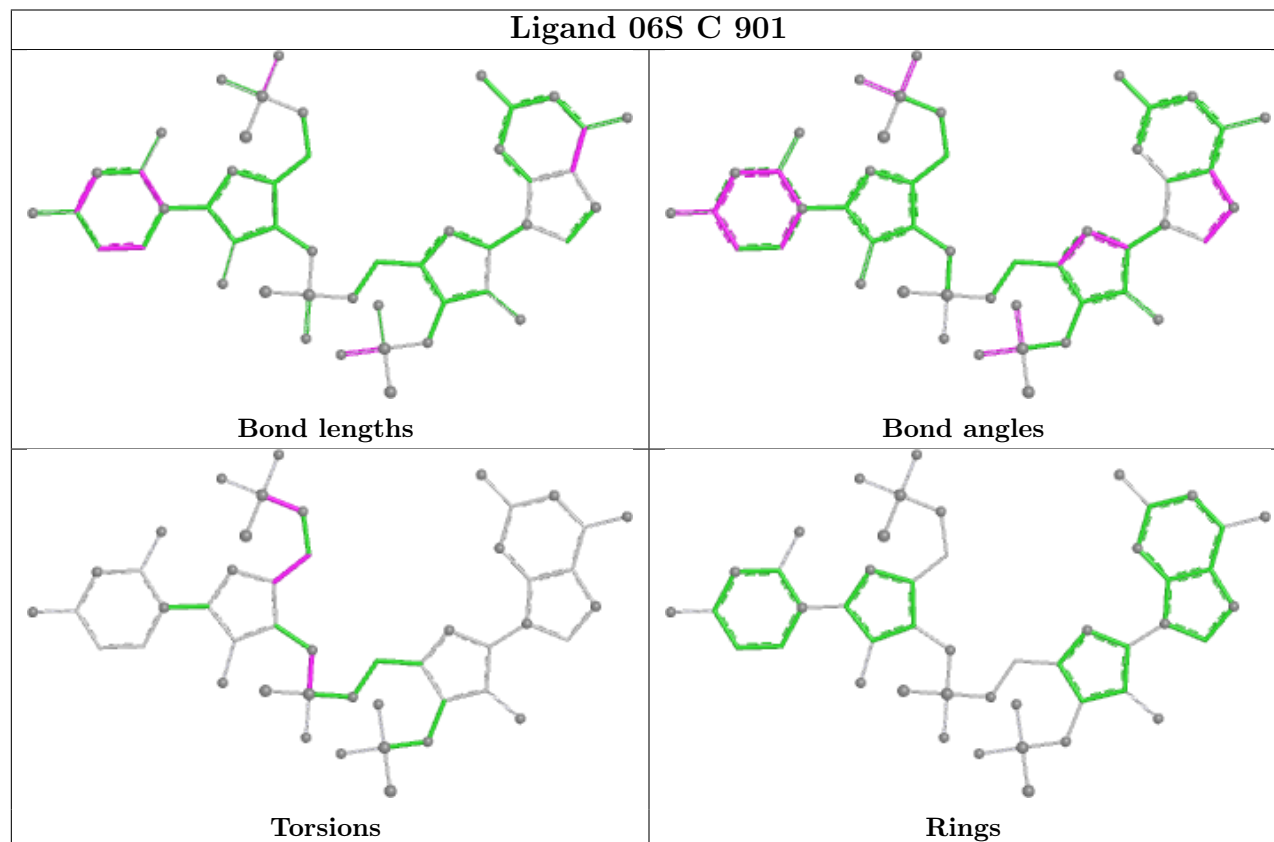
There are no ring outliers.

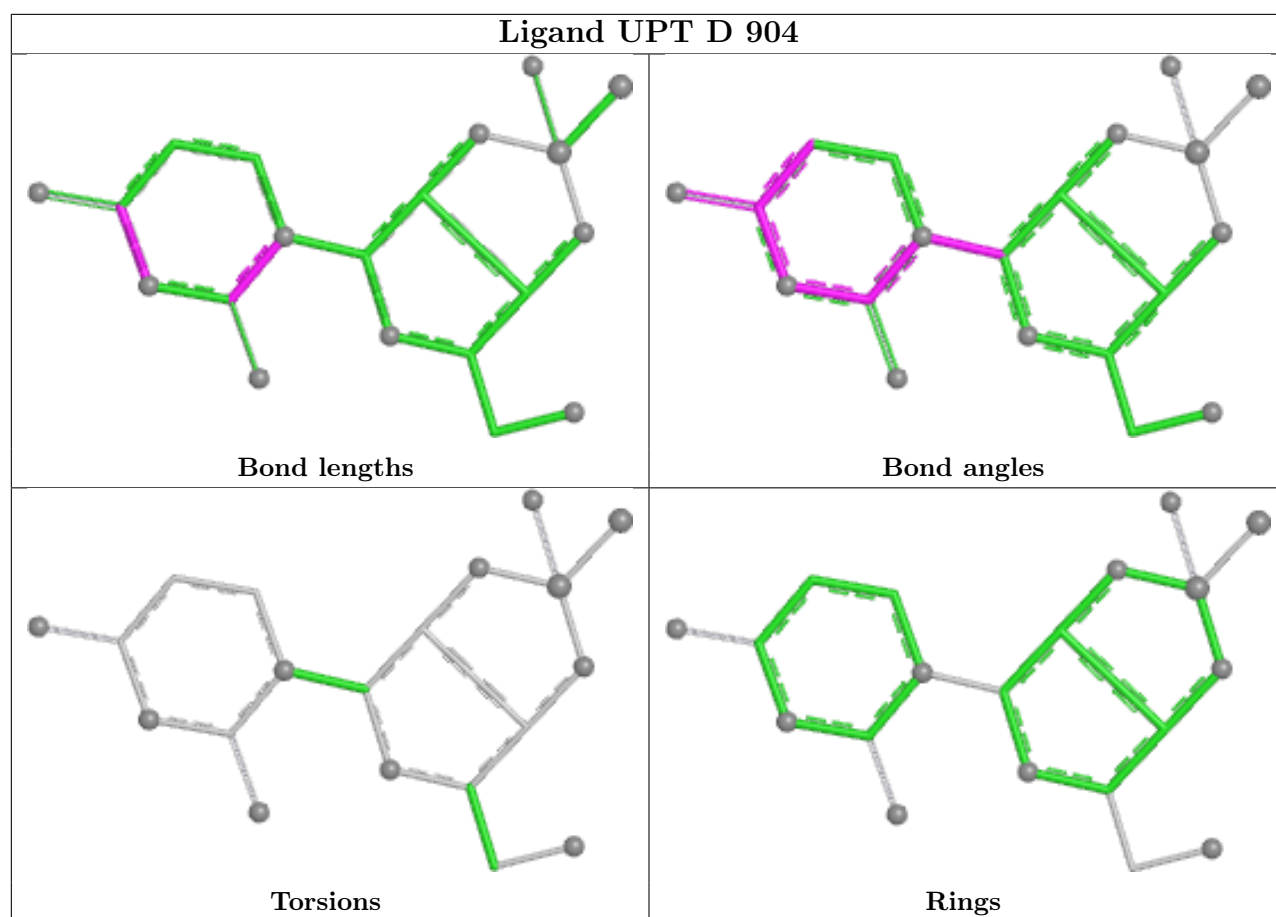
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	904	UPT	4	0
5	D	901	URI	1	0
7	C	902	UPT	1	0
6	D	903	06S	1	0
5	D	902	URI	2	0

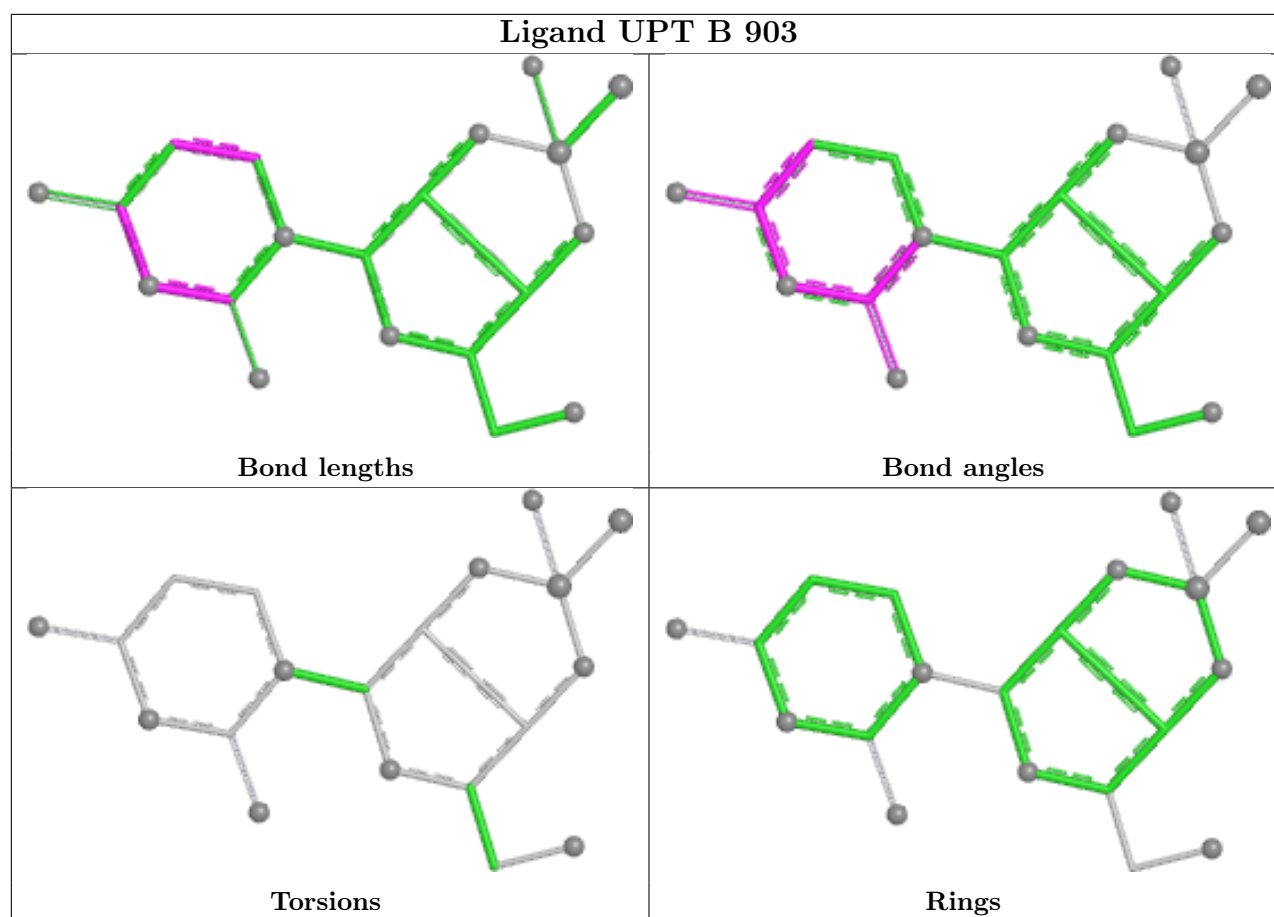
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

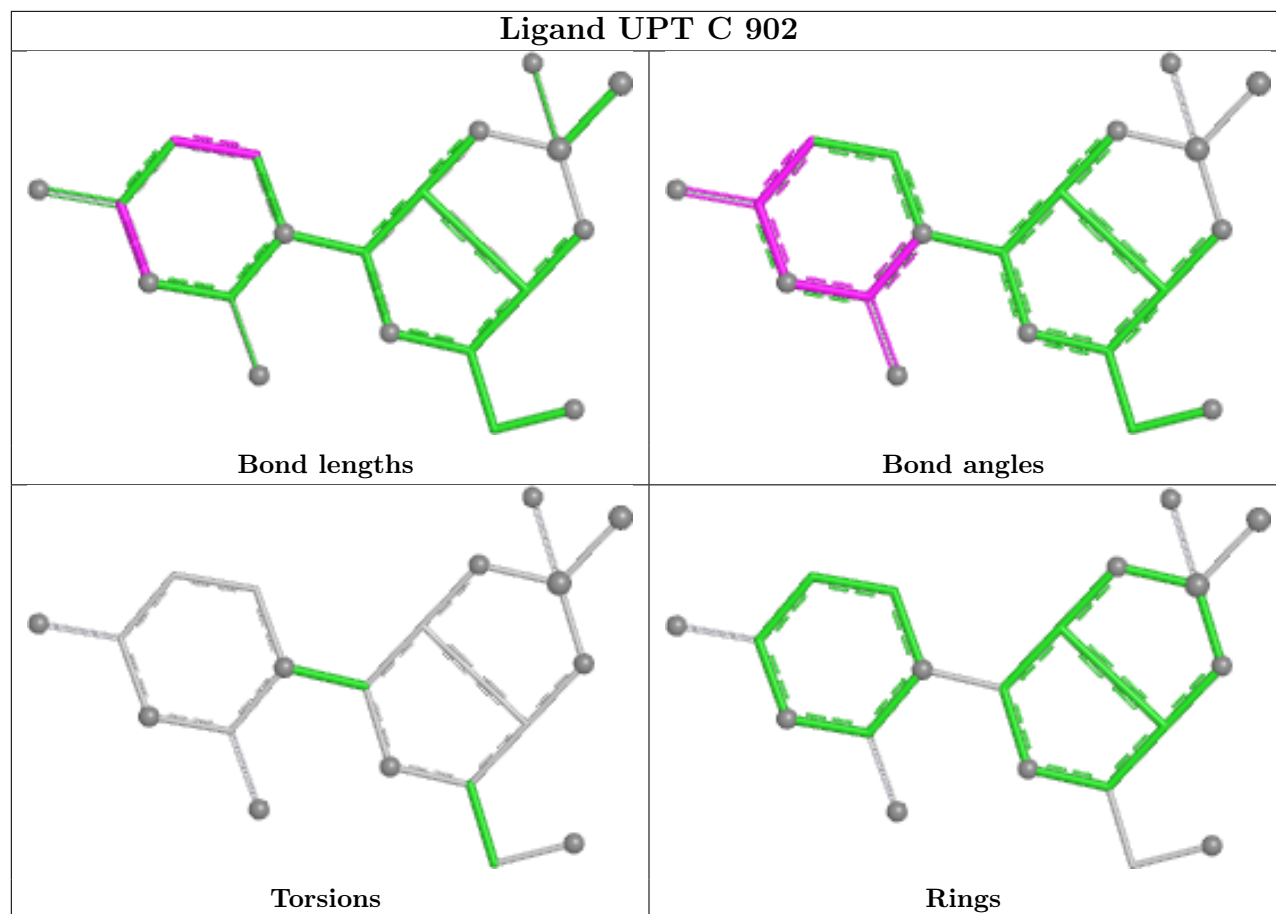




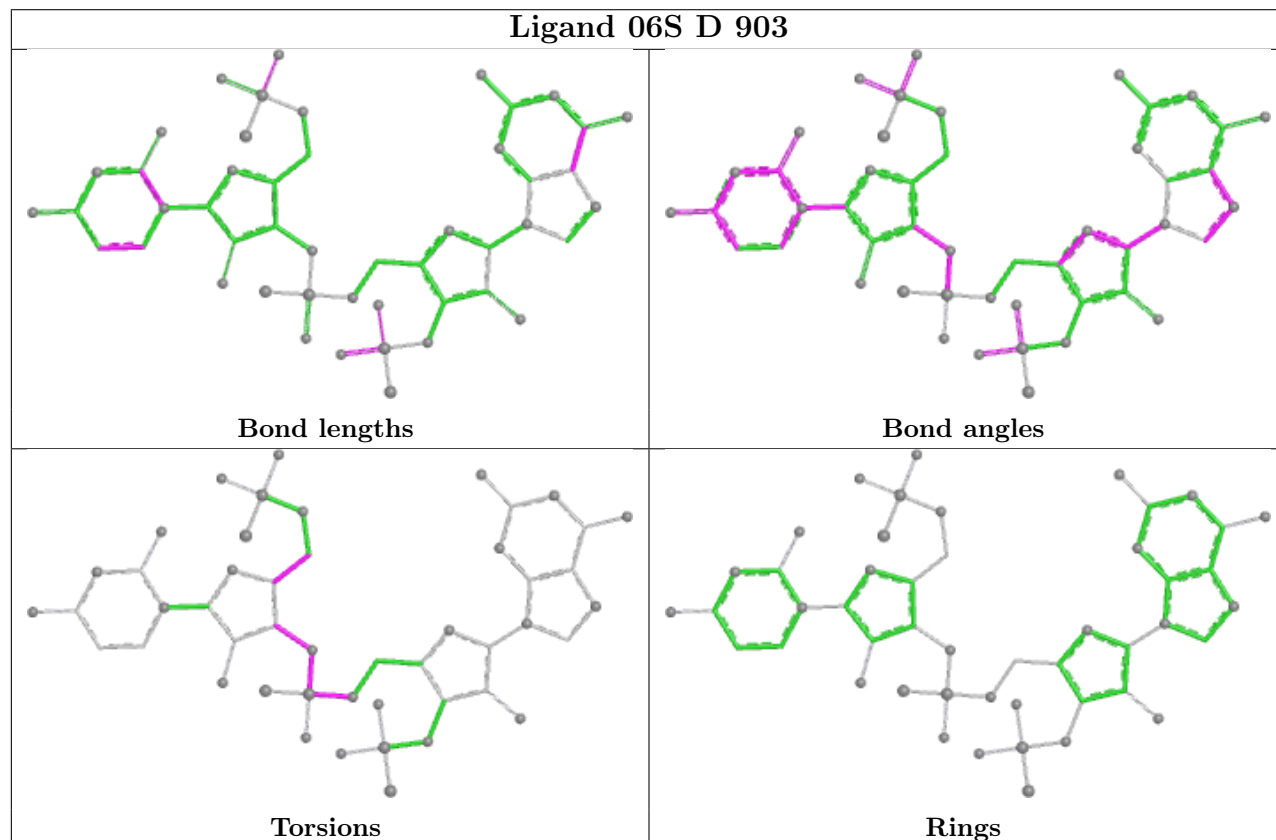


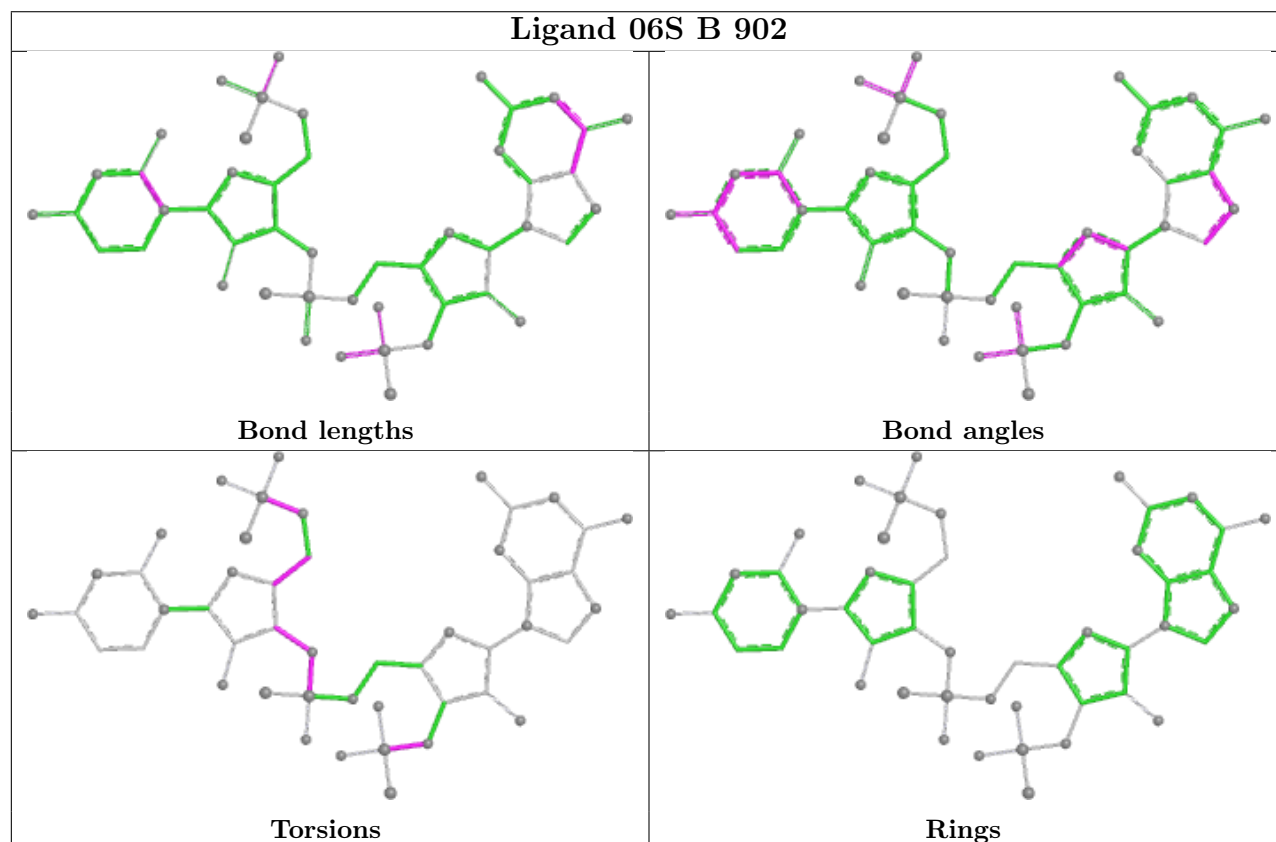
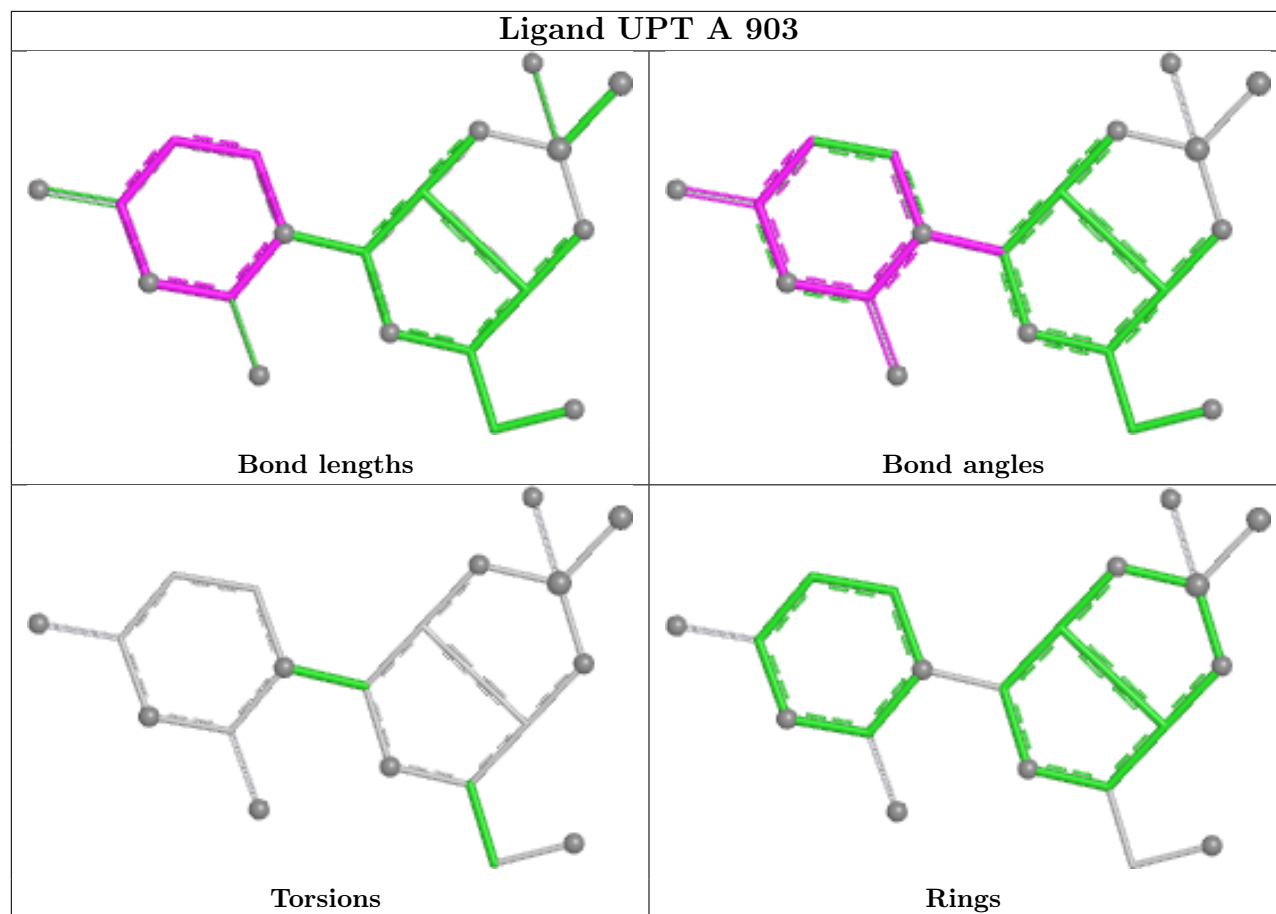


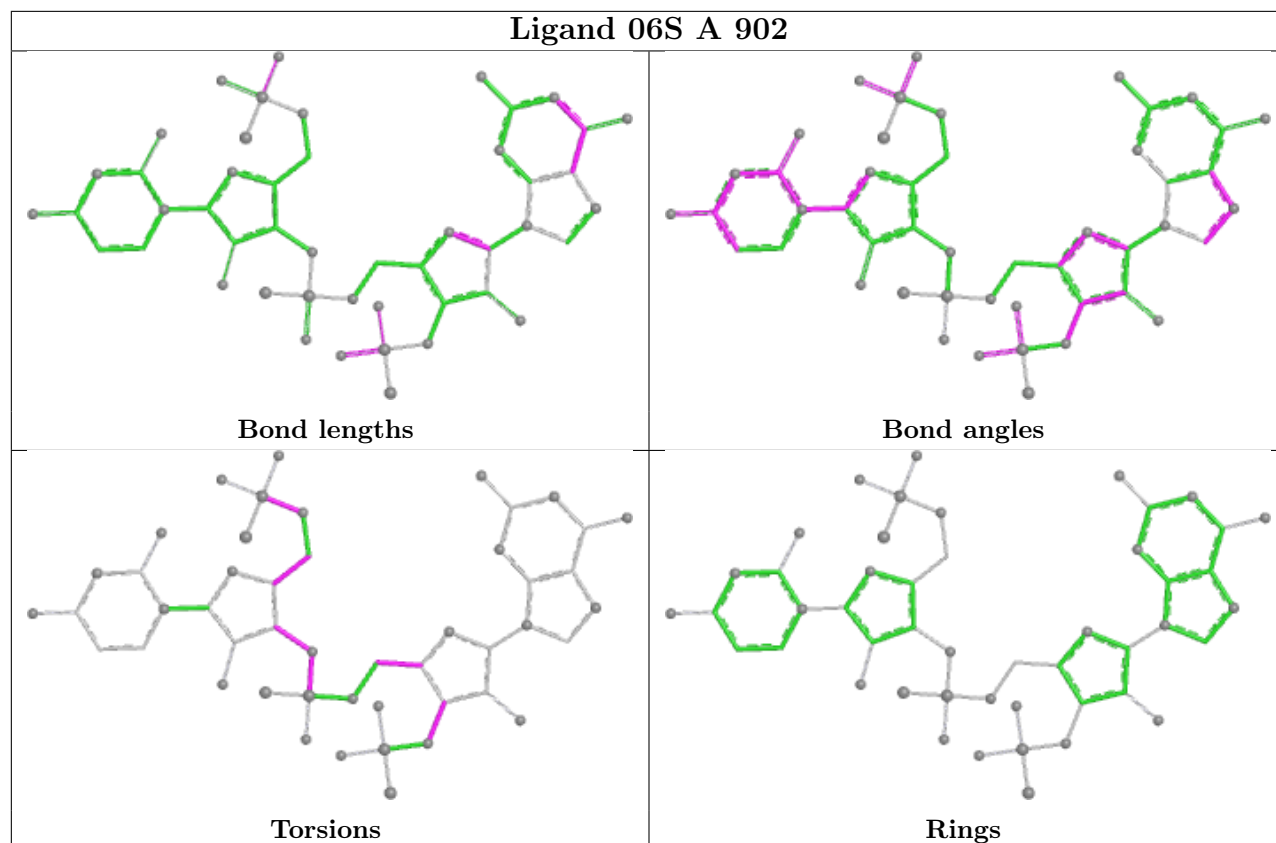
## Ligand UPT C 902



## Ligand 06S D 903







## 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	749/811 (92%)	-0.40	7 (0%) 81 77	29, 48, 83, 114	0
1	B	752/811 (92%)	-0.20	10 (1%) 74 71	29, 55, 99, 138	0
1	C	746/811 (91%)	0.04	16 (2%) 63 59	36, 65, 119, 170	0
1	D	746/811 (91%)	0.12	18 (2%) 59 55	37, 73, 118, 184	0
All	All	2993/3244 (92%)	-0.11	51 (1%) 69 65	29, 59, 110, 184	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	678	PHE	5.1
1	B	819	LEU	4.8
1	D	307	PHE	4.6
1	A	433	LEU	4.5
1	D	780	ILE	4.3
1	C	762	THR	4.3
1	C	760	THR	3.9
1	D	751	ILE	3.9
1	C	100	VAL	3.7
1	B	732	LEU	3.5
1	D	121	PHE	3.4
1	C	588	VAL	3.2
1	C	817	LEU	3.1
1	C	239	GLU	3.1
1	B	761	THR	3.0
1	D	74	PHE	2.9
1	D	753	LYS	2.8
1	D	678	PHE	2.7
1	D	124	LEU	2.7
1	A	761	THR	2.7
1	C	809	GLN	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	734	GLU	2.5
1	A	819	LEU	2.5
1	C	732	LEU	2.5
1	A	100	VAL	2.5
1	B	757	GLU	2.4
1	B	100	VAL	2.4
1	D	92	ILE	2.4
1	D	464	HIS	2.3
1	D	732	LEU	2.3
1	B	735	VAL	2.2
1	A	678	PHE	2.2
1	D	72	ASP	2.2
1	B	284	GLN	2.2
1	C	40	GLN	2.2
1	D	214	SER	2.2
1	C	756	LEU	2.2
1	C	758	THR	2.1
1	D	795	ILE	2.1
1	A	732	LEU	2.1
1	D	433	LEU	2.1
1	B	416	ASN	2.1
1	C	726	HIS	2.1
1	C	38	LYS	2.1
1	B	758	THR	2.1
1	C	774	PHE	2.0
1	A	39	LYS	2.0
1	C	776	CYS	2.0
1	D	60	THR	2.0
1	D	729	SER	2.0
1	D	816	SER	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 ⓘ

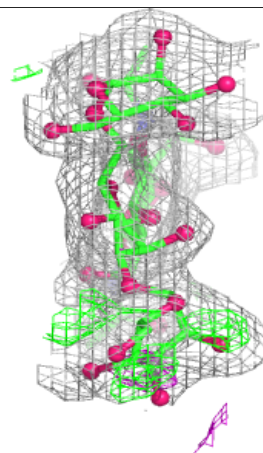
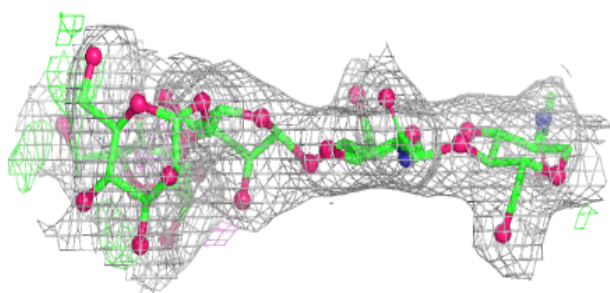
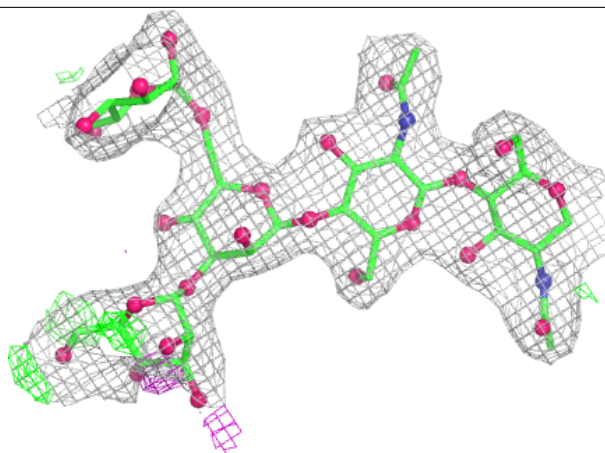
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MAN	E	4	11/12	0.69	0.19	54,70,80,83	0
2	MAN	K	5	11/12	0.73	0.10	70,72,77,78	0
2	MAN	K	4	11/12	0.79	0.12	61,67,75,87	0
4	BMA	N	3	11/12	0.80	0.09	61,70,73,77	0
4	BMA	L	3	11/12	0.83	0.10	73,80,84,89	0
4	BMA	H	3	11/12	0.83	0.10	48,54,57,60	0
2	MAN	E	5	11/12	0.85	0.10	59,67,73,75	0
3	NAG	J	2	14/15	0.86	0.10	38,41,49,54	0
3	NAG	O	2	14/15	0.87	0.10	46,50,55,56	0
3	NAG	F	2	14/15	0.87	0.09	46,53,62,62	0
3	NAG	G	2	14/15	0.89	0.08	34,37,40,49	0
3	NAG	I	2	14/15	0.89	0.09	48,55,66,67	0
2	BMA	K	3	11/12	0.89	0.07	52,59,66,70	0
3	NAG	M	2	14/15	0.89	0.09	42,49,57,59	0
3	NAG	M	1	14/15	0.91	0.09	49,55,61,66	0
2	BMA	E	3	11/12	0.91	0.08	46,56,64,64	0
4	NAG	N	2	14/15	0.92	0.10	53,57,63,65	0
4	NAG	L	2	14/15	0.92	0.09	55,64,74,82	0
3	NAG	G	1	14/15	0.93	0.07	30,36,41,42	0
3	NAG	J	1	14/15	0.94	0.06	36,40,41,42	0
2	NAG	K	1	14/15	0.95	0.09	40,43,46,46	0
4	NAG	H	1	14/15	0.95	0.08	38,41,44,46	0
4	NAG	N	1	14/15	0.95	0.09	53,58,62,64	0
4	NAG	H	2	14/15	0.95	0.07	42,45,52,52	0
3	NAG	O	1	14/15	0.95	0.07	39,44,49,54	0
4	NAG	L	1	14/15	0.96	0.08	43,45,54,65	0
3	NAG	F	1	14/15	0.96	0.06	34,40,45,50	0
2	NAG	K	2	14/15	0.96	0.07	42,49,54,56	0
2	NAG	E	2	14/15	0.97	0.05	31,36,38,44	0
3	NAG	I	1	14/15	0.97	0.06	33,36,39,39	0
2	NAG	E	1	14/15	0.97	0.06	31,32,37,38	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:**

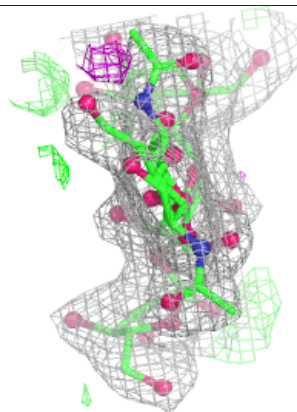
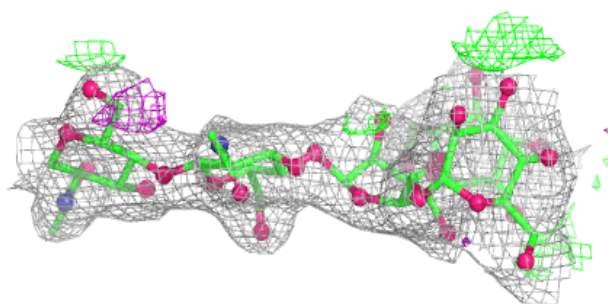
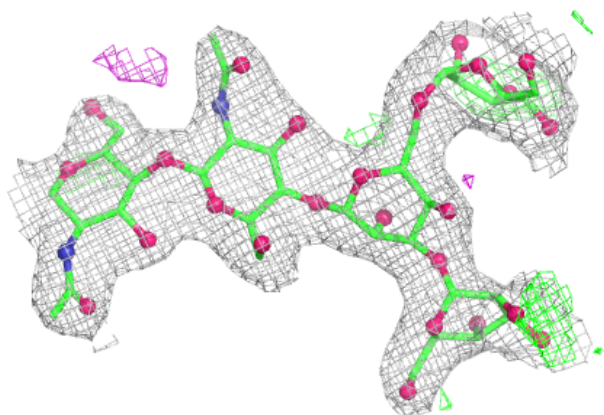
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





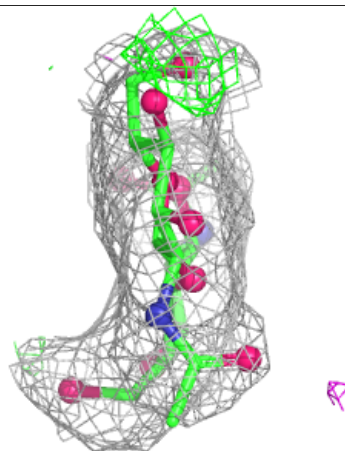
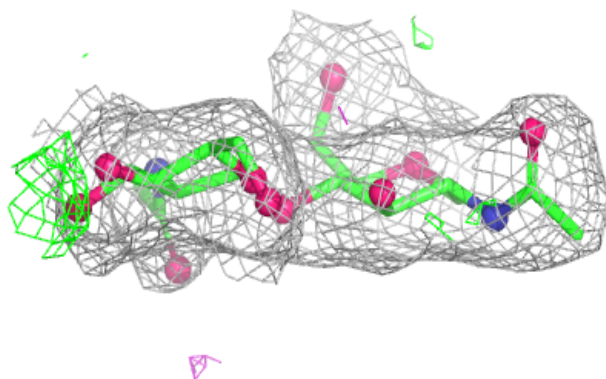
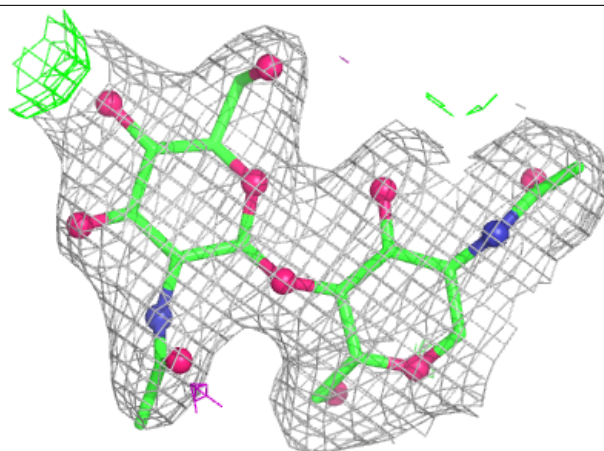
**Electron density around Chain K:**

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



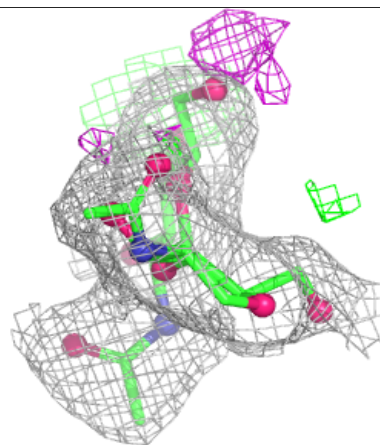
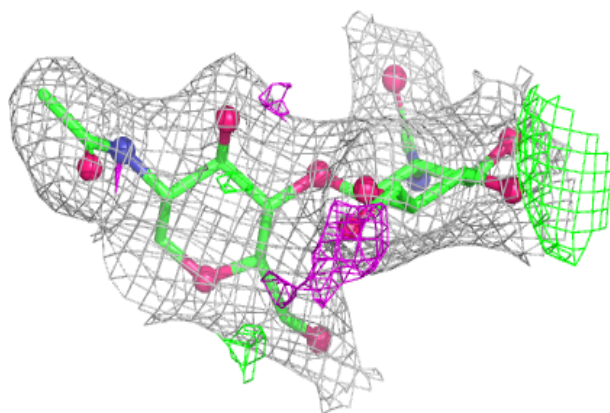
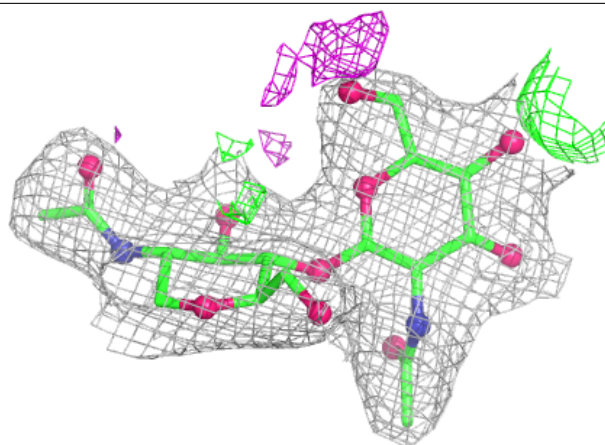
**Electron density around Chain F:**

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



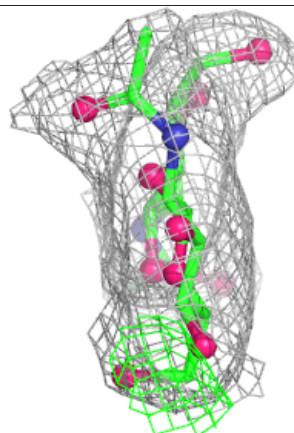
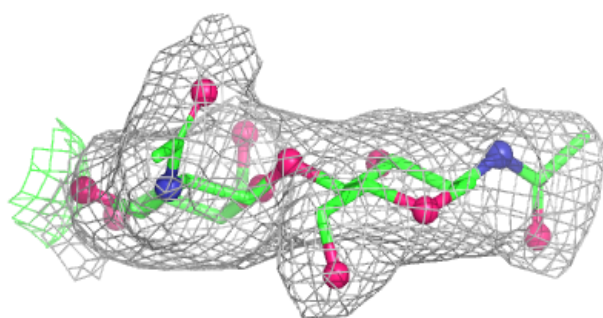
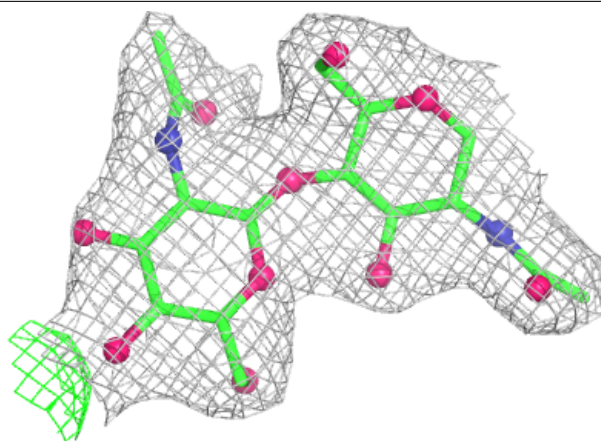
**Electron density around Chain G:**

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



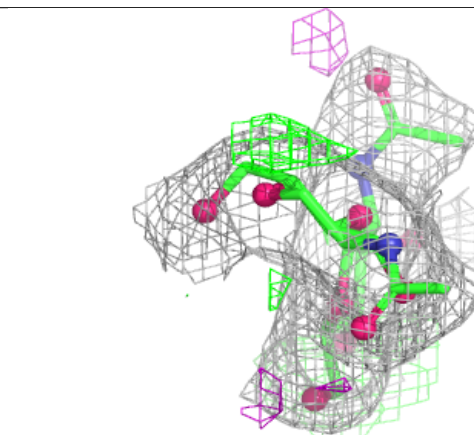
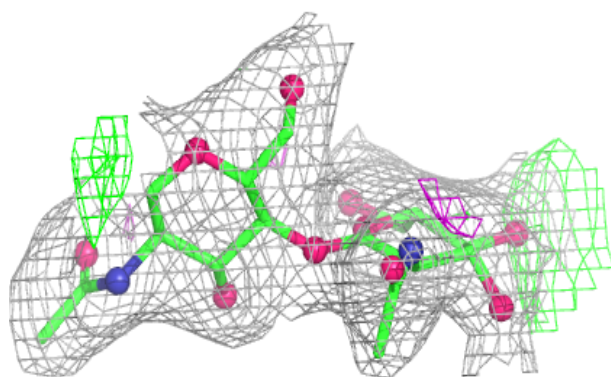
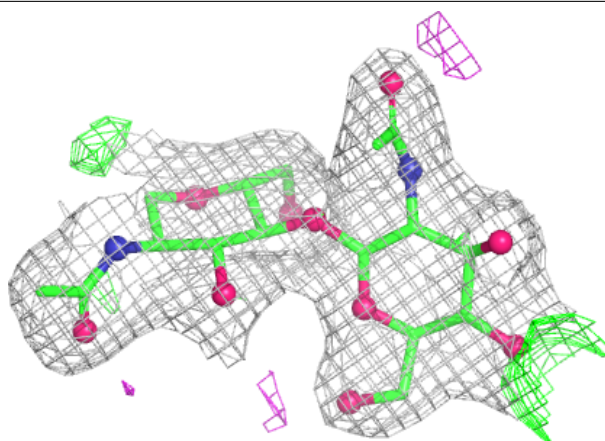
**Electron density around Chain I:**

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

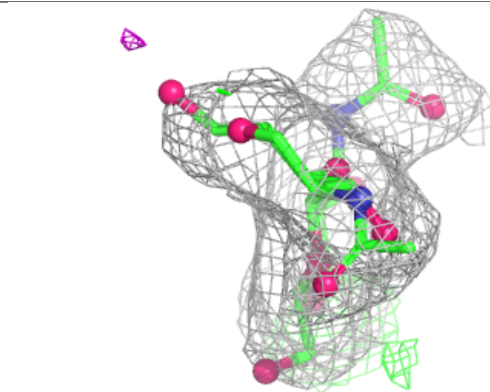
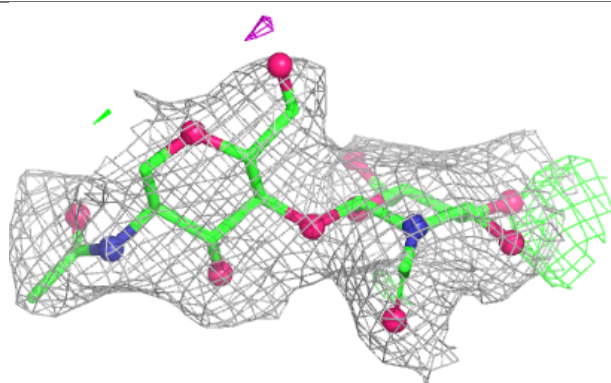
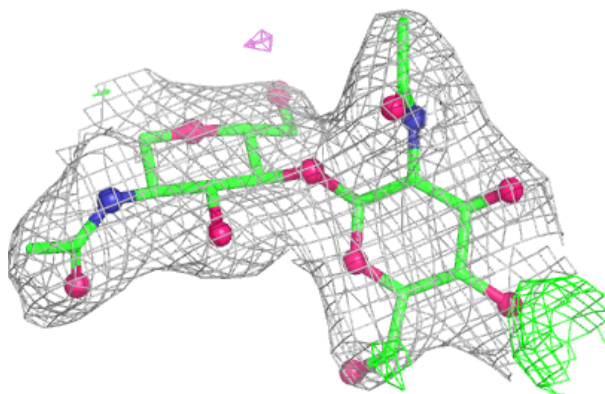


**Electron density around Chain J:**

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

**Electron density around Chain M:**

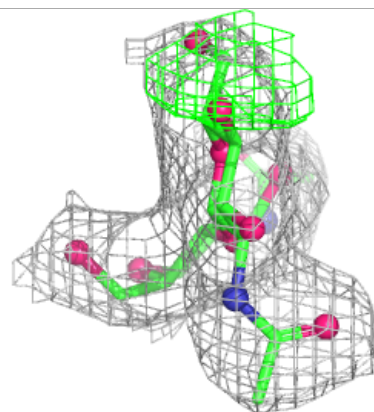
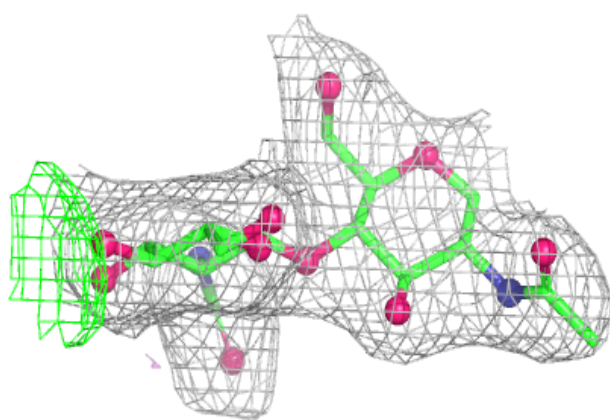
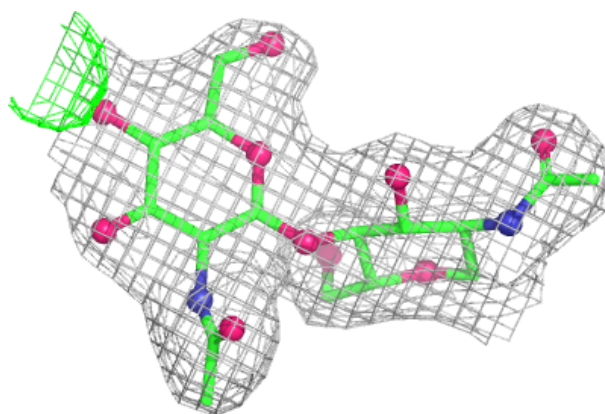
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





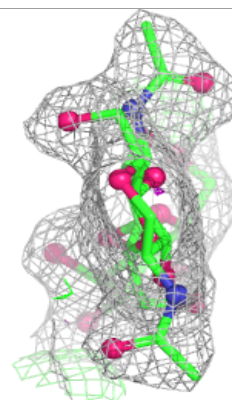
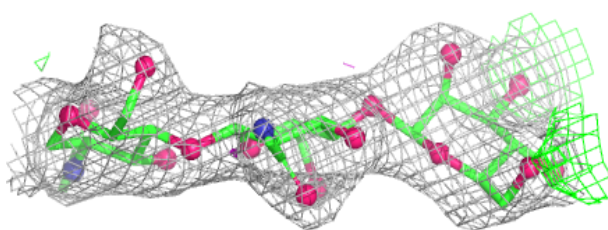
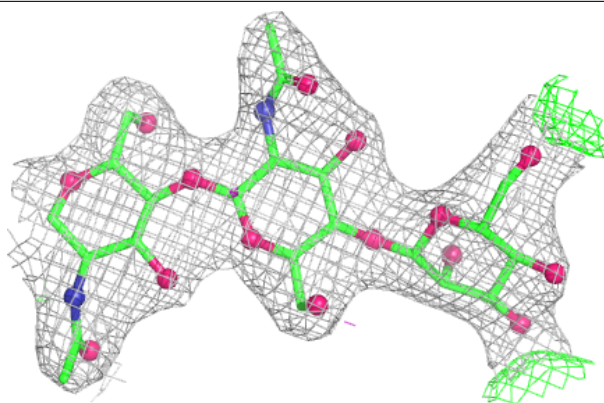
**Electron density around Chain O:**

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

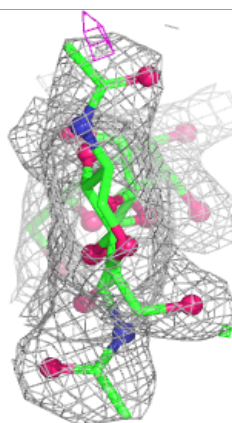
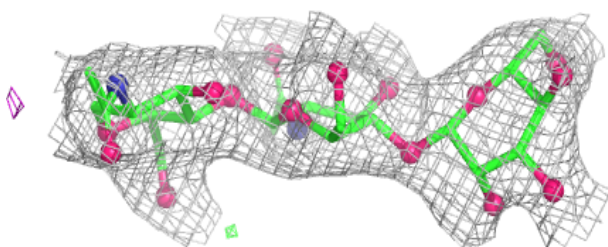
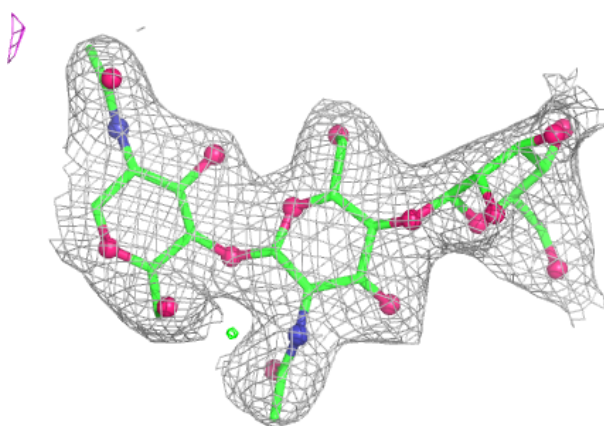


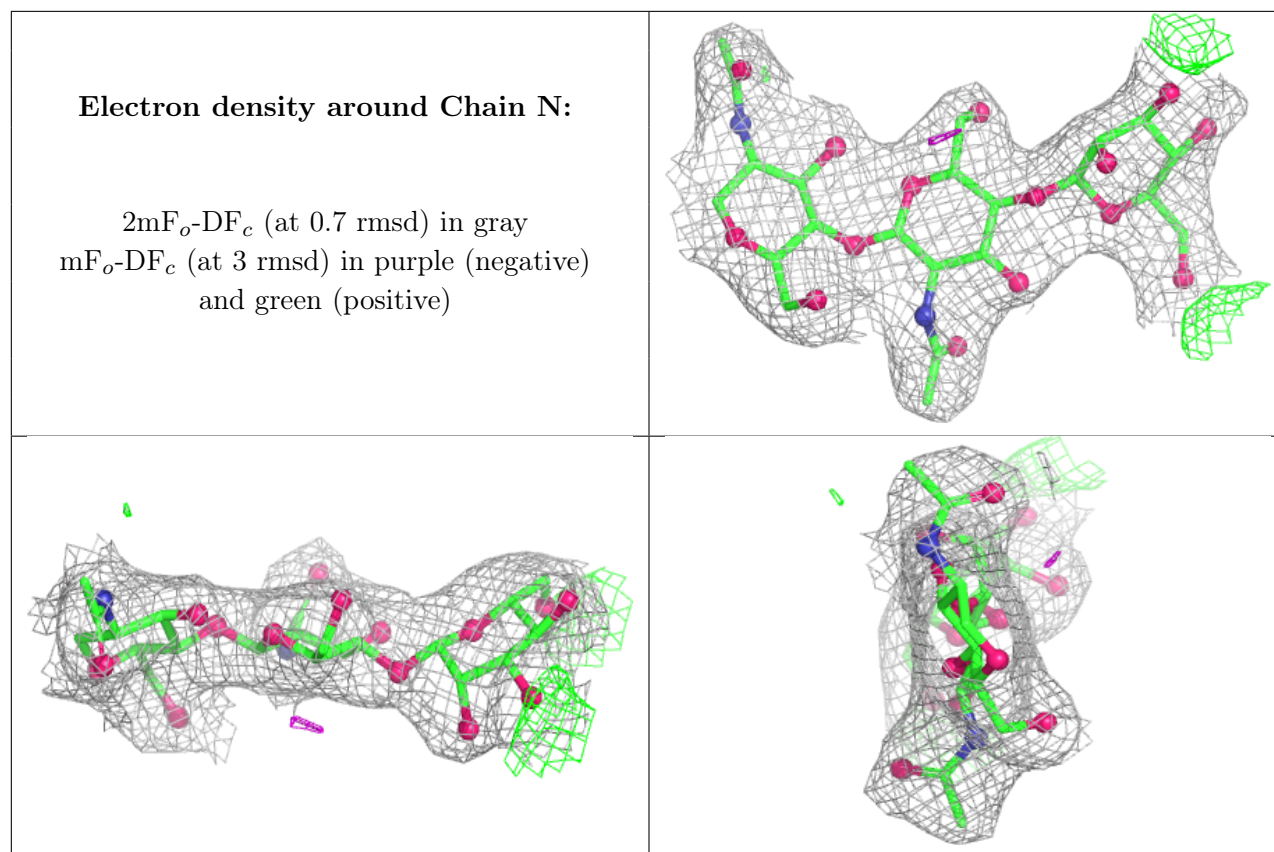
**Electron density around Chain H:**

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

**Electron density around Chain L:**

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





## 6.4 Ligands [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
8	NAG	B	911	14/15	0.86	0.09	56,61,64,64	0
5	URI	D	902	17/17	0.89	0.09	58,64,69,72	0
8	NAG	D	908	14/15	0.89	0.08	42,44,49,54	0
6	06S	D	903	48/48	0.90	0.09	57,70,87,90	0
8	NAG	A	913	14/15	0.90	0.08	56,61,67,70	0
5	URI	A	901	17/17	0.91	0.08	36,40,43,48	0
6	06S	C	901	48/48	0.91	0.08	47,61,77,87	0
5	URI	B	901	17/17	0.91	0.08	34,38,47,53	0
6	06S	B	902	48/48	0.92	0.09	45,59,82,90	0
5	URI	D	901	17/17	0.93	0.08	35,40,45,45	0
6	06S	A	902	48/48	0.94	0.07	36,52,75,87	0
7	UPT	D	904	20/20	0.95	0.07	57,65,75,76	0
7	UPT	A	903	20/20	0.96	0.07	36,40,44,45	0
7	UPT	B	903	20/20	0.97	0.07	37,43,50,52	0

*Continued on next page...*



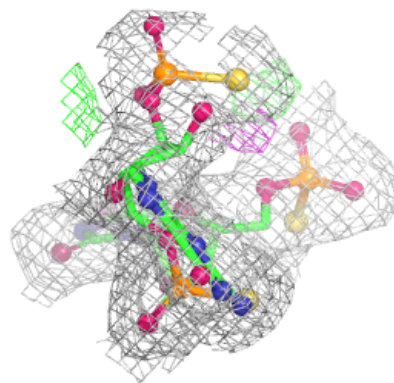
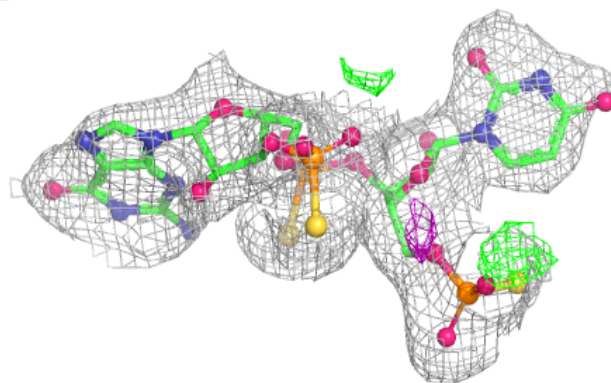
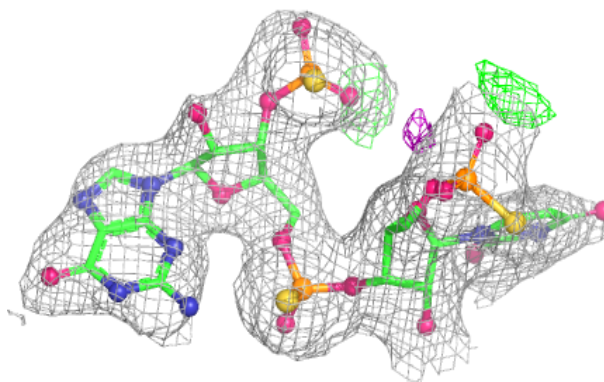
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	UPT	C	902	20/20	0.97	0.06	45,49,58,60	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.

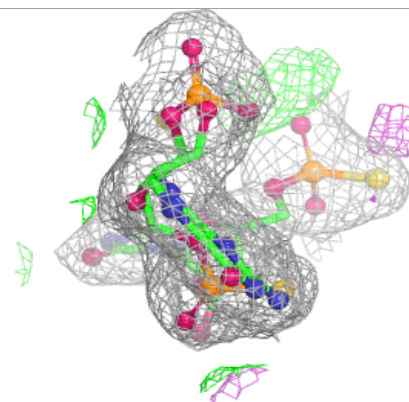
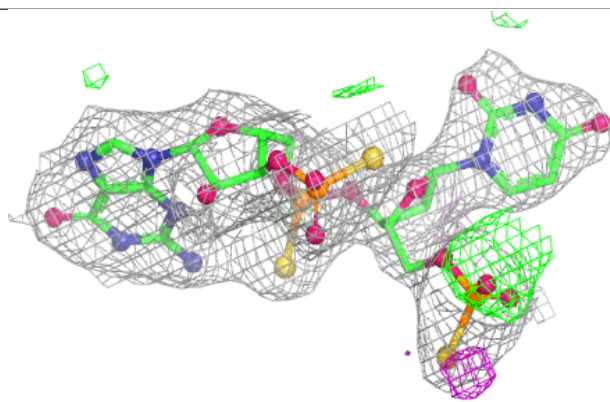
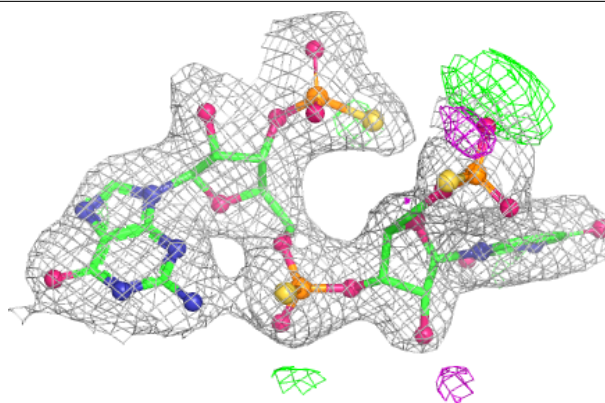
**Electron density around 06S D 903:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

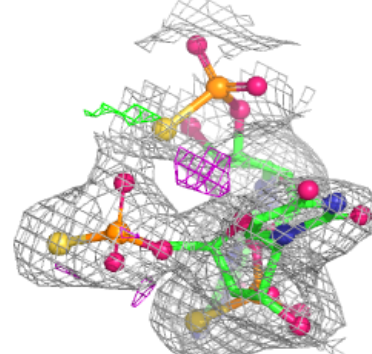
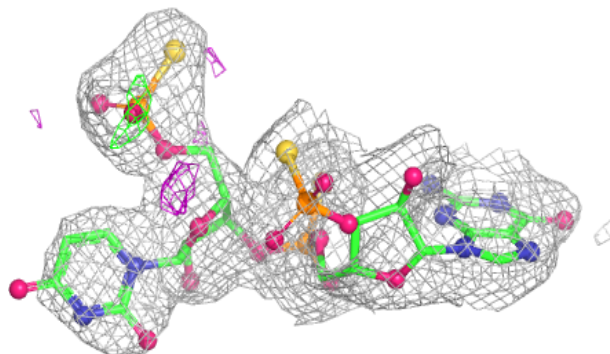
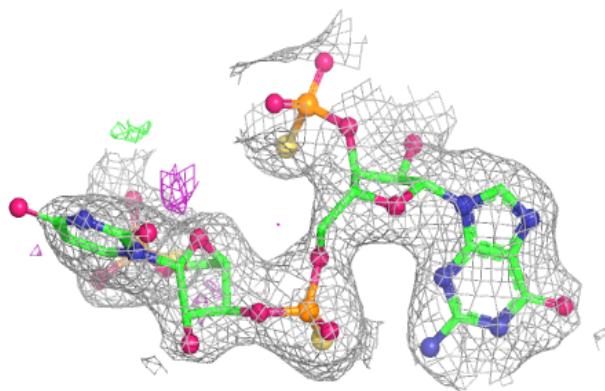


**Electron density around 06S C 901:**

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

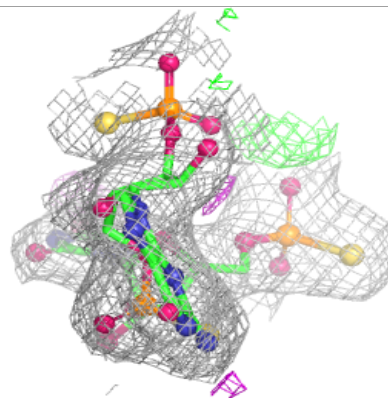
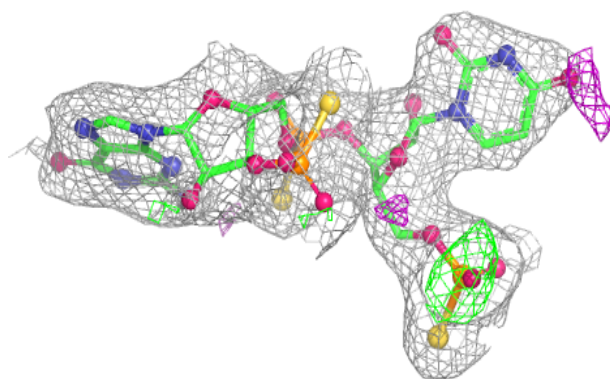
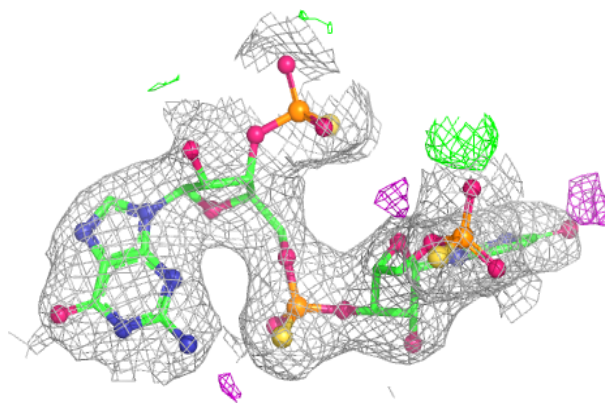
**Electron density around 06S B 902:**

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



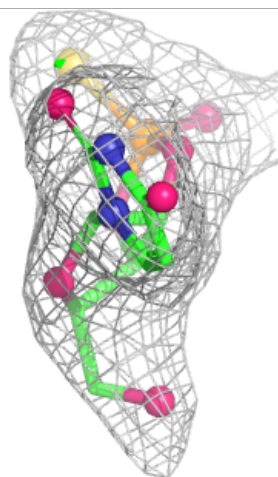
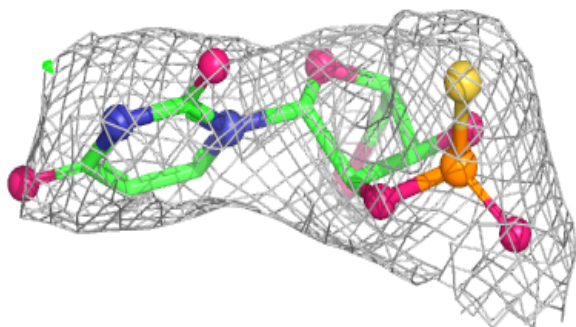
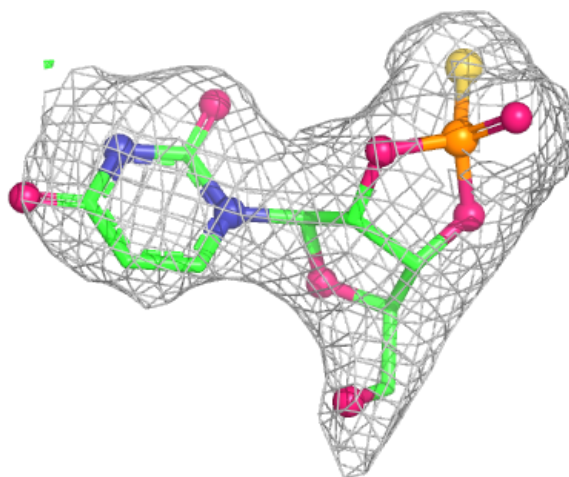
**Electron density around 06S A 902:**

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



**Electron density around UPT D 904:**

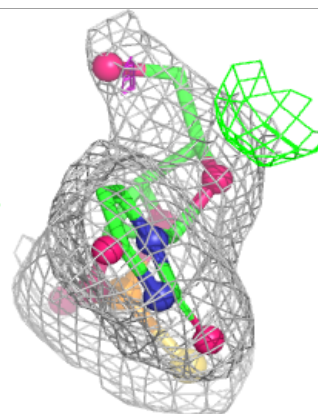
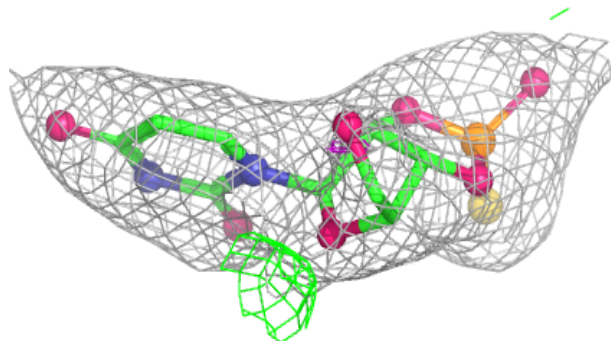
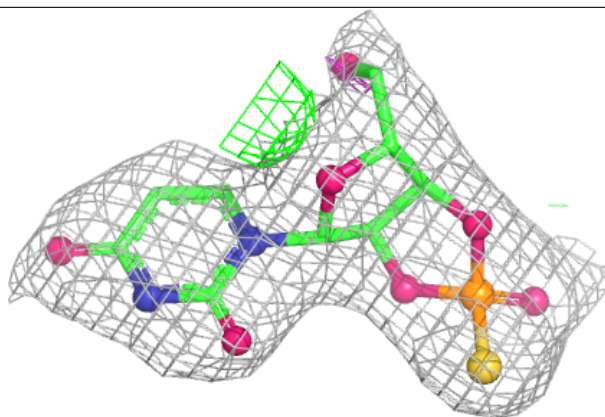
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



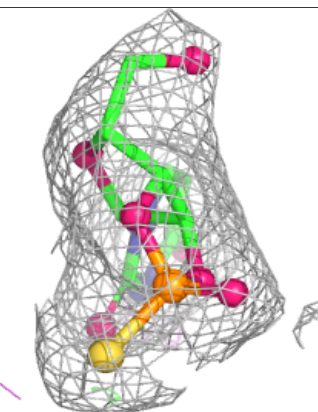
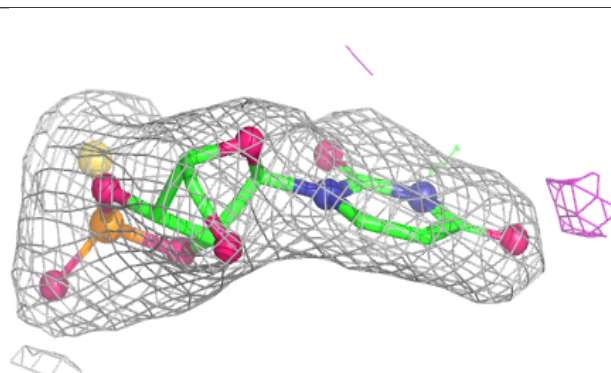
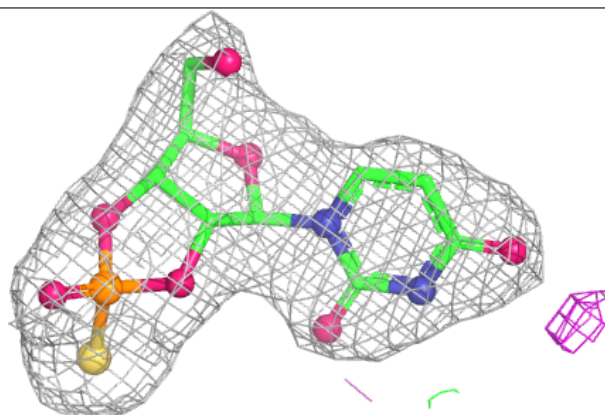


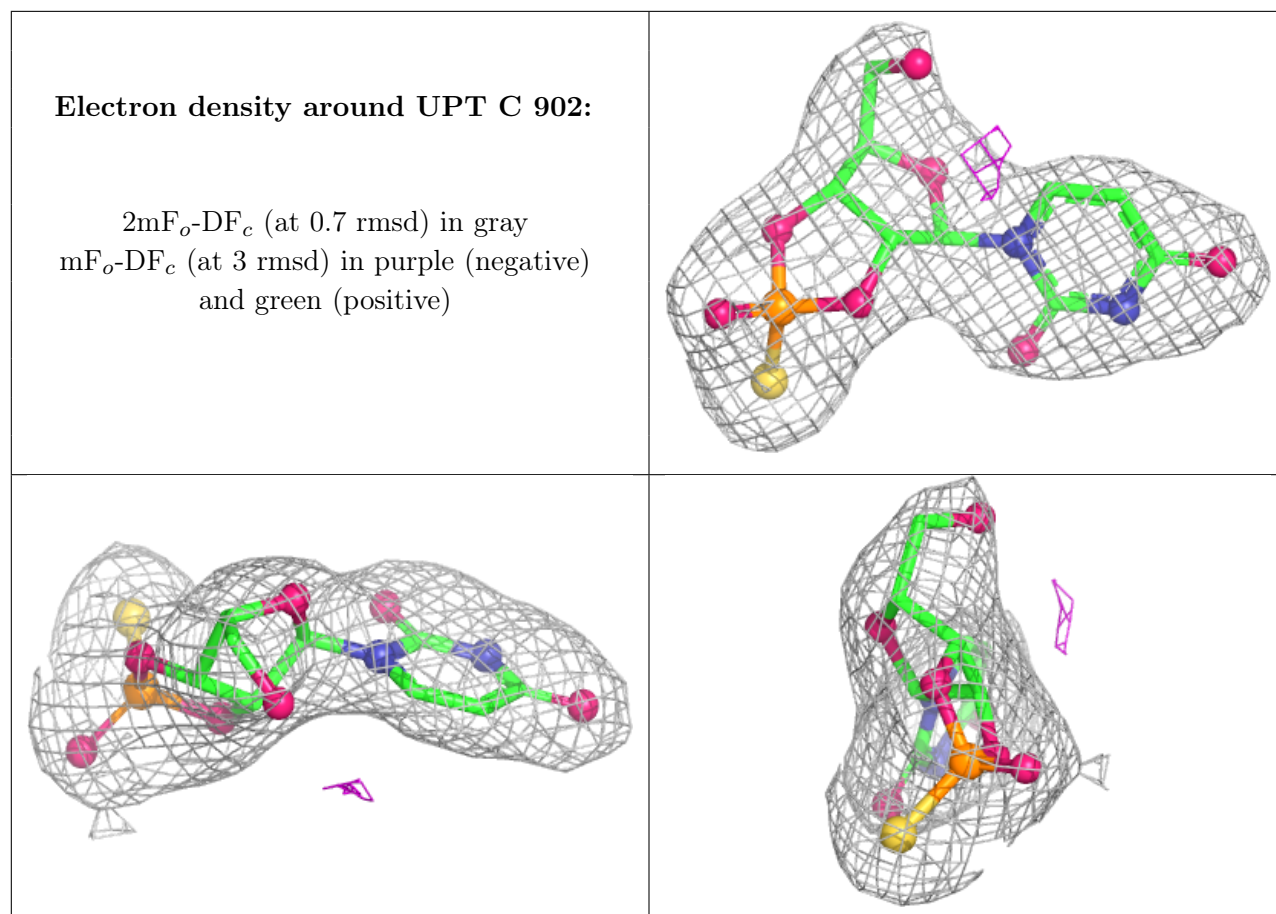
**Electron density around UPT A 903:**

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

**Electron density around UPT B 903:**

$2mF_o-DF_c$  (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.