wwPDB X-ray Structure Validation Summary Report (i)

Jun 22, 2024 – 01:44 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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *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 (i) 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 (i)) were used in the production of this report:

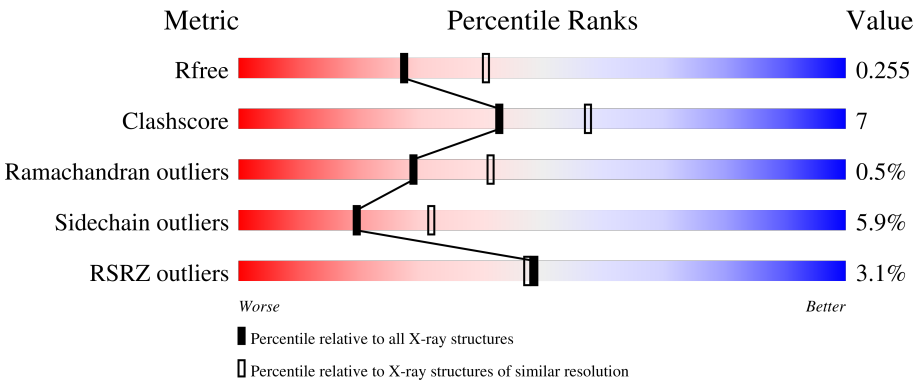
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 >=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 <=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	77% 14% • 8%
1	B	811	% 75% 15% • 9%
1	C	811	6% 66% 20% • 10%
1	D	811	4% 72% 18% • 8%
2	E	3	67% 33%

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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	50% 50%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	743	5992	3835	1017	1121	19	4	0	0
1	B	737	5941	3806	1009	1107	19	4	0	0
1	C	731	5898	3779	1000	1100	19	4	0	0
1	D	743	5989	3834	1016	1120	19	4	0	0

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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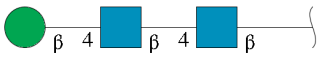
Chain	Residue	Modelled	Actual	Comment	Reference
C	23	SER	-	expression tag	UNP Q9NR97
C	24	PRO	-	expression tag	UNP Q9NR97
C	25	TRP	-	expression tag	UNP Q9NR97
C	828	GLU	-	expression tag	UNP Q9NR97
C	829	PHE	-	expression tag	UNP Q9NR97
C	830	LEU	-	expression tag	UNP Q9NR97
C	831	VAL	-	expression tag	UNP 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
			Total	C	N	O			
2	E	3	39	22	2	15	0	0	0
2	F	3	39	22	2	15	0	0	0
2	H	3	39	22	2	15	0	0	0
2	I	3	39	22	2	15	0	0	0
2	K	3	39	22	2	15	0	0	0
2	L	3	39	22	2	15	0	0	0
2	N	3	39	22	2	15	0	0	0

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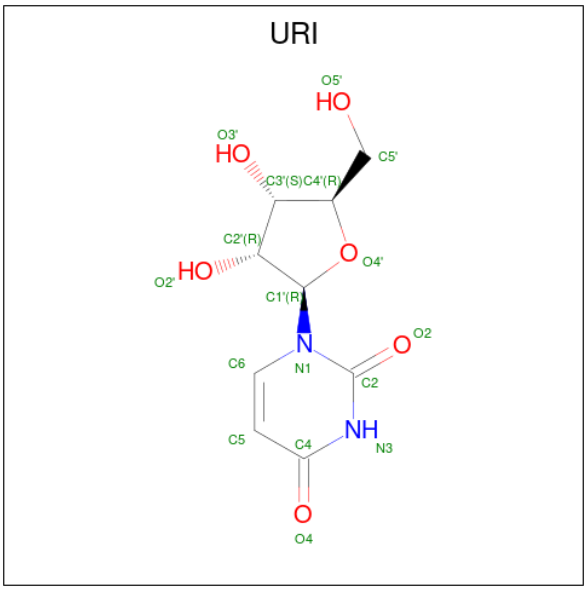
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	O	3	39	22	2	15	0	0	0

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

- Molecule 4 is URIDINE (three-letter code: URI) (formula: $C_9H_{12}N_2O_6$).



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

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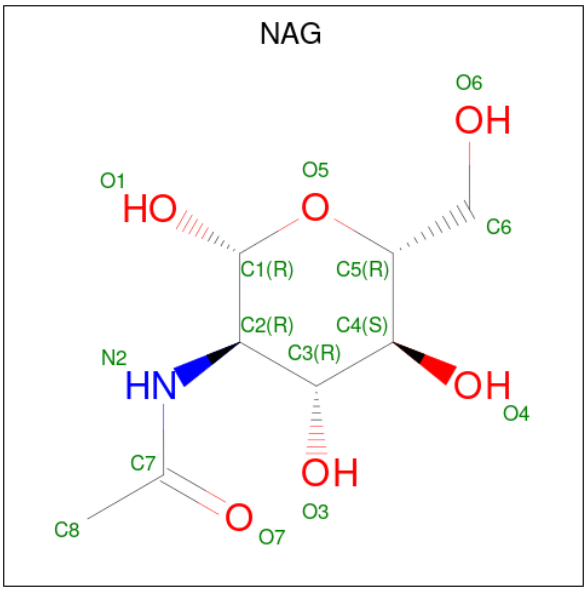
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	17	9	2	6	0	0
			Total	C	N	O		
4	C	1	17	9	2	6	0	0
			Total	C	N	O		
4	D	1	17	9	2	6	0	0

- 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
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	B	1	14	8	1	5	0	0
			Total	C	N	O		
5	B	1	14	8	1	5	0	0
			Total	C	N	O		
5	B	1	14	8	1	5	0	0

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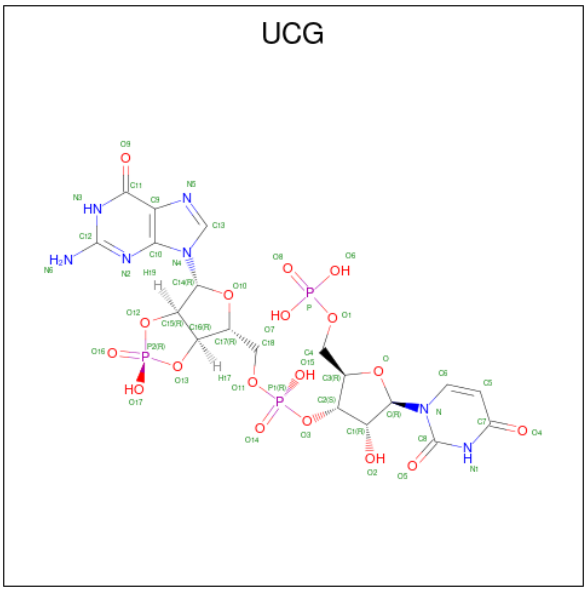
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	14	8	1	5	0	0
			Total	C	N	O		
5	B	1	14	8	1	5	0	0
			Total	C	N	O		
5	C	1	14	8	1	5	0	0
			Total	C	N	O		
5	C	1	14	8	1	5	0	0
			Total	C	N	O		
5	C	1	14	8	1	5	0	0
			Total	C	N	O		
5	C	1	14	8	1	5	0	0
			Total	C	N	O		
5	D	1	14	8	1	5	0	0
			Total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

- 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: $C_{19}H_{24}N_7O_{18}P_3$).



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

- Molecule 7 is water.

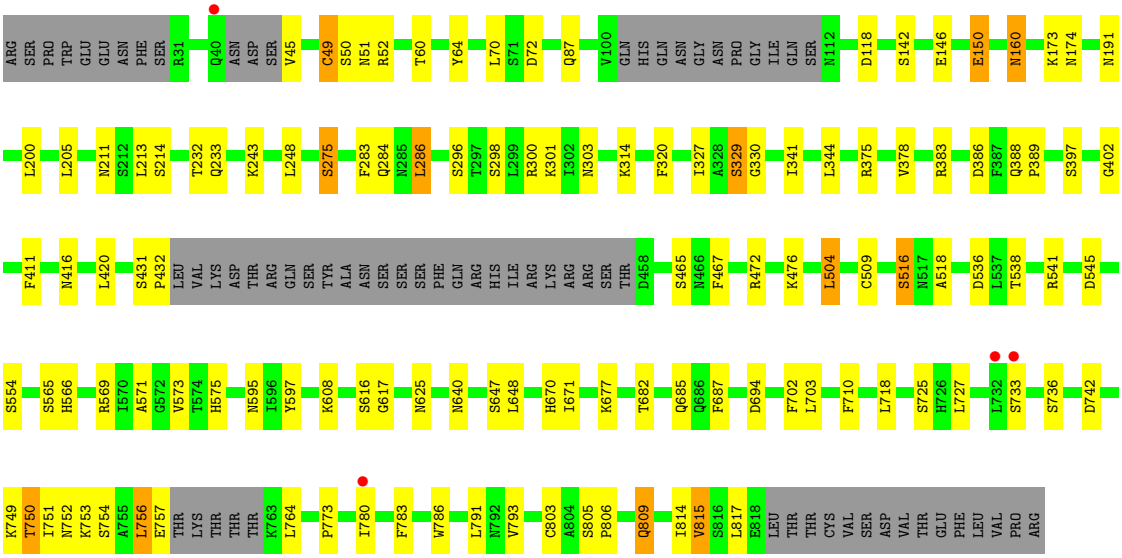
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	300	300	300	0	0
7	B	250	250	250	0	0
7	C	192	192	192	0	0
7	D	182	182	182	0	0

3 Residue-property plots (i)

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

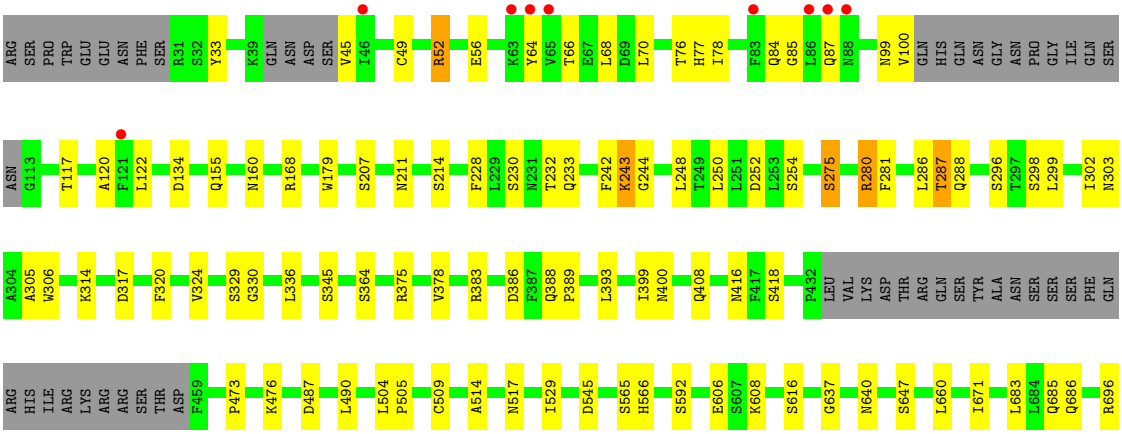
• Molecule 1: Toll-like receptor 8

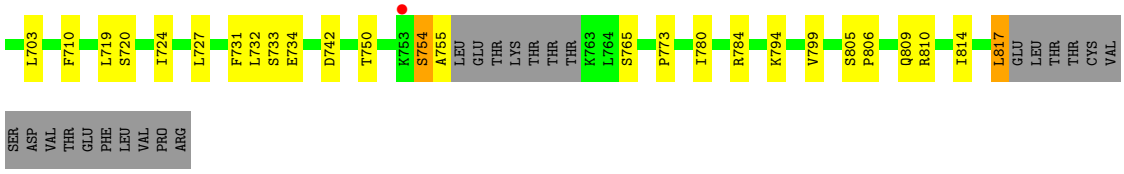
Chain A: 77% 14% • 8%



• Molecule 1: Toll-like receptor 8

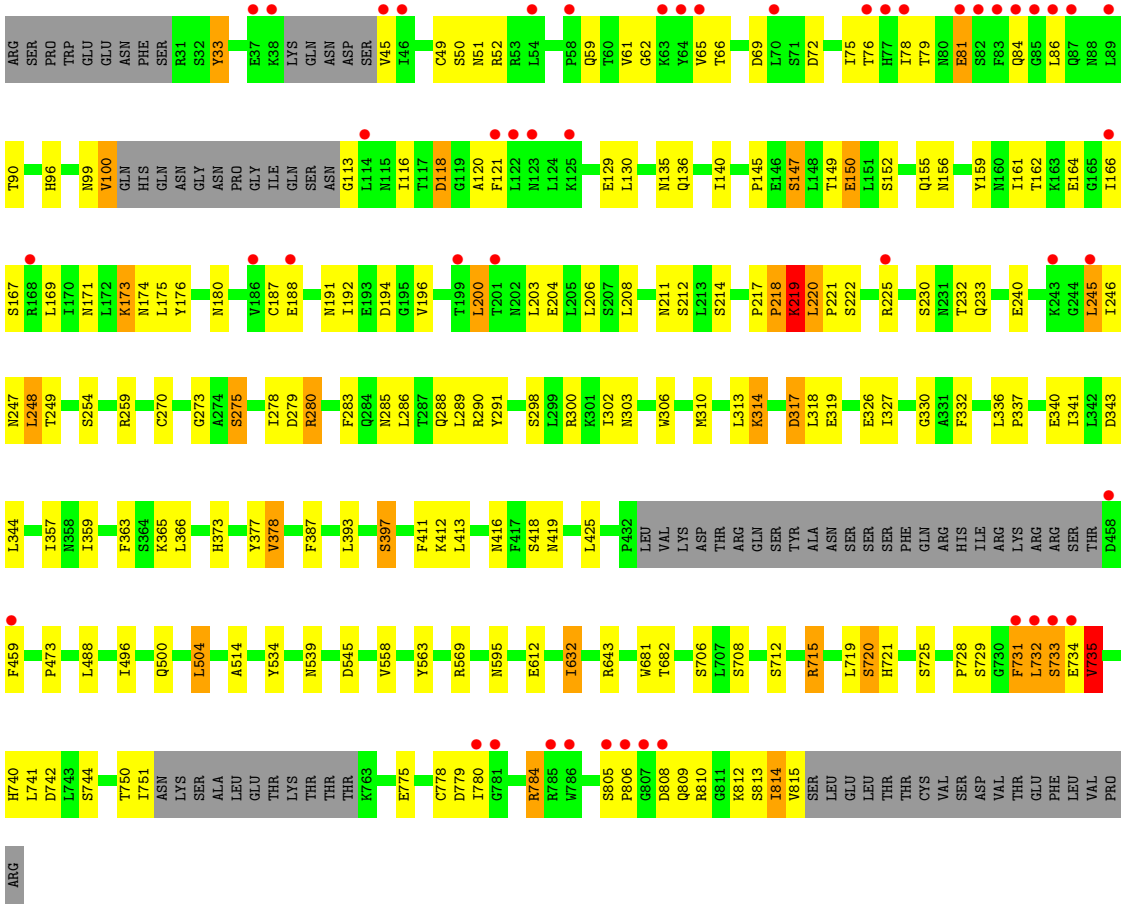
Chain B: % 75% 15% • 9%





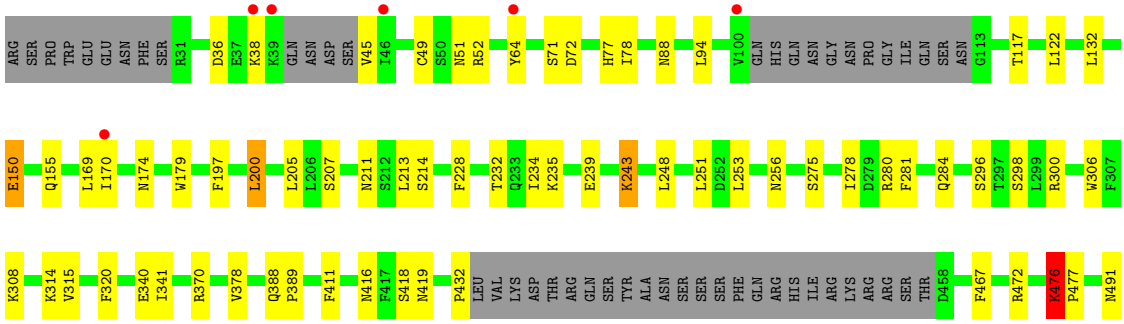
• Molecule 1: Toll-like receptor 8

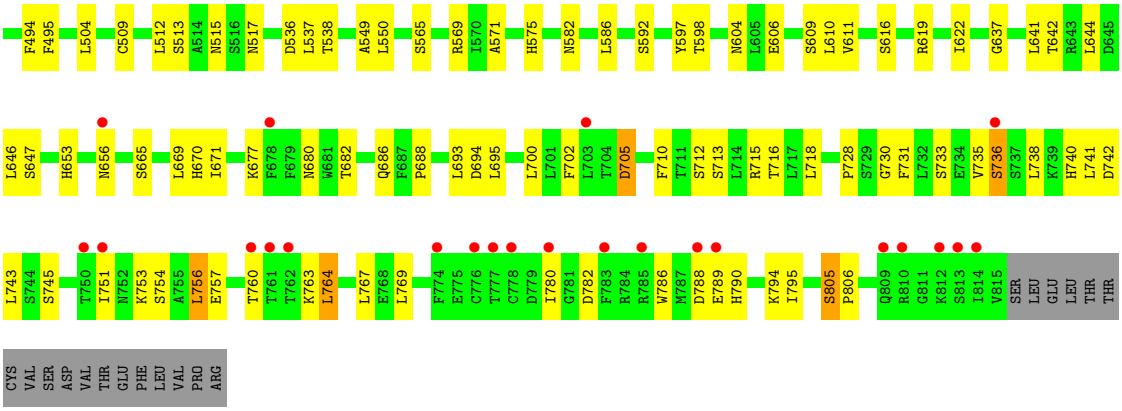
Chain C:



• Molecule 1: Toll-like receptor 8

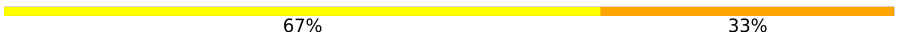
Chain D:





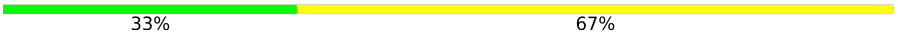
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



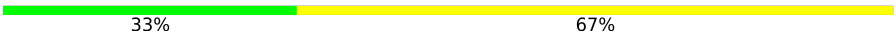
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



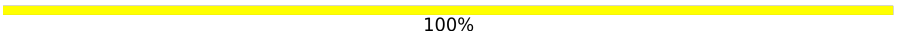
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



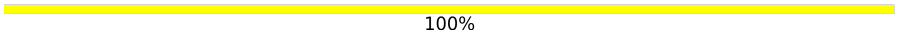
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



• 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:



• 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%

NAG1 NAG2 BMA3

• 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%

NAG1 NAG2 BMA3

• 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%

NAG1 NAG2 BMA3

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

Chain G: 100%

NAG1 NAG2

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

Chain J: 100%

NAG1 NAG2

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

Chain M: 100%

NAG1 NAG2

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

Chain P: 50% 50%

NAG1
NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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^2)	34.6	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	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^2)	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.49	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(^{o})	Ideal(^{o})
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.

The worst 5 of 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

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	733/811 (90%)	672 (92%)	59 (8%)	2 (0%)	41	55
1	B	727/811 (90%)	669 (92%)	53 (7%)	5 (1%)	22	32
1	C	721/811 (89%)	643 (89%)	72 (10%)	6 (1%)	19	29
1	D	735/811 (91%)	671 (91%)	61 (8%)	3 (0%)	34	48
All	All	2916/3244 (90%)	2655 (91%)	245 (8%)	16 (0%)	29	41

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	243	LYS

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Mol	Chain	Res	Type
1	C	220	LEU
1	C	219	LYS
1	C	733	SER
1	D	243	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	690/755 (91%)	646 (94%)	44 (6%)	17	28
1	B	684/755 (91%)	656 (96%)	28 (4%)	30	48
1	C	679/755 (90%)	627 (92%)	52 (8%)	13	20
1	D	690/755 (91%)	652 (94%)	38 (6%)	21	35
All	All	2743/3020 (91%)	2581 (94%)	162 (6%)	19	32

5 of 162 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	720	SER
1	D	509	CYS
1	C	732	LEU
1	D	122	LEU
1	D	705	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	285	ASN
1	D	247	ASN
1	D	686	GLN
1	D	123	ASN
1	D	284	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	1,2	14,14,15	0.99	1 (7%)	17,19,21	2.19	4 (23%)
2	NAG	E	2	2	14,14,15	0.68	0	17,19,21	1.25	2 (11%)
2	BMA	E	3	2	11,11,12	1.08	1 (9%)	15,15,17	1.81	6 (40%)
2	NAG	F	1	1,2	14,14,15	0.75	0	17,19,21	1.43	2 (11%)
2	NAG	F	2	2	14,14,15	0.70	0	17,19,21	1.05	0
2	BMA	F	3	2	11,11,12	0.55	0	15,15,17	1.68	3 (20%)
3	NAG	G	1	3,1	14,14,15	0.65	0	17,19,21	1.07	1 (5%)
3	NAG	G	2	3	14,14,15	0.75	1 (7%)	17,19,21	1.41	4 (23%)
2	NAG	H	1	1,2	14,14,15	0.80	0	17,19,21	1.33	4 (23%)
2	NAG	H	2	2	14,14,15	0.61	0	17,19,21	1.28	1 (5%)
2	BMA	H	3	2	11,11,12	0.25	0	15,15,17	0.64	0
2	NAG	I	1	1,2	14,14,15	0.76	0	17,19,21	1.51	5 (29%)
2	NAG	I	2	2	14,14,15	0.98	1 (7%)	17,19,21	1.31	3 (17%)
2	BMA	I	3	2	11,11,12	0.44	0	15,15,17	1.12	1 (6%)
3	NAG	J	1	3,1	14,14,15	0.98	1 (7%)	17,19,21	1.93	3 (17%)
3	NAG	J	2	3	14,14,15	0.66	0	17,19,21	1.60	4 (23%)
2	NAG	K	1	1,2	14,14,15	0.58	0	17,19,21	1.40	4 (23%)
2	NAG	K	2	2	14,14,15	0.67	0	17,19,21	1.27	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	BMA	K	3	2	11,11,12	0.71	0	15,15,17	1.46	3 (20%)
2	NAG	L	1	1,2	14,14,15	0.49	0	17,19,21	1.45	3 (17%)
2	NAG	L	2	2	14,14,15	0.78	0	17,19,21	0.84	0
2	BMA	L	3	2	11,11,12	0.53	0	15,15,17	0.99	1 (6%)
3	NAG	M	1	3,1	14,14,15	0.85	1 (7%)	17,19,21	1.74	5 (29%)
3	NAG	M	2	3	14,14,15	0.57	0	17,19,21	1.42	3 (17%)
2	NAG	N	1	1,2	14,14,15	0.87	1 (7%)	17,19,21	1.90	4 (23%)
2	NAG	N	2	2	14,14,15	0.78	0	17,19,21	1.57	4 (23%)
2	BMA	N	3	2	11,11,12	0.98	1 (9%)	15,15,17	2.62	6 (40%)
2	NAG	O	1	1,2	14,14,15	0.72	0	17,19,21	1.04	1 (5%)
2	NAG	O	2	2	14,14,15	0.59	0	17,19,21	0.89	0
2	BMA	O	3	2	11,11,12	0.43	0	15,15,17	1.36	2 (13%)
3	NAG	P	1	3,1	14,14,15	0.70	0	17,19,21	1.31	2 (11%)
3	NAG	P	2	3	14,14,15	0.64	0	17,19,21	1.12	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	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	1,2	-	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	1,2	-	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	1,2	-	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	1,2	-	1/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	K	3	2	-	2/2/19/22	0/1/1/1
2	NAG	L	1	1,2	-	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	1,2	-	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	1,2	-	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

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	O5-C1	-2.96	1.39	1.43
2	E	3	BMA	O5-C1	-2.81	1.39	1.43
2	N	1	NAG	O5-C1	-2.69	1.39	1.43
3	J	1	NAG	O5-C1	-2.48	1.39	1.43
2	N	3	BMA	O5-C1	-2.43	1.39	1.43

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	NAG	C1-O5-C5	6.77	121.36	112.19
2	N	3	BMA	O5-C1-C2	-5.66	102.04	110.77
3	J	1	NAG	C1-O5-C5	4.81	118.72	112.19
3	J	1	NAG	O5-C5-C6	-4.72	99.80	107.20
2	N	1	NAG	O5-C1-C2	-4.51	104.17	111.29

There are no chirality outliers.

5 of 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

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Mol	Chain	Res	Type	Atoms
2	K	3	BMA	O5-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6

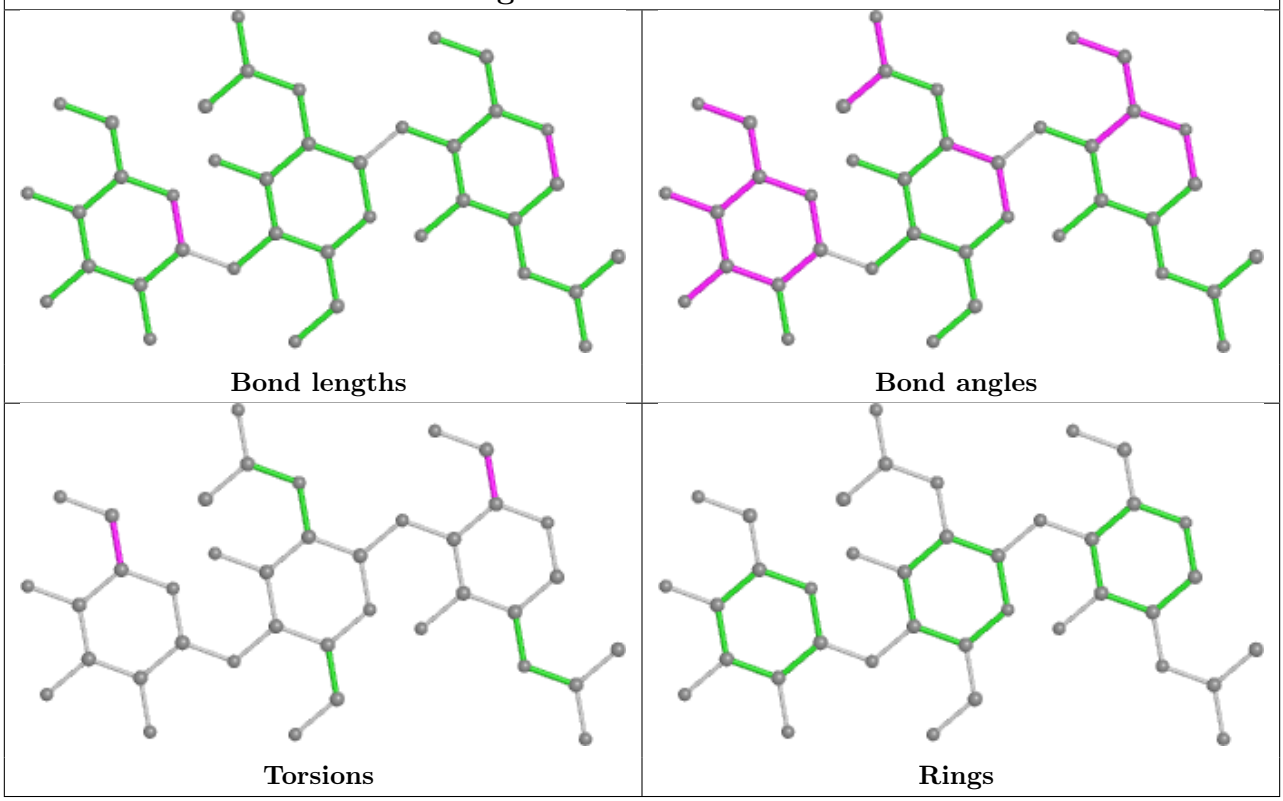
There are no ring outliers.

2 monomers are involved in 4 short contacts:

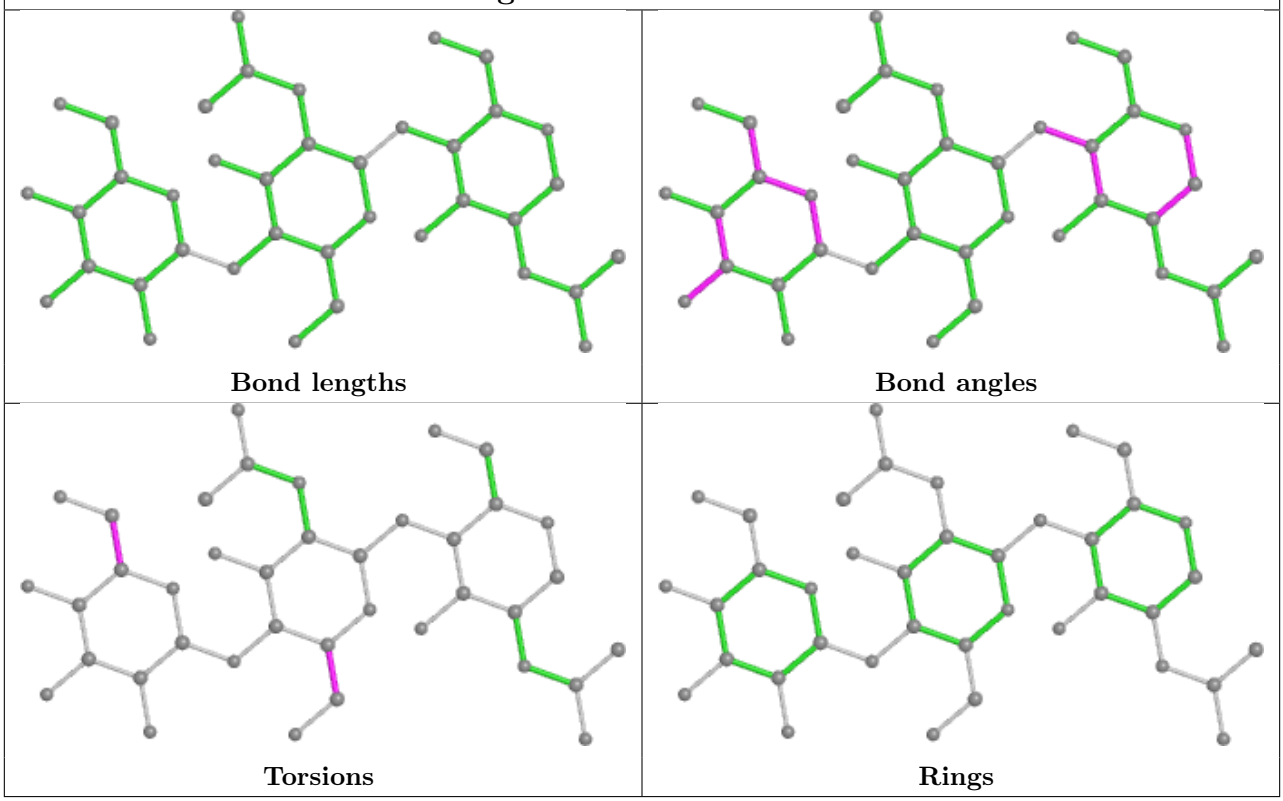
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	1	NAG	2	0
2	E	1	NAG	2	0

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

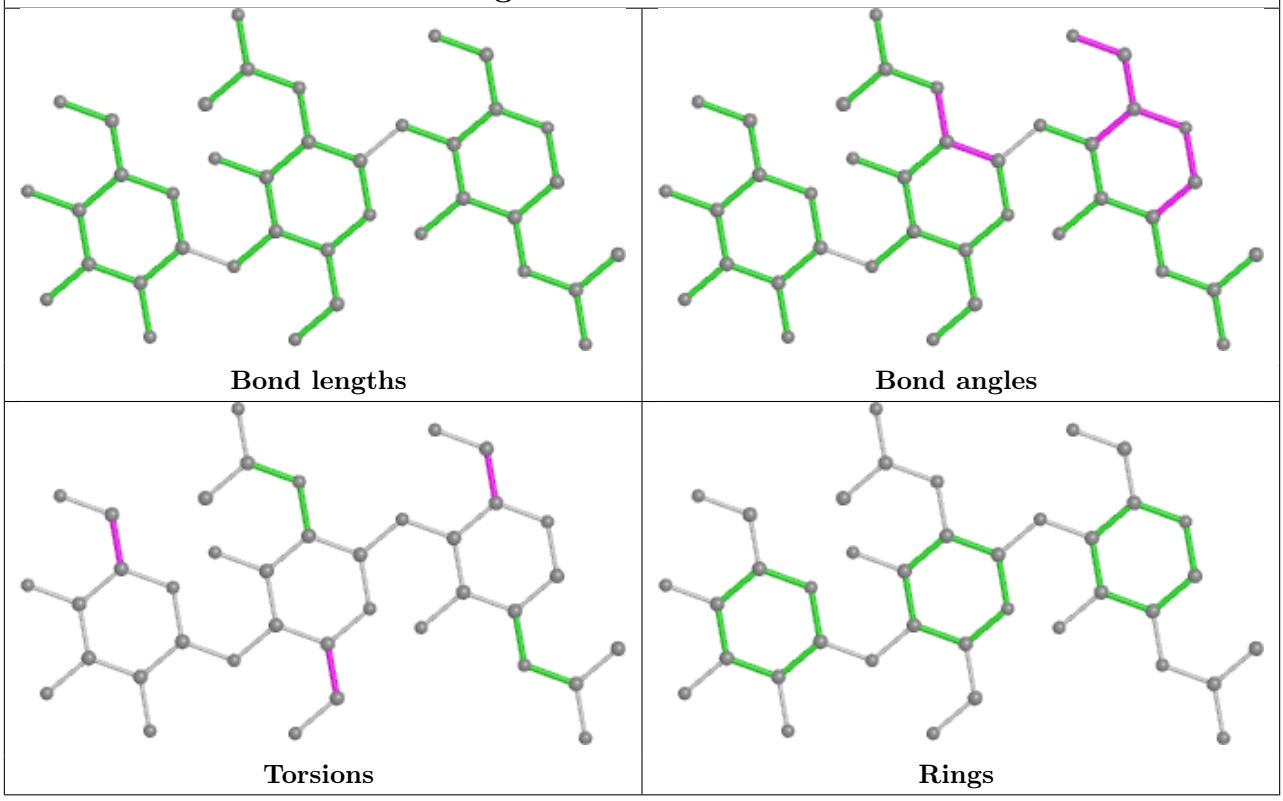
Oligosaccharide Chain E



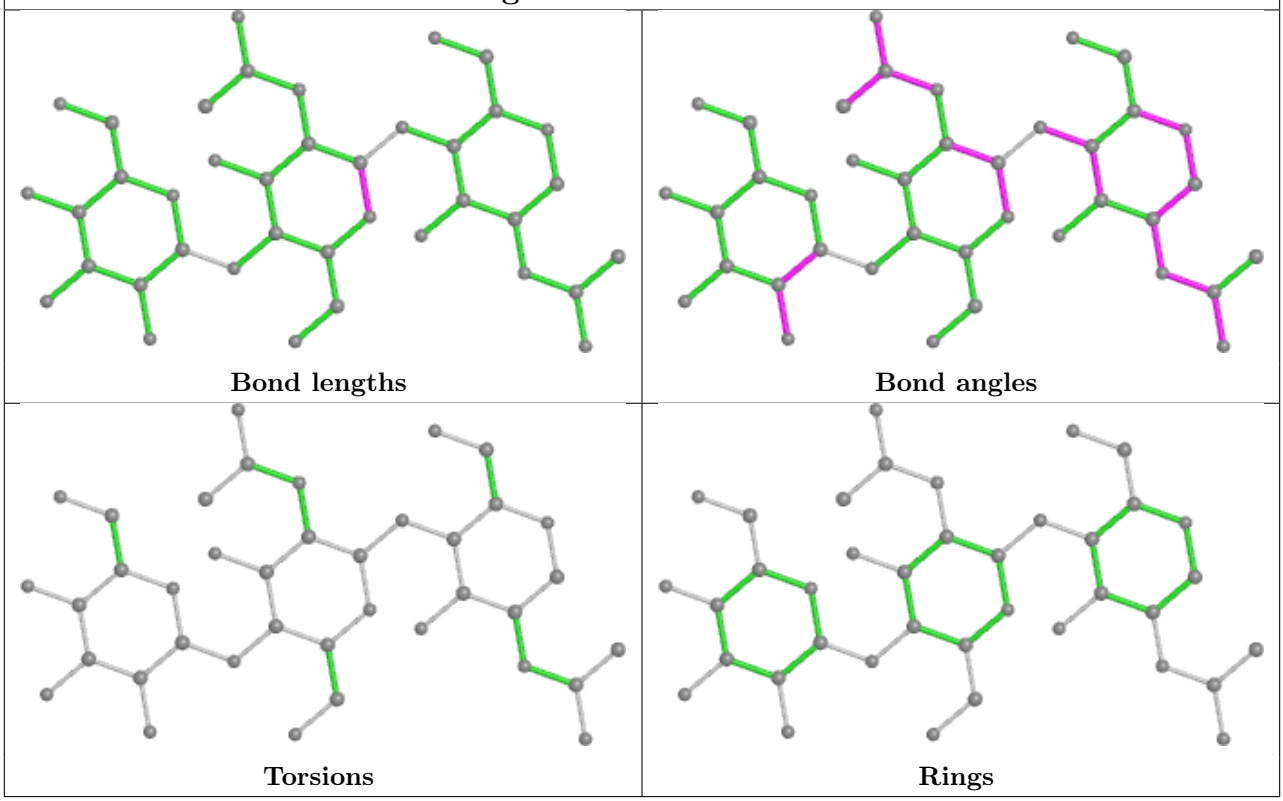
Oligosaccharide Chain F



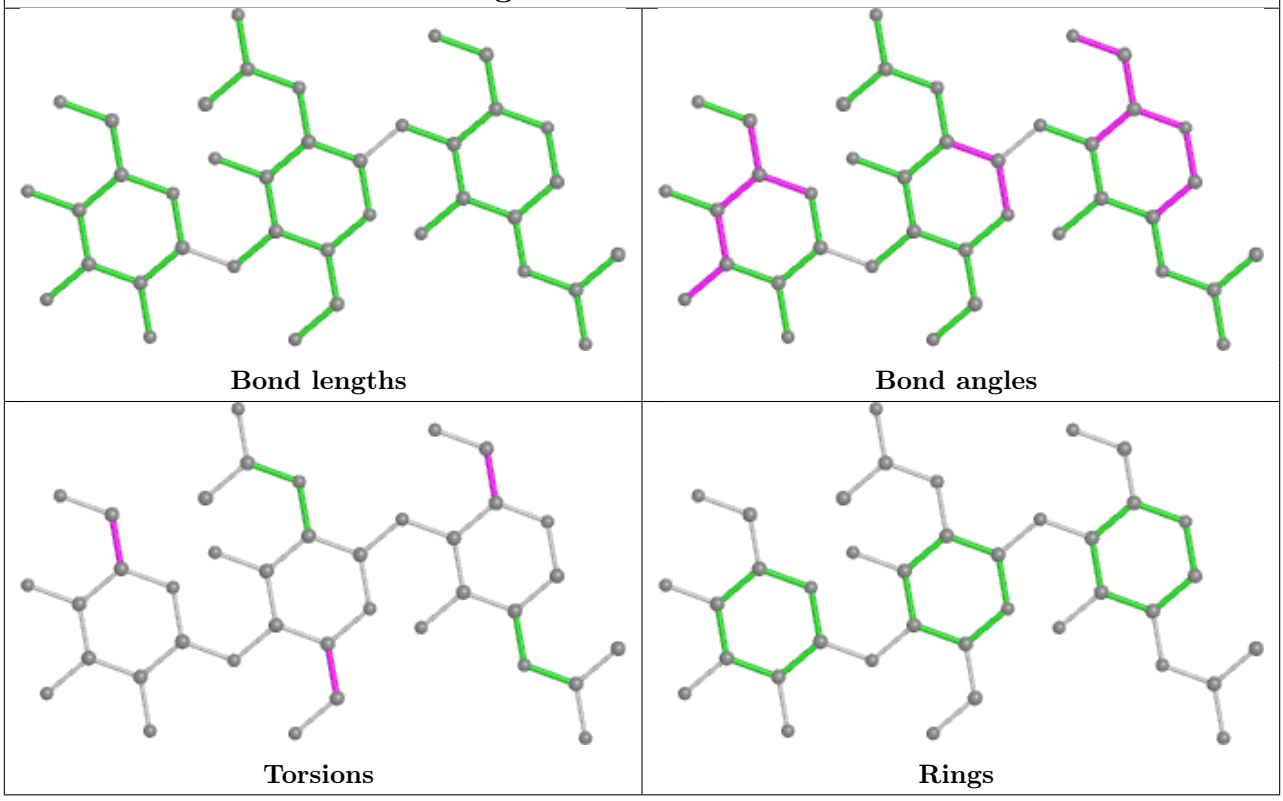
Oligosaccharide Chain H



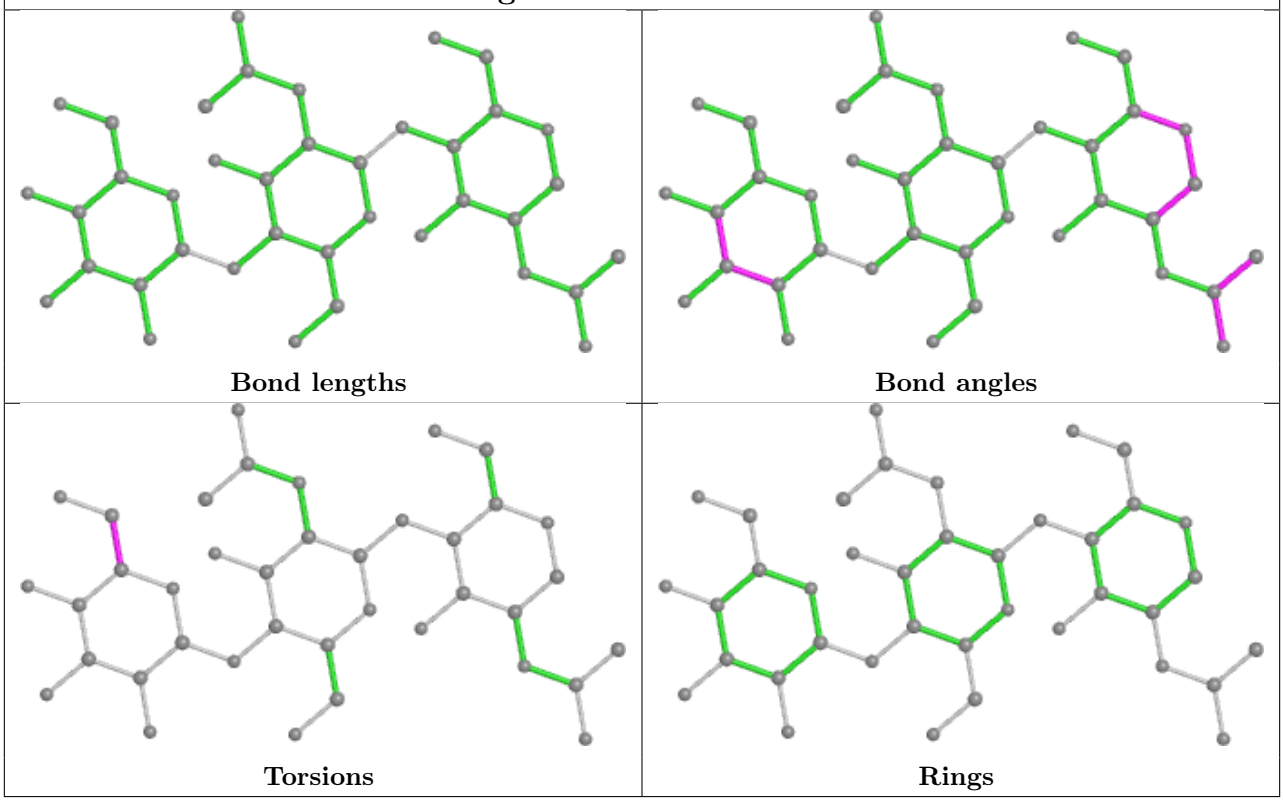
Oligosaccharide Chain I



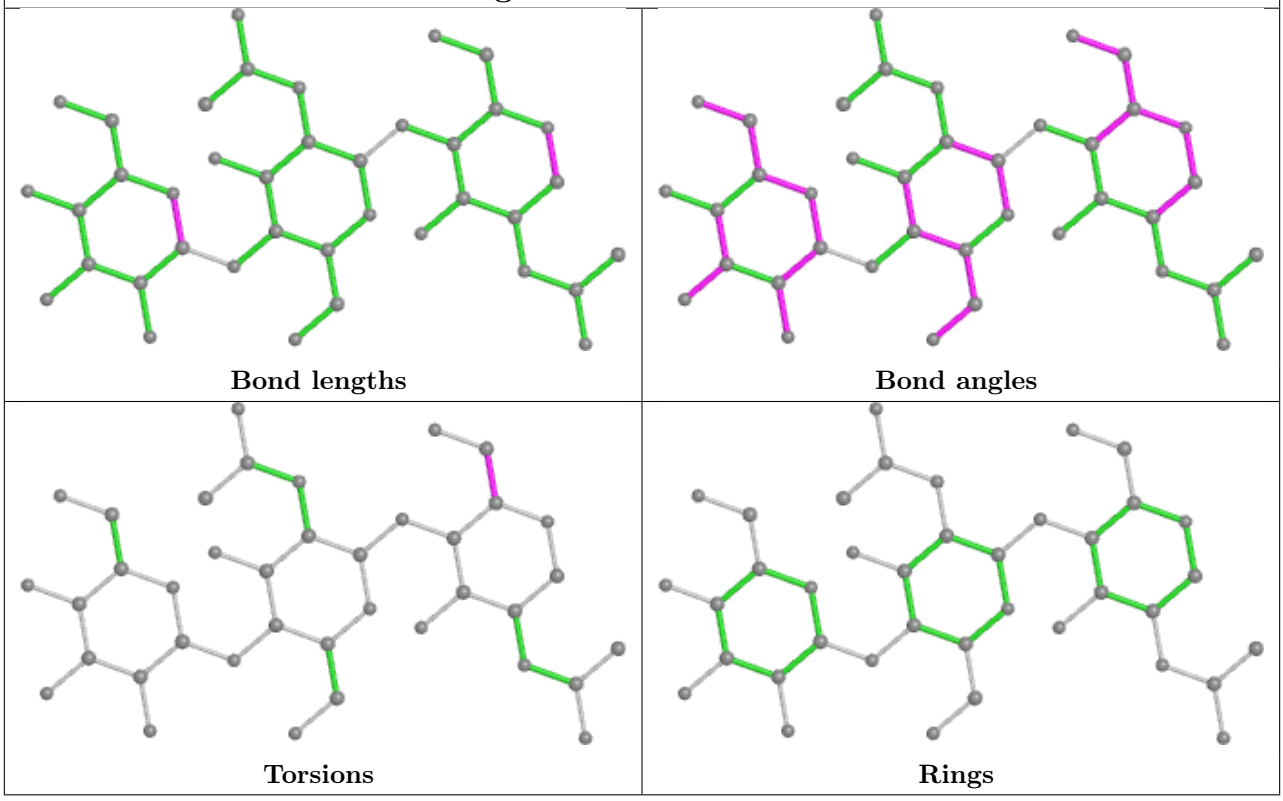
Oligosaccharide Chain K



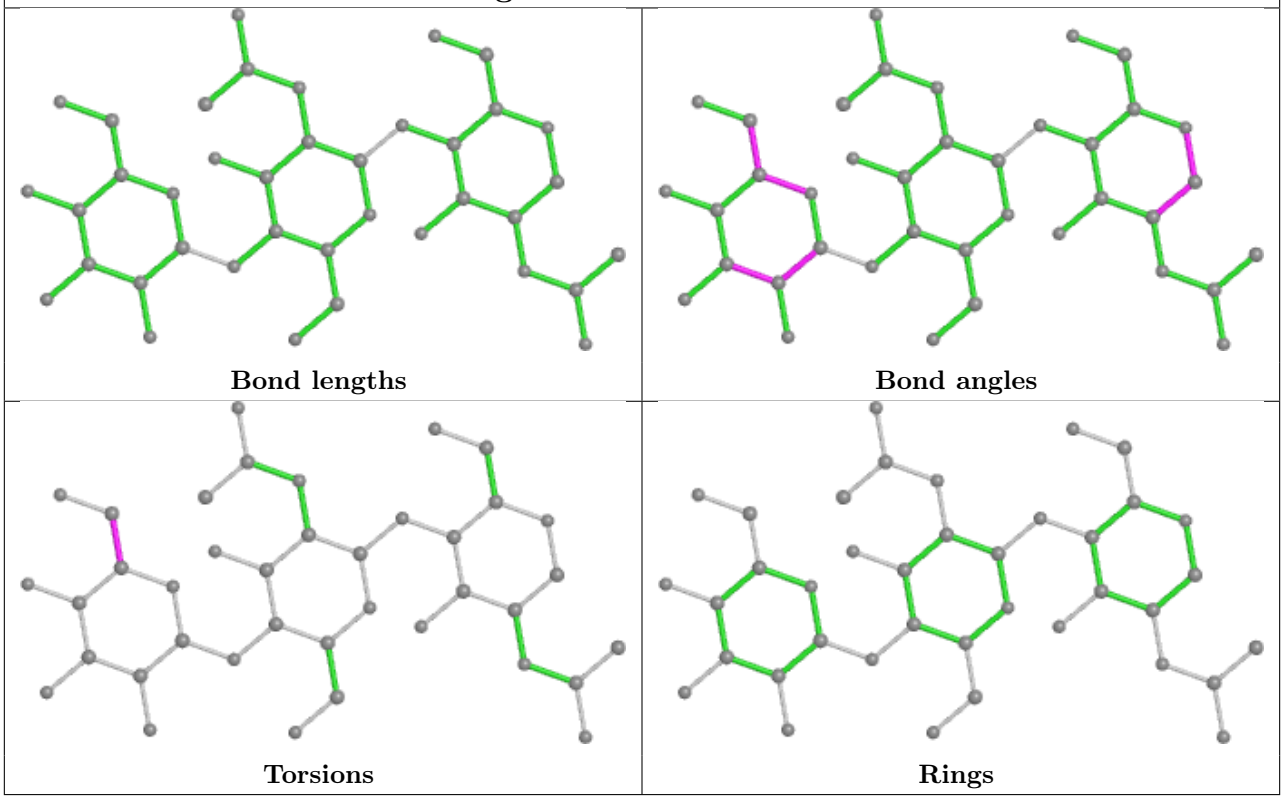
Oligosaccharide Chain L



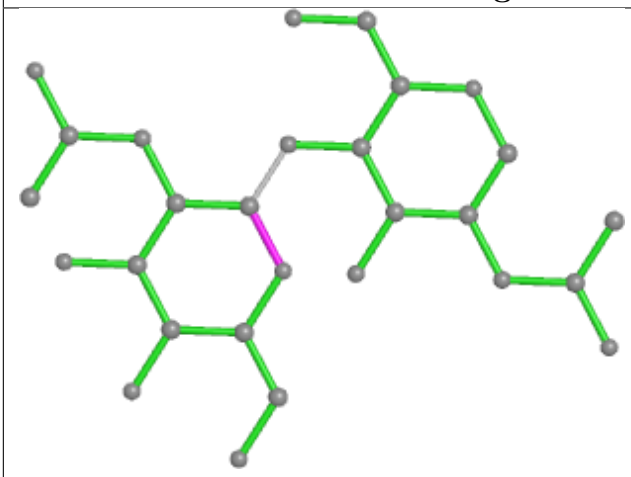
Oligosaccharide Chain N



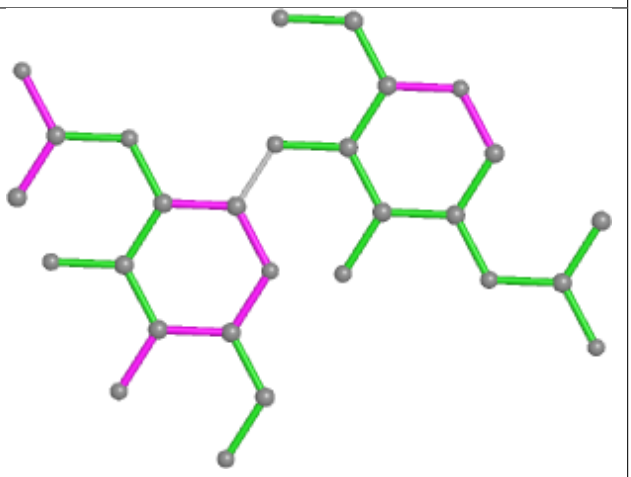
Oligosaccharide Chain O



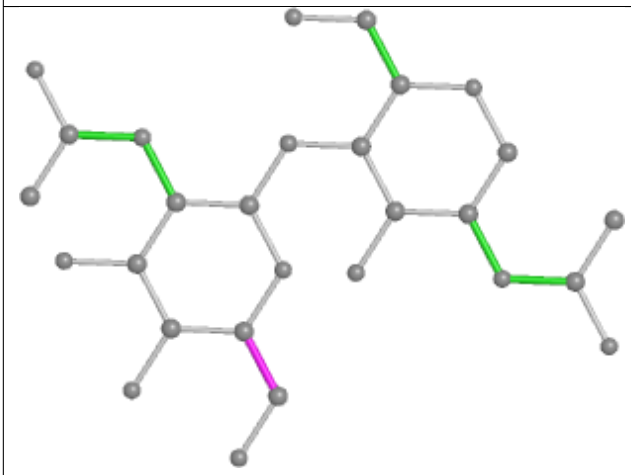
Oligosaccharide Chain G



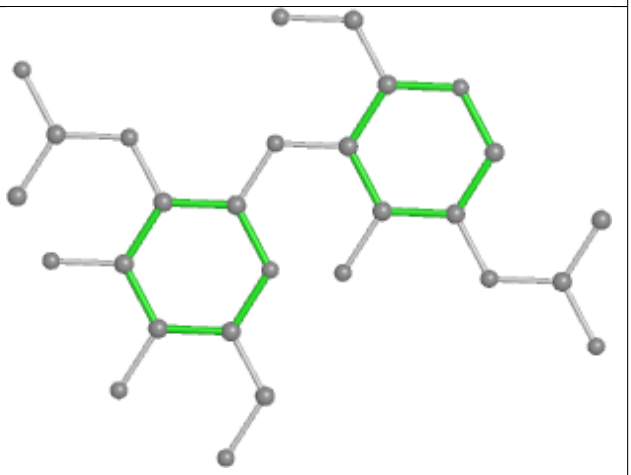
Bond lengths



Bond angles

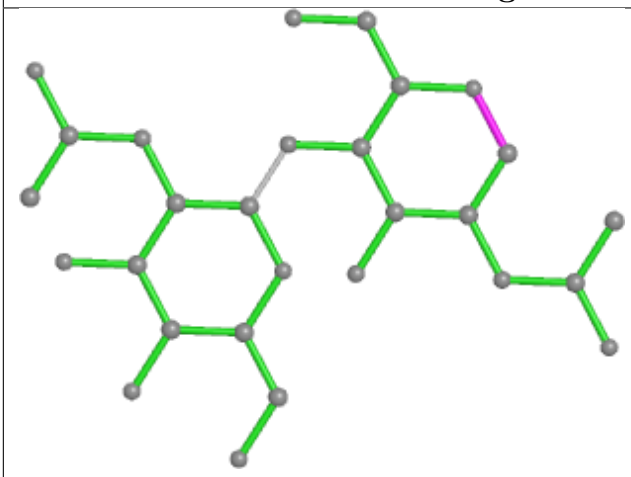


Torsions

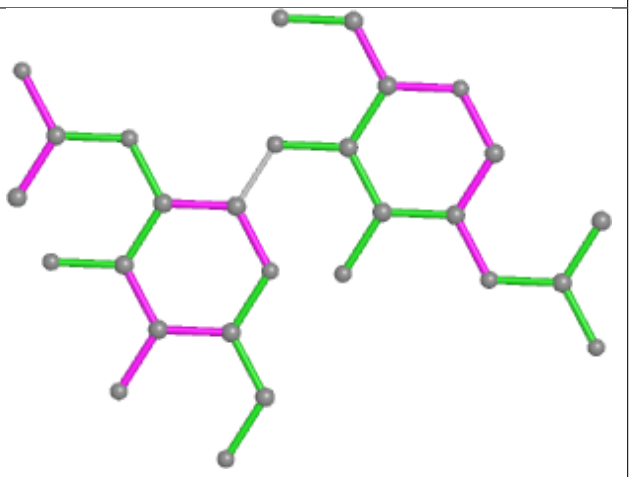


Rings

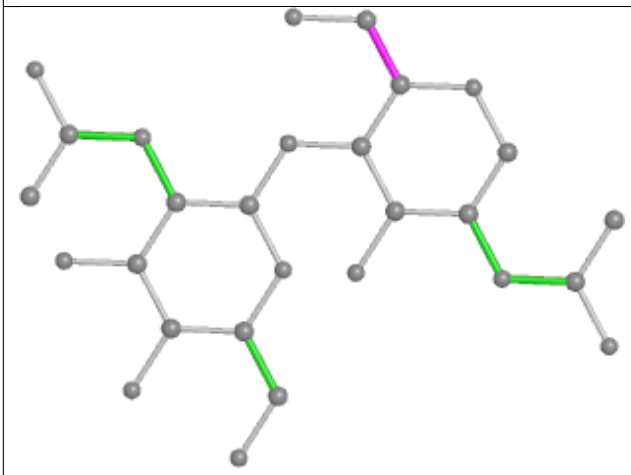
Oligosaccharide Chain J



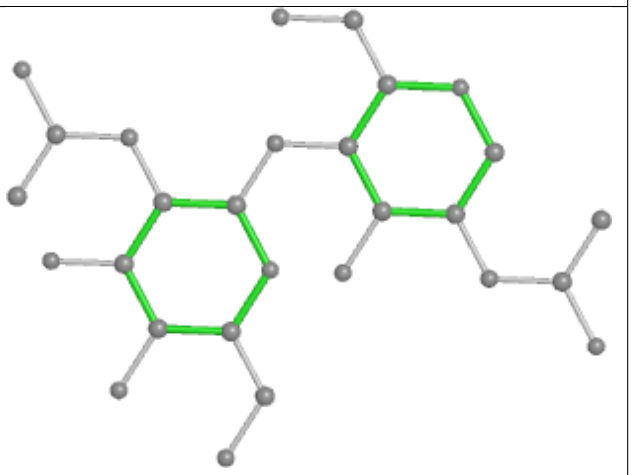
Bond lengths



Bond angles

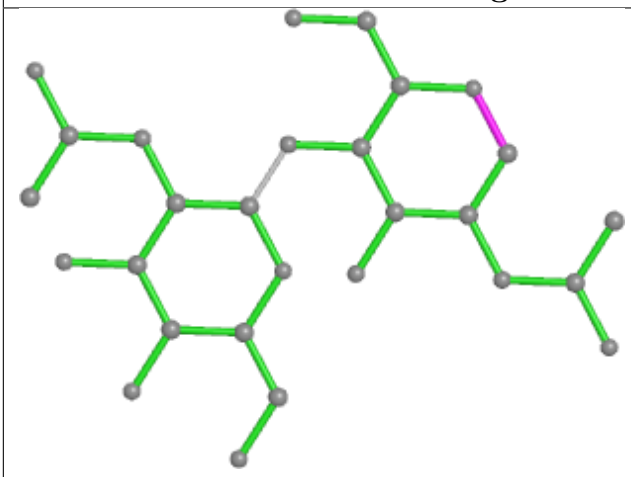


Torsions

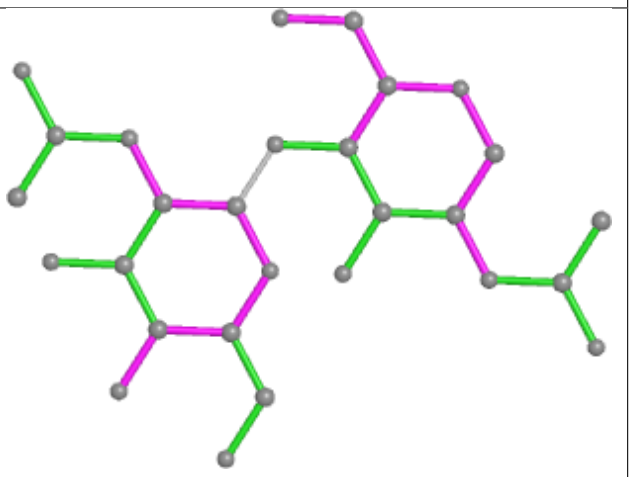


Rings

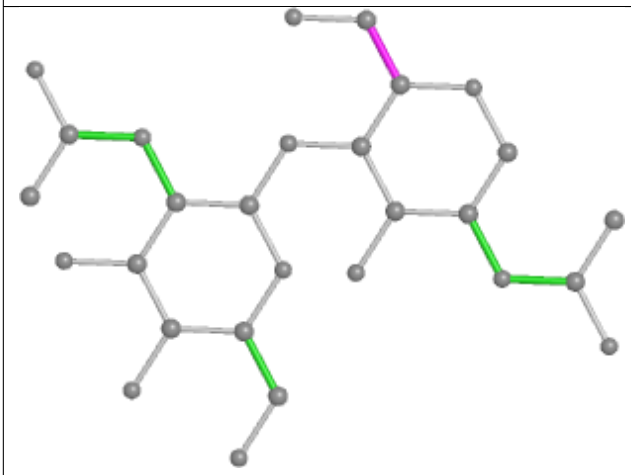
Oligosaccharide Chain M



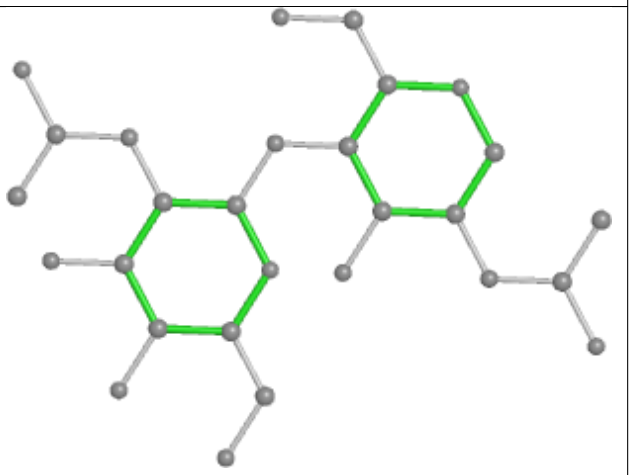
Bond lengths



Bond angles

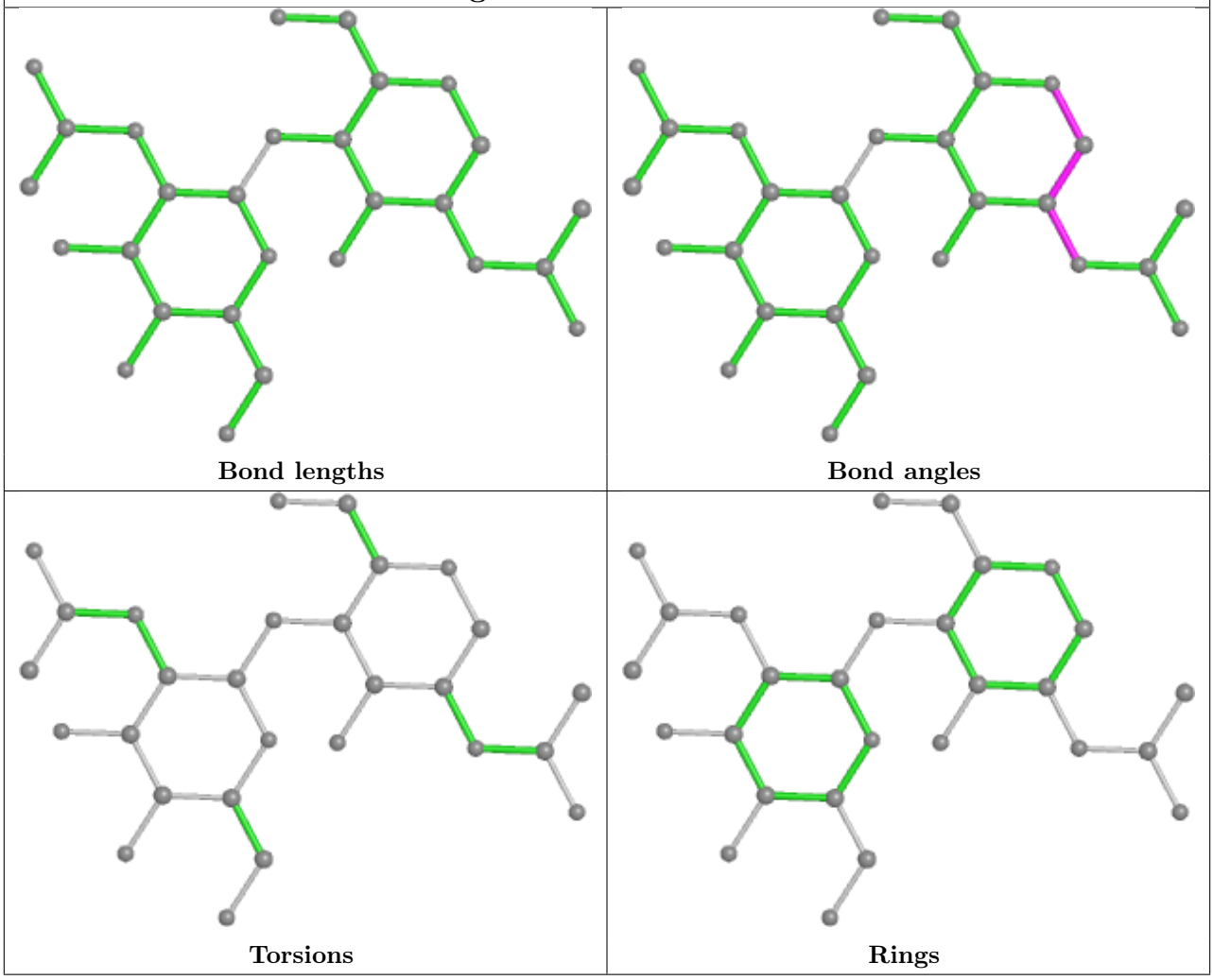


Torsions



Rings

Oligosaccharide Chain P



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	$\#\|Z\| > 2$
4	URI	B	901	-	18,18,18	1.35	3 (16%)	26,26,26	1.66	5 (19%)
4	URI	C	902	-	18,18,18	1.50	4 (22%)	26,26,26	2.13	10 (38%)
4	URI	D	901	-	18,18,18	1.39	3 (16%)	26,26,26	1.94	7 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	B	911	1	14,14,15	0.30	0	17,19,21	0.62	0
5	NAG	A	908	1	14,14,15	0.29	0	17,19,21	0.61	0
5	NAG	B	913	1	14,14,15	0.58	0	17,19,21	1.30	1 (5%)
5	NAG	A	911	1	14,14,15	0.29	0	17,19,21	0.62	0
5	NAG	D	909	1	14,14,15	0.80	0	17,19,21	2.52	5 (29%)
5	NAG	C	909	1	14,14,15	0.55	0	17,19,21	1.16	1 (5%)
5	NAG	A	914	1	14,14,15	0.71	0	17,19,21	1.31	3 (17%)
5	NAG	C	914	1	14,14,15	0.51	0	17,19,21	1.69	4 (23%)
5	NAG	D	912	1	14,14,15	0.64	0	17,19,21	1.32	1 (5%)
5	NAG	B	908	1	14,14,15	0.64	0	17,19,21	0.74	1 (5%)
5	NAG	B	912	1	14,14,15	0.53	0	17,19,21	1.66	3 (17%)
5	NAG	C	912	1	14,14,15	0.83	1 (7%)	17,19,21	1.26	1 (5%)
6	UCG	B	915	-	45,52,52	1.35	5 (11%)	60,82,82	2.48	18 (30%)
6	UCG	C	901	-	45,52,52	1.36	4 (8%)	60,82,82	2.59	14 (23%)
4	URI	A	901	-	18,18,18	1.23	3 (16%)	26,26,26	1.70	5 (19%)
5	NAG	B	914	1	14,14,15	0.30	0	17,19,21	0.61	0
5	NAG	A	913	1	14,14,15	0.60	0	17,19,21	1.21	2 (11%)
6	UCG	D	902	-	45,52,52	1.42	5 (11%)	60,82,82	2.68	18 (30%)
5	NAG	D	914	1	14,14,15	0.53	0	17,19,21	2.18	3 (17%)
5	NAG	D	913	1	14,14,15	0.28	0	17,19,21	0.61	0
6	UCG	A	915	-	45,52,52	1.36	5 (11%)	60,82,82	2.59	20 (33%)
5	NAG	A	912	1	14,14,15	0.29	0	17,19,21	0.61	0
5	NAG	C	913	1	14,14,15	0.57	0	17,19,21	1.42	3 (17%)

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
4	URI	B	901	-	-	4/6/22/22	0/2/2/2
4	URI	C	902	-	-	6/6/22/22	0/2/2/2
4	URI	D	901	-	-	4/6/22/22	0/2/2/2
5	NAG	B	911	1	-	2/6/23/26	0/1/1/1
5	NAG	A	908	1	-	0/6/23/26	0/1/1/1
5	NAG	B	913	1	-	0/6/23/26	0/1/1/1
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	D	909	1	-	2/6/23/26	0/1/1/1
5	NAG	C	909	1	-	2/6/23/26	0/1/1/1
5	NAG	A	914	1	-	1/6/23/26	0/1/1/1
5	NAG	C	914	1	-	2/6/23/26	0/1/1/1
5	NAG	D	912	1	-	0/6/23/26	0/1/1/1
5	NAG	B	908	1	-	0/6/23/26	0/1/1/1
5	NAG	B	912	1	-	2/6/23/26	0/1/1/1
5	NAG	C	912	1	-	2/6/23/26	0/1/1/1
6	UCG	B	915	-	-	1/21/67/67	0/6/6/6
6	UCG	C	901	-	-	5/21/67/67	0/6/6/6
4	URI	A	901	-	-	4/6/22/22	0/2/2/2
5	NAG	B	914	1	-	2/6/23/26	0/1/1/1
5	NAG	A	913	1	-	2/6/23/26	0/1/1/1
6	UCG	D	902	-	-	5/21/67/67	0/6/6/6
5	NAG	D	914	1	-	0/6/23/26	0/1/1/1
5	NAG	D	913	1	-	1/6/23/26	0/1/1/1
6	UCG	A	915	-	-	5/21/67/67	0/6/6/6
5	NAG	A	912	1	-	2/6/23/26	0/1/1/1
5	NAG	C	913	1	-	2/6/23/26	0/1/1/1

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	915	UCG	P2-O16	4.47	1.66	1.50
6	B	915	UCG	P2-O16	4.36	1.66	1.50
6	C	901	UCG	P2-O16	4.23	1.65	1.50
6	D	902	UCG	C9-C11	-4.20	1.38	1.47
6	D	902	UCG	P2-O16	4.18	1.65	1.50

The worst 5 of 125 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	915	UCG	O12-C15-C16	10.10	123.61	105.08
6	C	901	UCG	O13-C16-C15	9.39	122.29	105.08
6	C	901	UCG	O12-C15-C16	9.27	122.07	105.08
6	D	902	UCG	O12-C15-C16	9.10	121.76	105.08
6	B	915	UCG	O12-C15-C16	9.09	121.74	105.08

There are no chirality outliers.

5 of 59 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

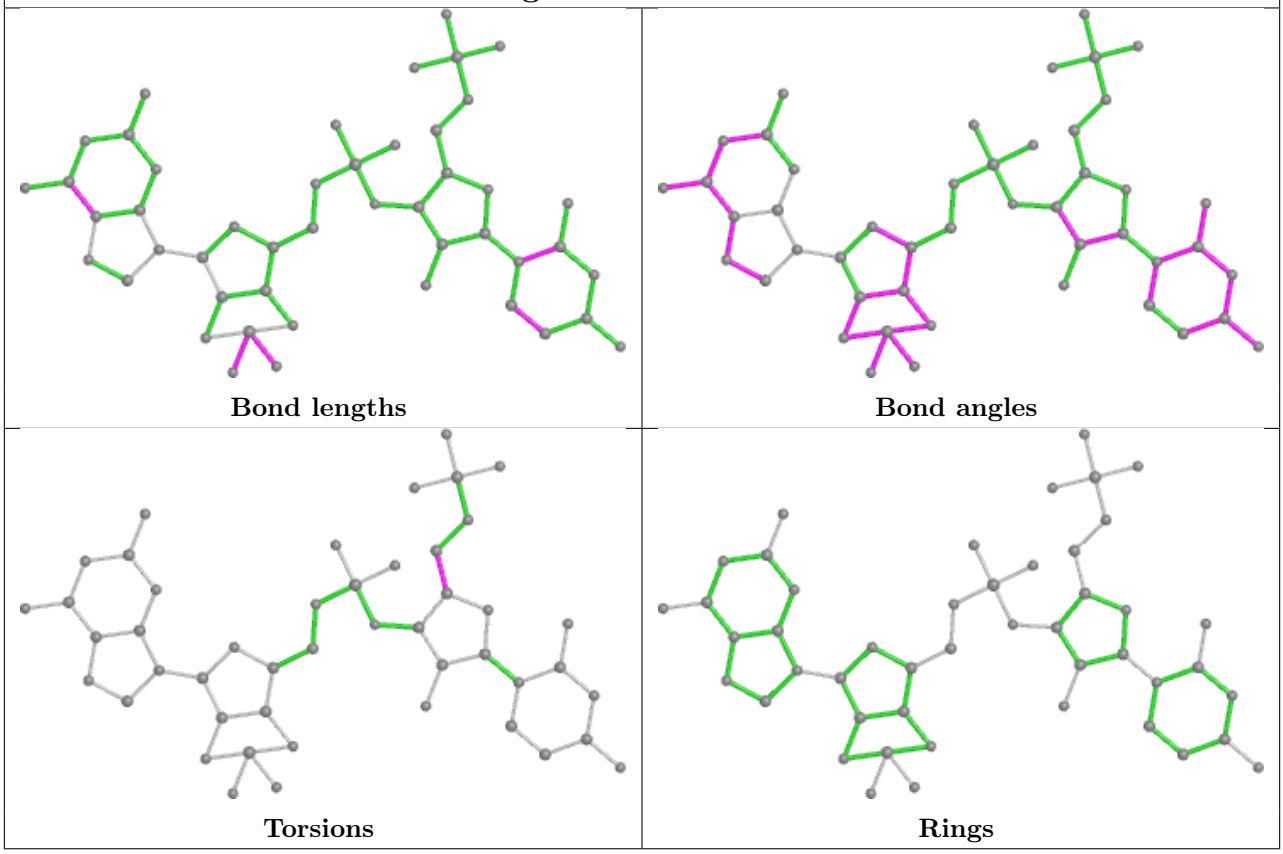
There are no ring outliers.

8 monomers are involved in 11 short contacts:

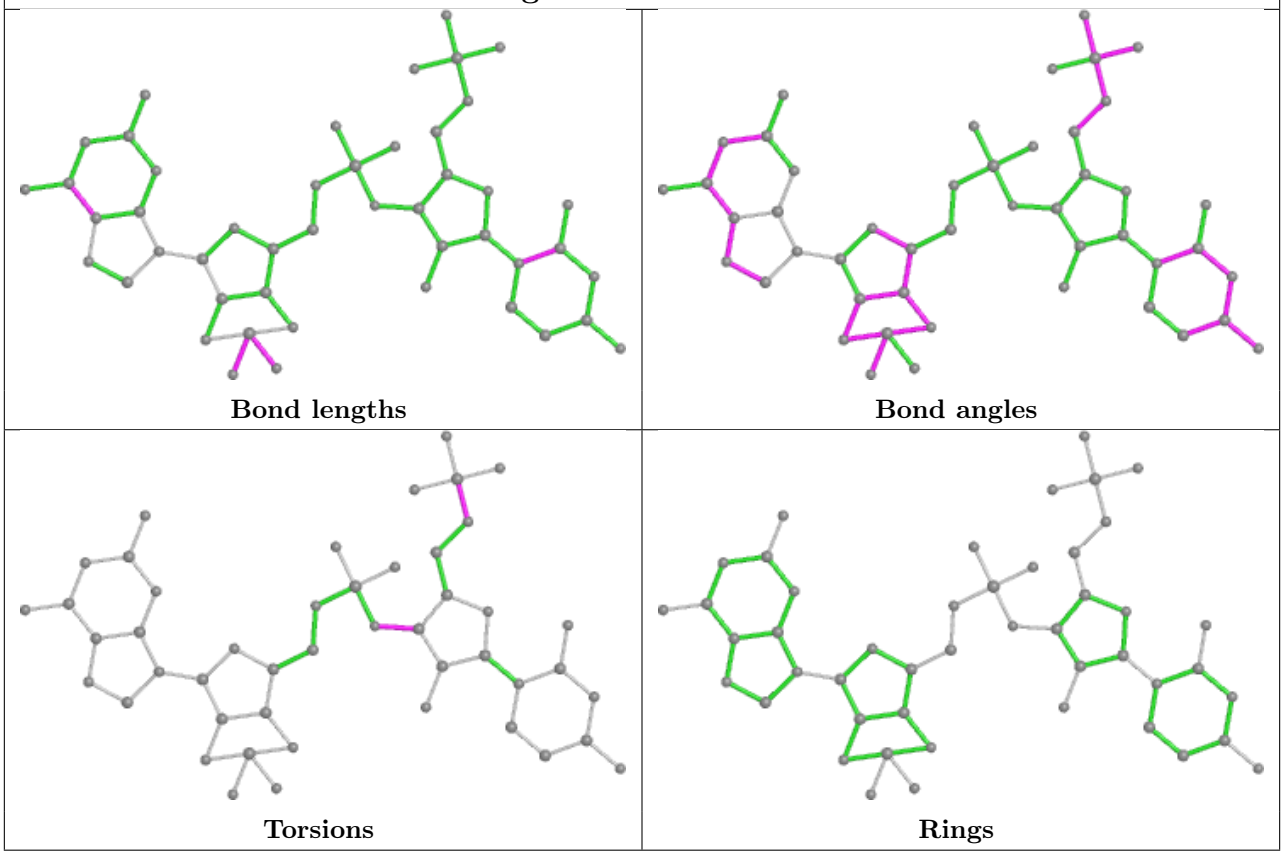
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	911	NAG	1	0
5	D	909	NAG	1	0
5	A	914	NAG	1	0
6	B	915	UCG	1	0
6	C	901	UCG	3	0
5	B	914	NAG	1	0
6	D	902	UCG	1	0
6	A	915	UCG	2	0

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 then 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.

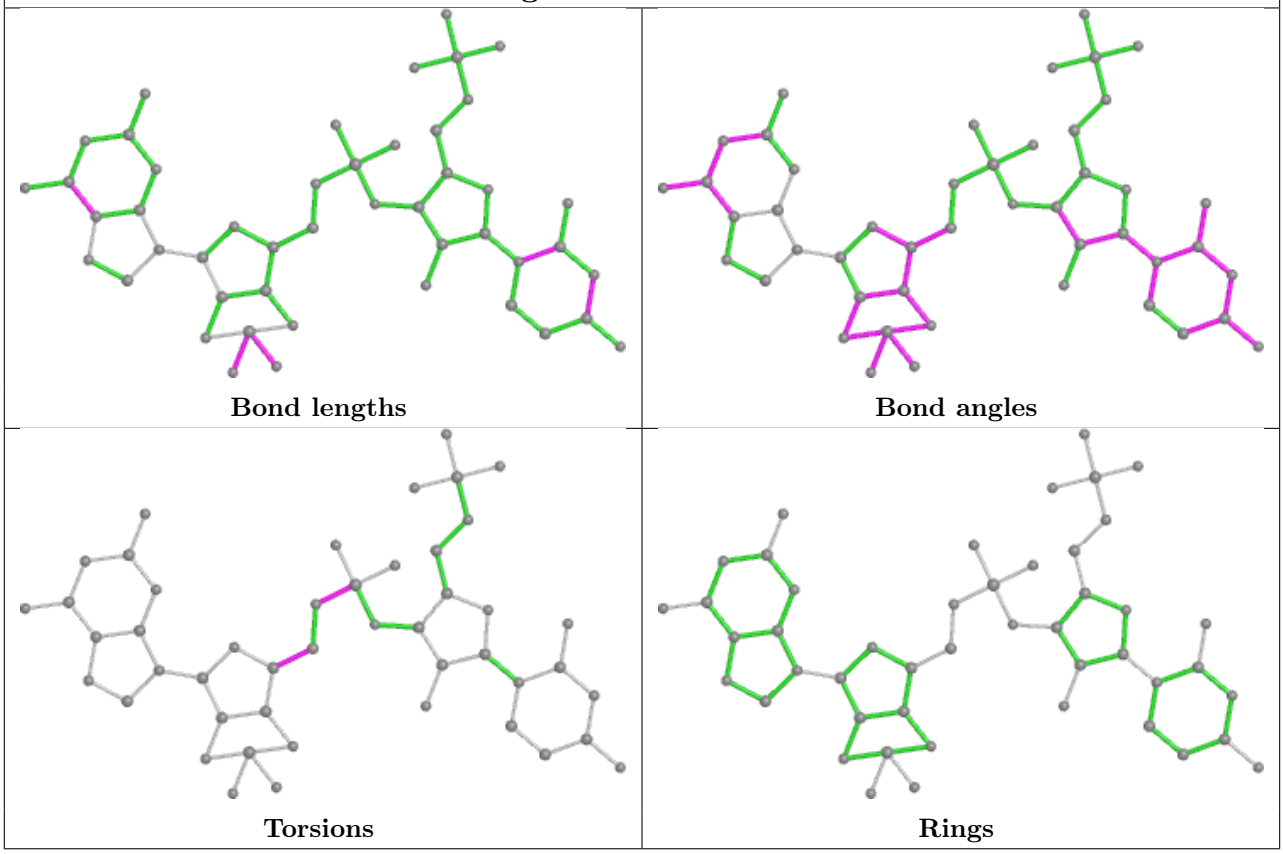
Ligand UCG B 915



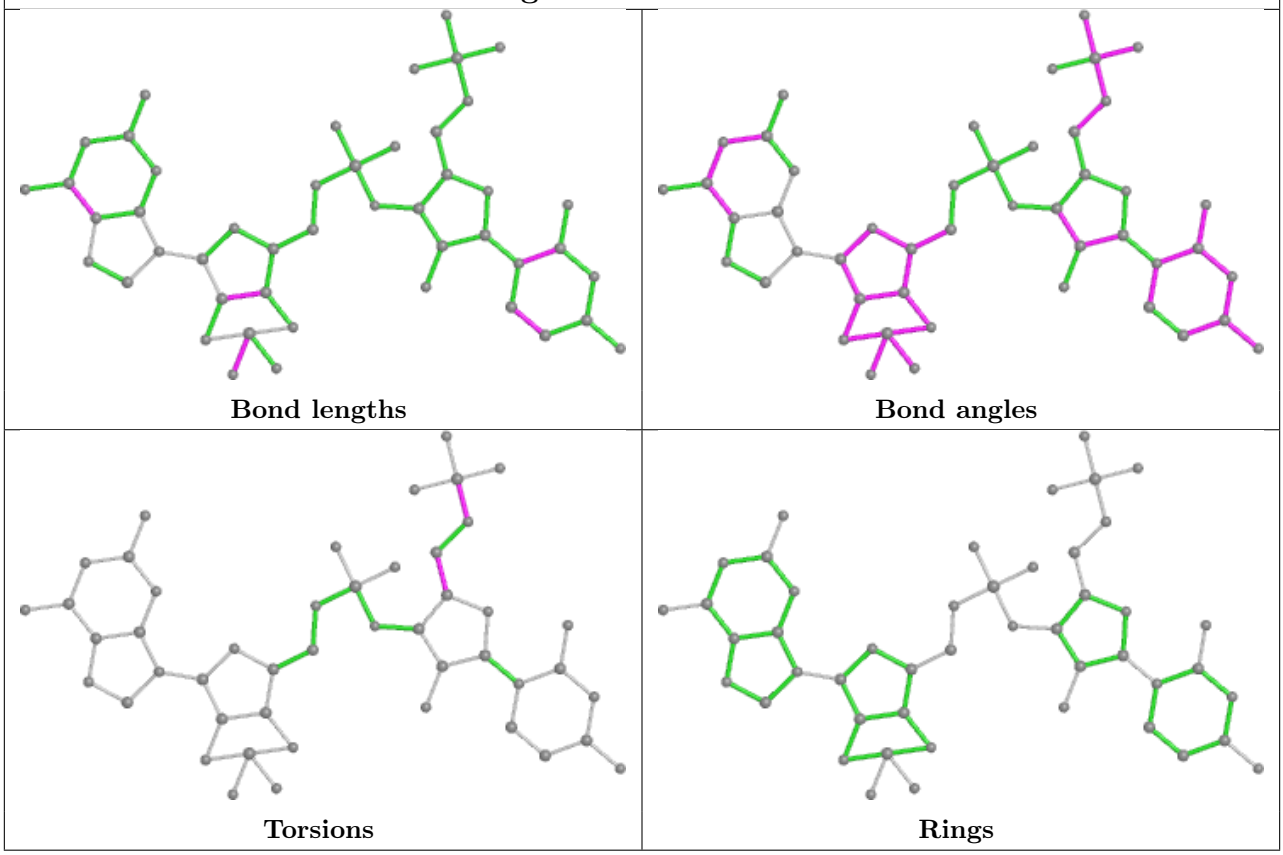
Ligand UCG C 901



Ligand UCG D 902



Ligand UCG A 915



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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^2)	Q<0.9
1	A	743/811 (91%)	-0.47	4 (0%)	91	89	17, 35, 71, 113	1 (0%)
1	B	737/811 (90%)	-0.44	10 (1%)	75	73	17, 41, 77, 108	1 (0%)
1	C	731/811 (90%)	0.05	49 (6%)	17	16	18, 54, 110, 157	1 (0%)
1	D	743/811 (91%)	-0.24	29 (3%)	39	38	18, 44, 97, 146	1 (0%)
All	All	2954/3244 (91%)	-0.28	92 (3%)	49	47	17, 42, 96, 157	4 (0%)

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	64	TYR	8.8
1	D	751	ILE	8.2
1	C	733	SER	6.3
1	B	65	VAL	6.0
1	C	81	GLU	5.6

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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^2)	Q<0.9
2	BMA	H	3	11/12	0.82	0.16	44,50,54,55	0
2	BMA	N	3	11/12	0.83	0.14	40,48,51,56	0

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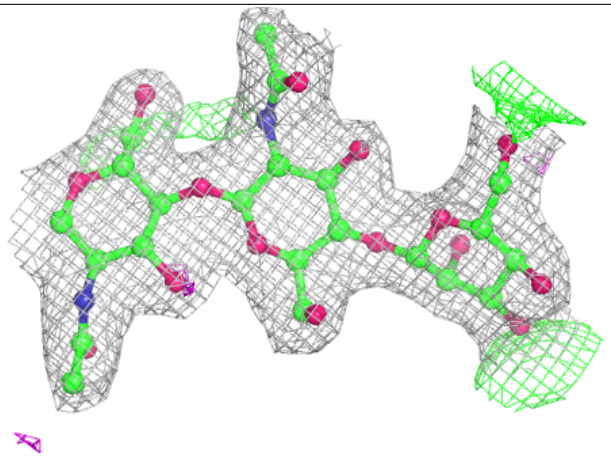
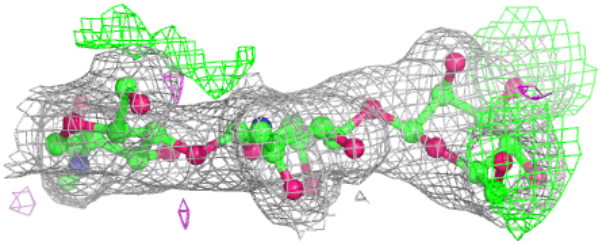
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMA	E	3	11/12	0.85	0.10	34,37,43,45	0
2	BMA	K	3	11/12	0.90	0.10	52,57,59,61	0
2	BMA	O	3	11/12	0.91	0.12	50,57,63,68	0
2	BMA	F	3	11/12	0.92	0.17	41,43,50,51	0
2	BMA	L	3	11/12	0.92	0.19	43,50,57,59	0
3	NAG	M	2	14/15	0.92	0.13	33,40,46,51	0
2	NAG	K	1	14/15	0.94	0.19	39,44,49,50	0
2	BMA	I	3	11/12	0.94	0.17	40,45,54,54	0
3	NAG	P	2	14/15	0.94	0.13	36,46,52,52	0
3	NAG	G	2	14/15	0.95	0.10	27,33,40,43	0
2	NAG	L	2	14/15	0.96	0.13	28,32,38,39	0
2	NAG	F	2	14/15	0.96	0.10	23,27,35,36	0
3	NAG	J	2	14/15	0.96	0.10	32,37,41,44	0
2	NAG	F	1	14/15	0.96	0.09	18,25,27,28	0
2	NAG	O	1	14/15	0.96	0.08	29,33,35,36	0
2	NAG	L	1	14/15	0.97	0.08	19,23,25,26	0
2	NAG	O	2	14/15	0.97	0.10	39,42,48,50	0
2	NAG	E	2	14/15	0.97	0.10	23,27,32,36	0
2	NAG	K	2	14/15	0.97	0.13	46,49,52,53	0
3	NAG	J	1	14/15	0.97	0.12	19,23,28,35	0
2	NAG	N	1	14/15	0.97	0.12	17,23,29,38	0
3	NAG	M	1	14/15	0.97	0.09	22,28,36,42	0
2	NAG	N	2	14/15	0.97	0.10	27,32,33,41	0
3	NAG	P	1	14/15	0.97	0.13	24,31,38,38	0
2	NAG	H	1	14/15	0.97	0.14	23,26,31,45	0
2	NAG	I	2	14/15	0.98	0.13	22,27,31,34	0
2	NAG	H	2	14/15	0.98	0.10	29,35,42,48	0
3	NAG	G	1	14/15	0.98	0.11	17,20,25,25	0
2	NAG	E	1	14/15	0.98	0.12	22,24,28,31	0
2	NAG	I	1	14/15	0.98	0.07	23,25,27,27	0

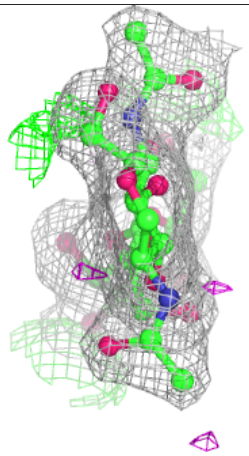
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

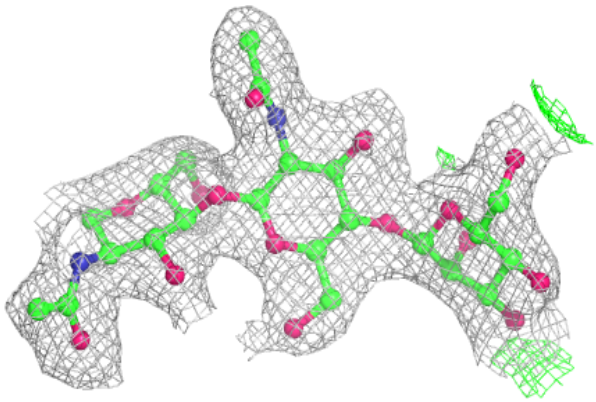


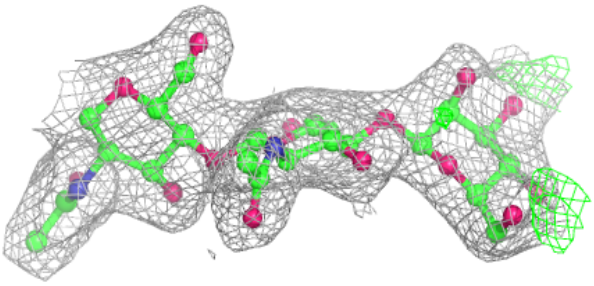


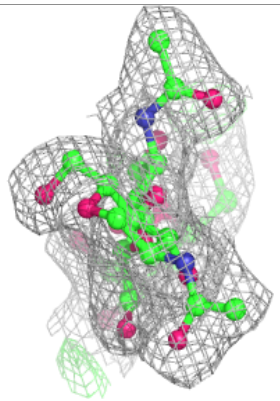


Electron density around Chain F:

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

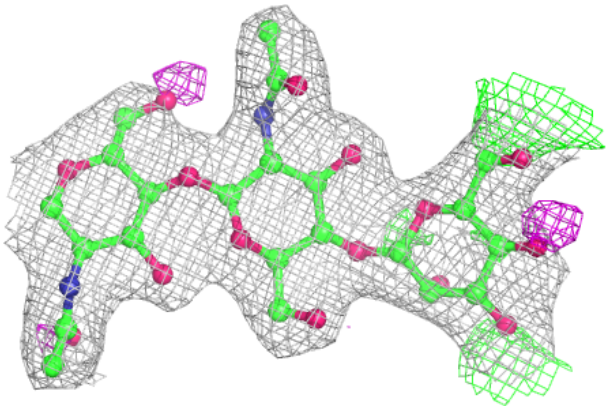


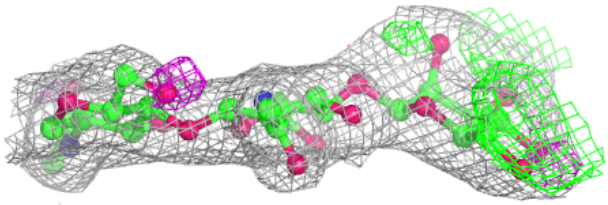


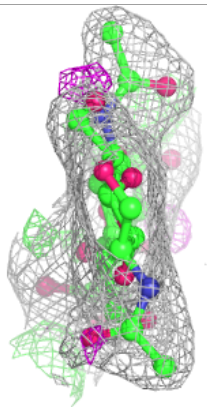


Electron density around Chain H:

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

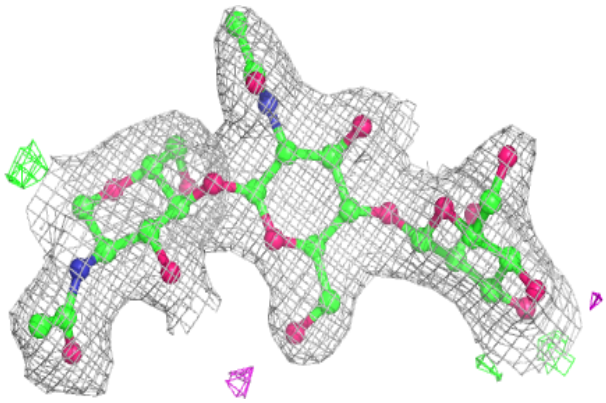


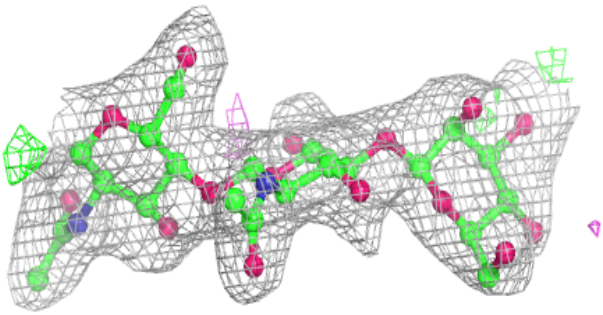


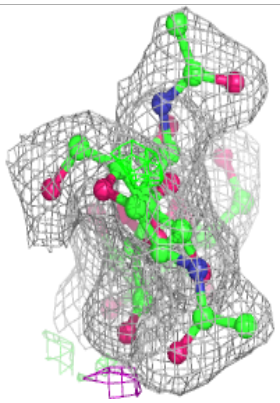


Electron density around Chain I:

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

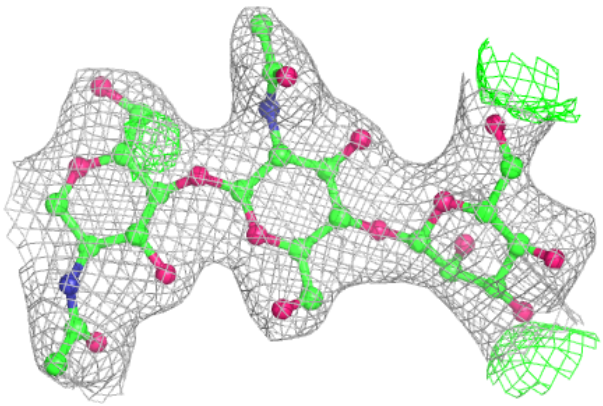


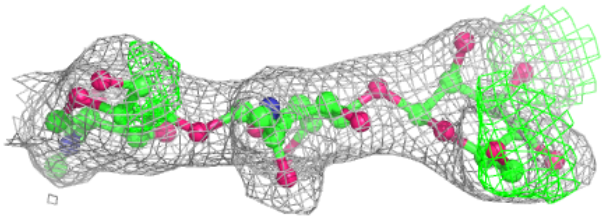


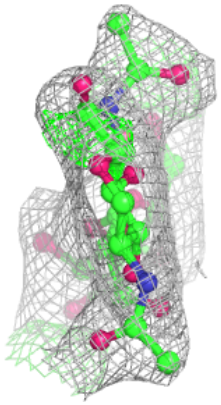


Electron density around Chain K:

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

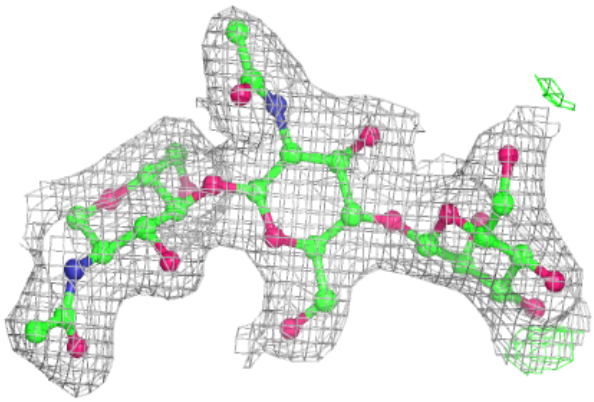


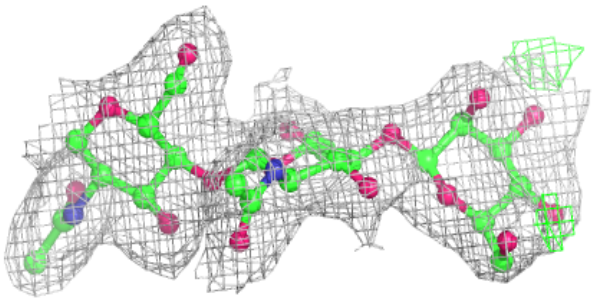


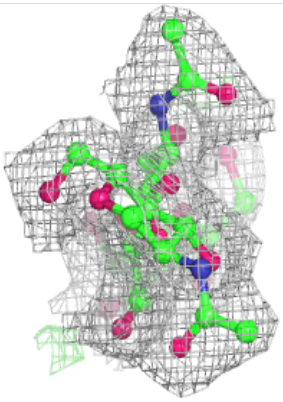


Electron density around Chain L:

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

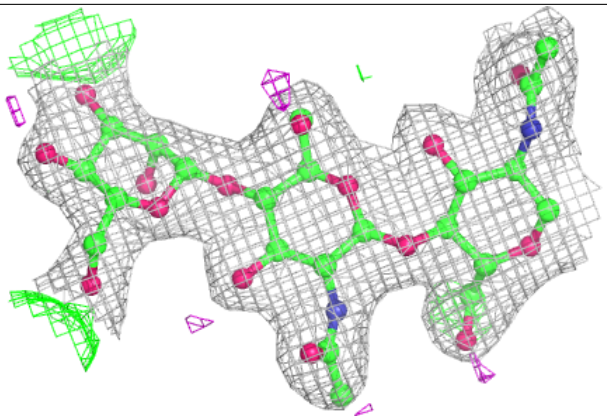


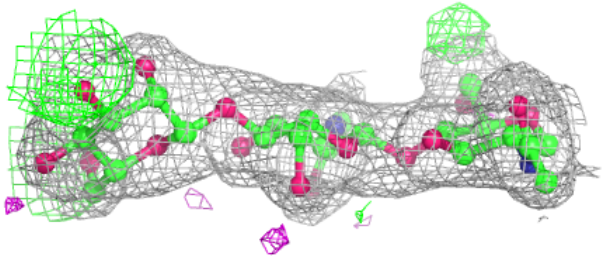


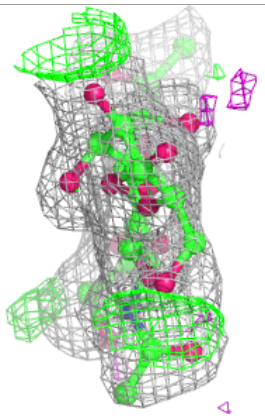


Electron density around Chain N:

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

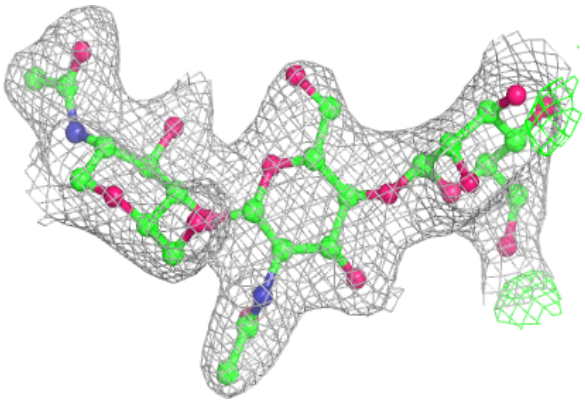


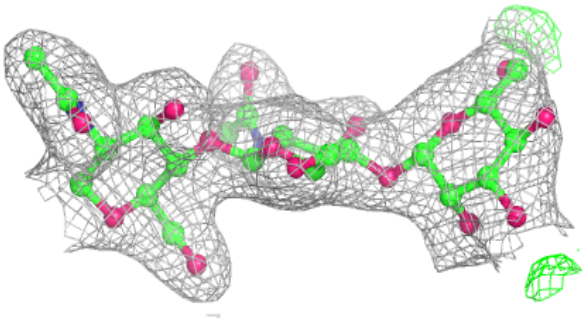


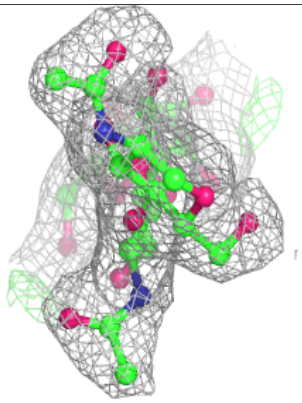


Electron density around Chain O:

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

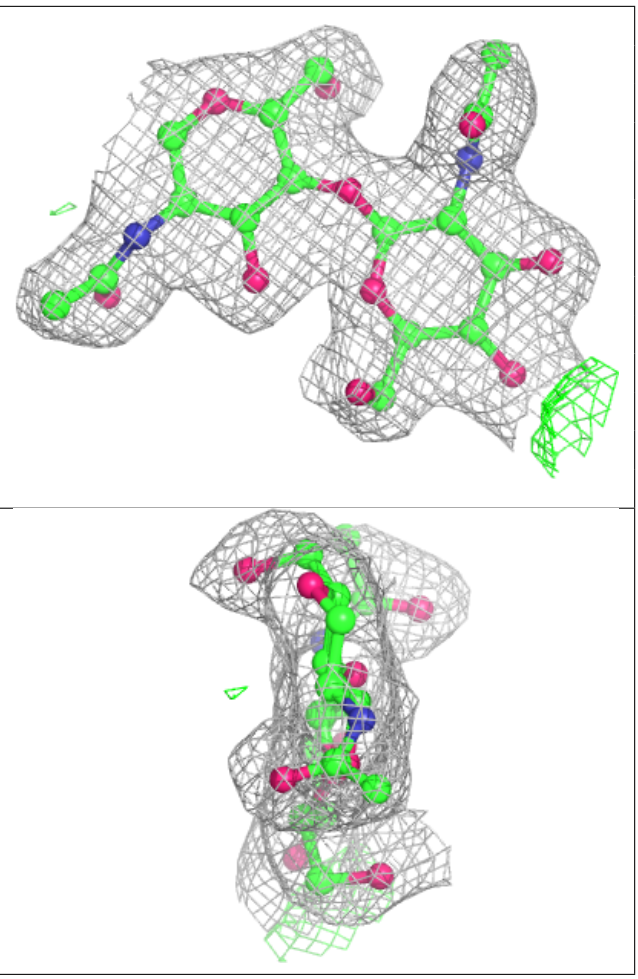






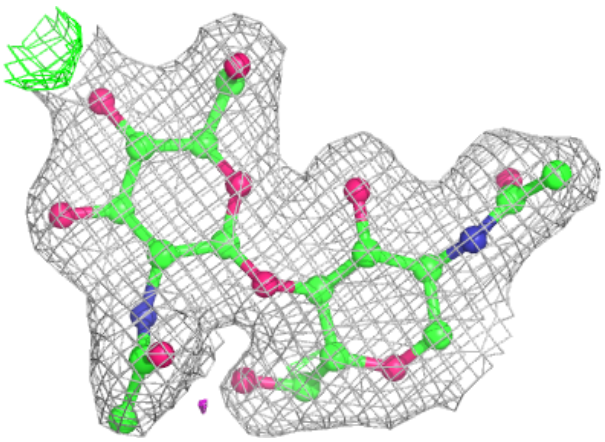
Electron density around Chain G:

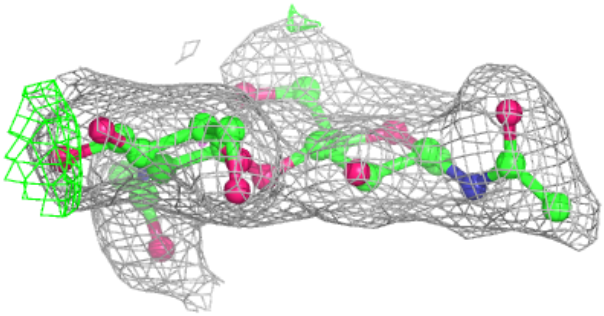
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

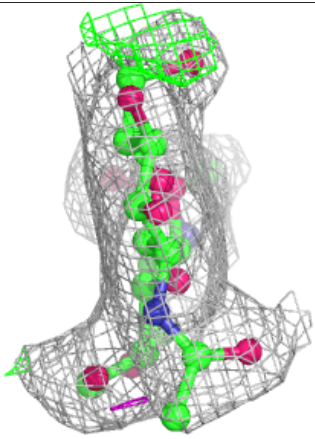


Electron density around Chain J:

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

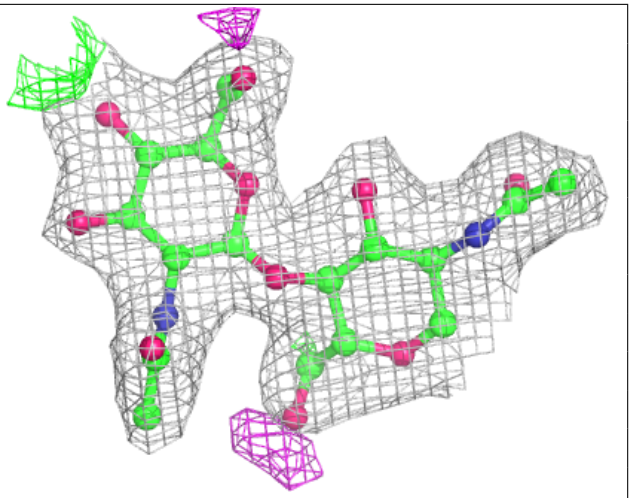


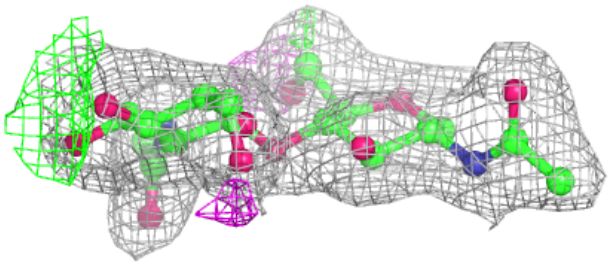




Electron density around Chain M:

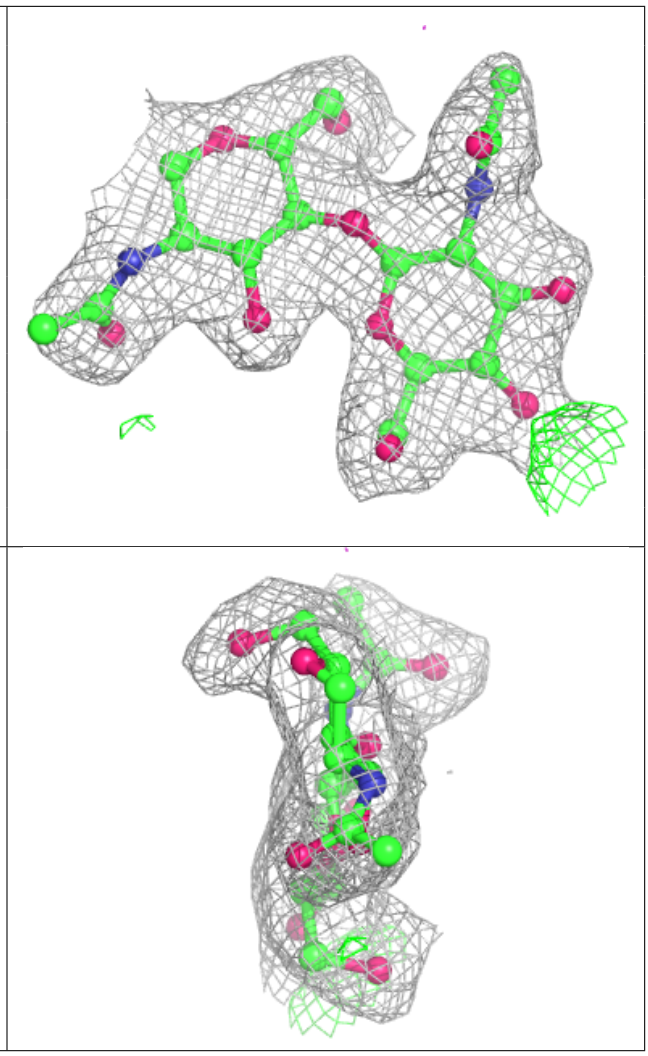
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around Chain P:

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



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, 95th 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^2)	Q<0.9
5	NAG	A	912	14/15	0.83	0.22	64,73,80,83	0
5	NAG	B	911	14/15	0.84	0.25	50,61,76,77	0
5	NAG	D	913	14/15	0.84	0.24	62,72,76,80	0
5	NAG	A	913	14/15	0.85	0.19	54,65,69,69	0
5	NAG	C	909	14/15	0.86	0.14	62,71,82,85	0
5	NAG	A	911	14/15	0.88	0.17	46,52,56,60	0
5	NAG	B	908	14/15	0.90	0.33	71,83,94,111	0
5	NAG	B	914	14/15	0.91	0.23	53,60,69,71	0
5	NAG	C	914	14/15	0.92	0.12	52,60,68,68	0

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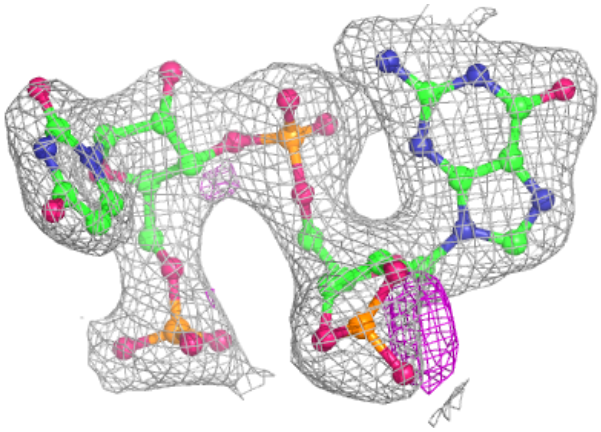
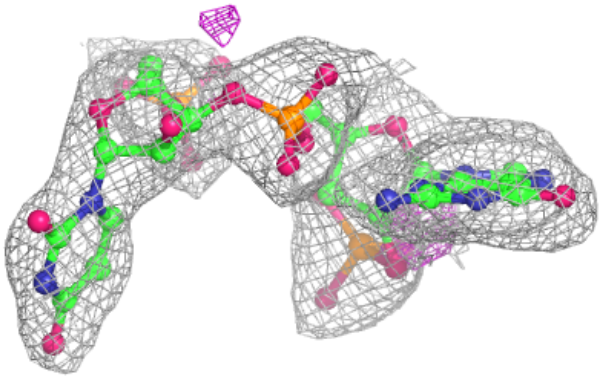
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	B	913	14/15	0.92	0.12	46,53,59,61	0
5	NAG	A	908	14/15	0.94	0.14	32,38,46,52	0
5	NAG	D	912	14/15	0.94	0.12	54,62,64,66	0
5	NAG	C	912	14/15	0.94	0.12	44,50,78,87	0
5	NAG	D	914	14/15	0.94	0.13	59,69,79,79	0
6	UCG	B	915	47/47	0.94	0.12	36,49,83,96	0
5	NAG	B	912	14/15	0.95	0.11	40,45,51,56	0
5	NAG	C	913	14/15	0.95	0.12	38,57,68,76	0
5	NAG	A	914	14/15	0.95	0.15	38,49,54,57	0
5	NAG	D	909	14/15	0.95	0.14	37,41,47,51	0
6	UCG	D	902	47/47	0.95	0.12	21,38,65,81	0
4	URI	C	902	17/17	0.96	0.12	26,35,45,48	0
6	UCG	C	901	47/47	0.96	0.11	40,48,83,106	0
6	UCG	A	915	47/47	0.96	0.12	24,31,70,79	0
4	URI	A	901	17/17	0.98	0.10	21,28,34,36	0
4	URI	D	901	17/17	0.98	0.10	17,23,29,34	0
4	URI	B	901	17/17	0.98	0.11	23,25,30,35	0

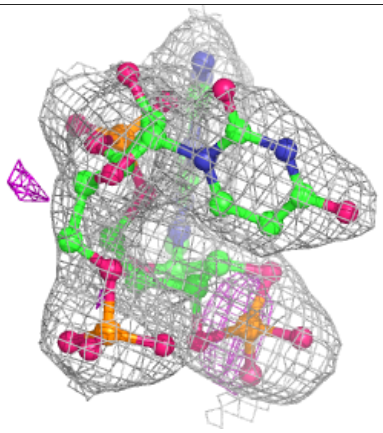
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UCG B 915:

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

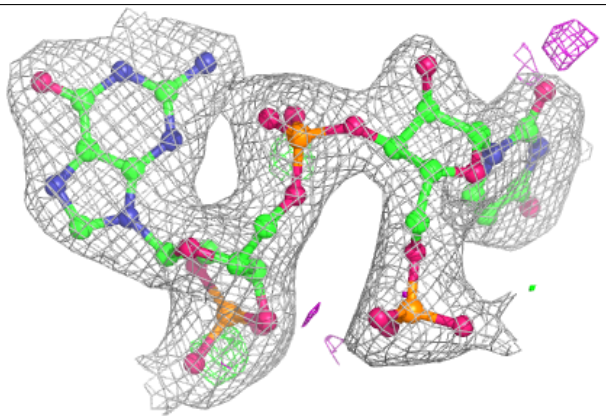


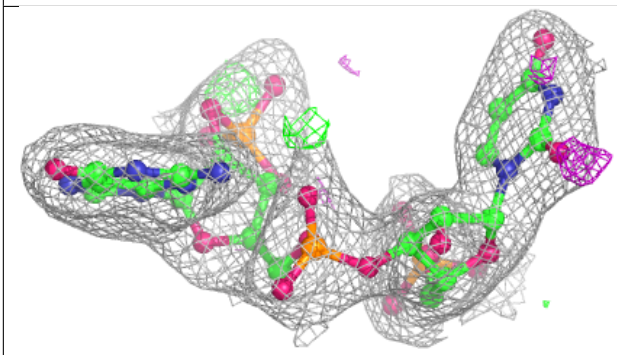


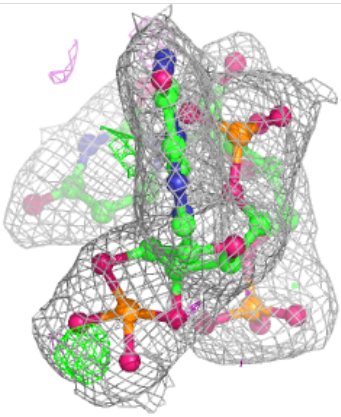


Electron density around UCG D 902:

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

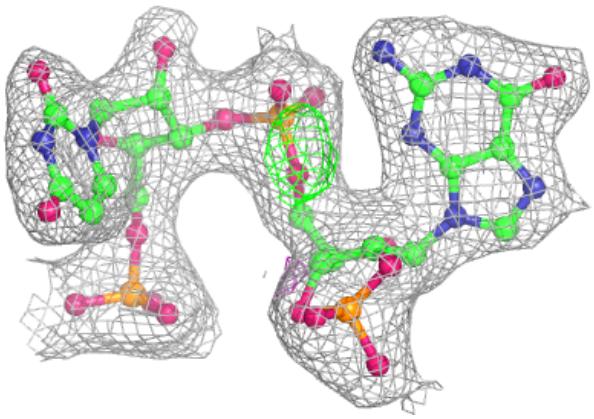


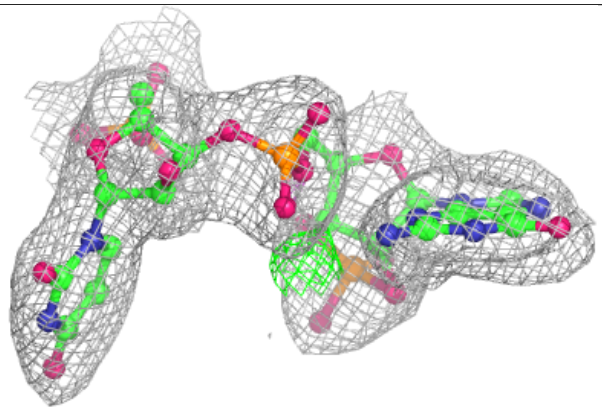


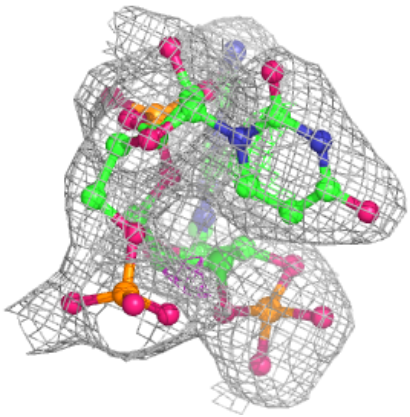


Electron density around UCG C 901:

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

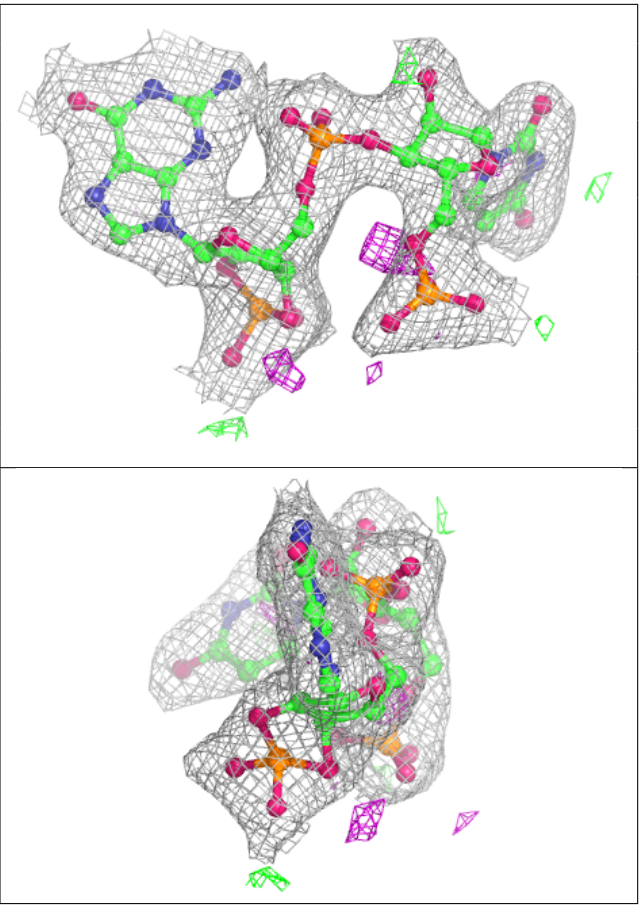






Electron density around UCG A 915:

$2mF_o$-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.