



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:58 AM UTC

PDB ID : 6WML / pdb_00006wml
Title : Human TLR8 bound to the potent agonist, GS-9688 (Selgantolimod)
Authors : Appleby, T.C.; Perry, J.K.; Mish, M.; Villasenor, A.G.; Mackman, R.L.
Deposited on : 2020-04-21
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

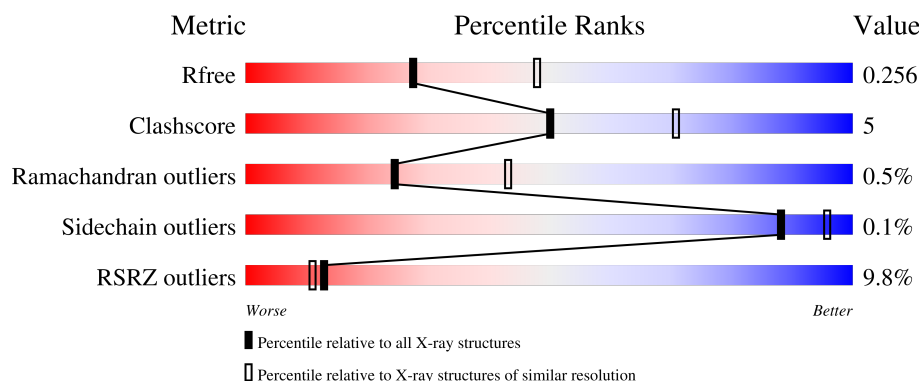
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	4% 84% 8% 8%
1	B	811	7% 80% 12% 7%
1	C	811	10% 72% 12% 16%
1	D	811	14% 76% 11% 13%
2	E	4	50% 50%

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	NAG	C	916	X	-	-	-
8	NAG	D	916	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 23787 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Toll-like receptor 8.

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

There are 40 discrepancies between the modelled and reference sequences:

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

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

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



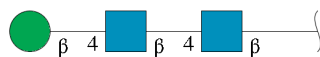
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



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

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



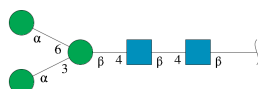
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	L	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	M	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	O	3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

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



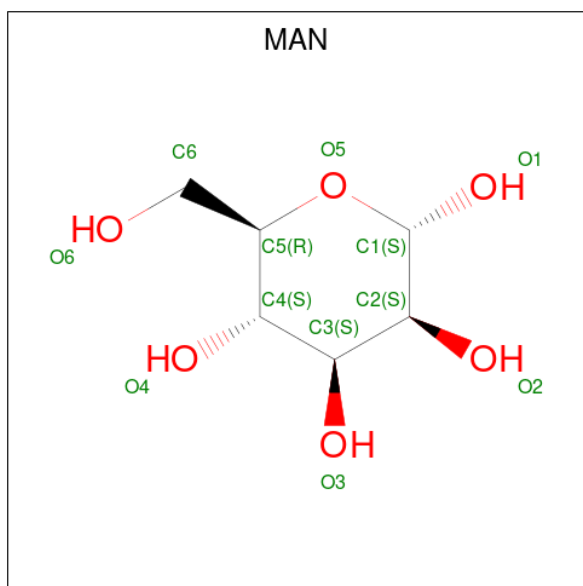
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	K	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	P	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

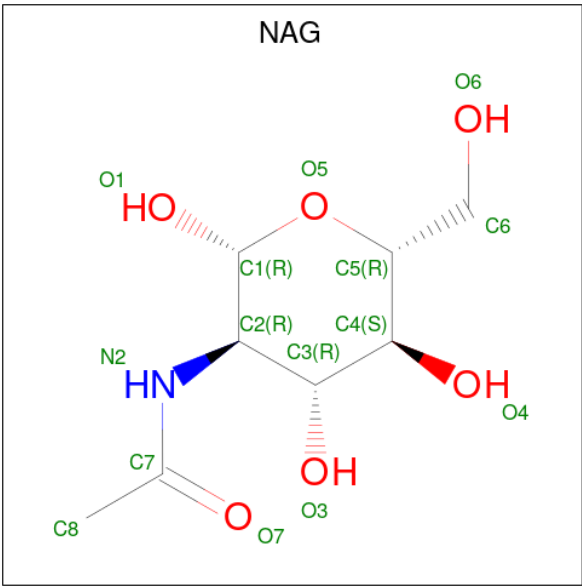
- Molecule 7 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).



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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆).



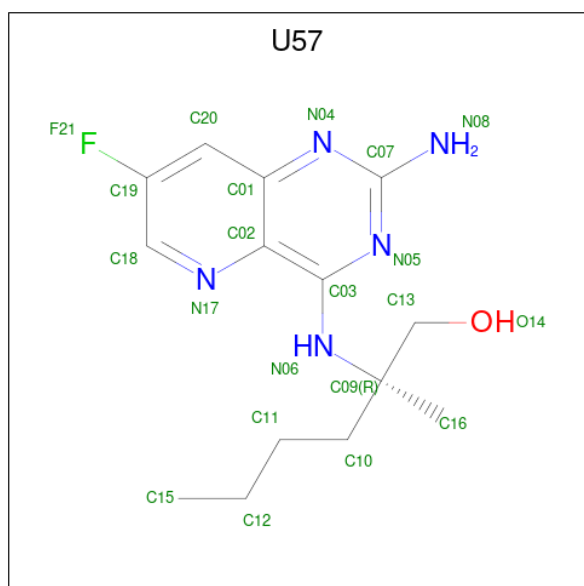
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1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

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

- Molecule 9 is (2R)-2-[(2-amino-7-fluoropyrido[3,2-d]pyrimidin-4-yl)amino]-2-methylhexan-1-ol (CCD ID: U57) (formula: C₁₄H₂₀FN₅O) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	155	Total	O	0	0
			155	155		
10	B	110	Total	O	0	0
			110	110		

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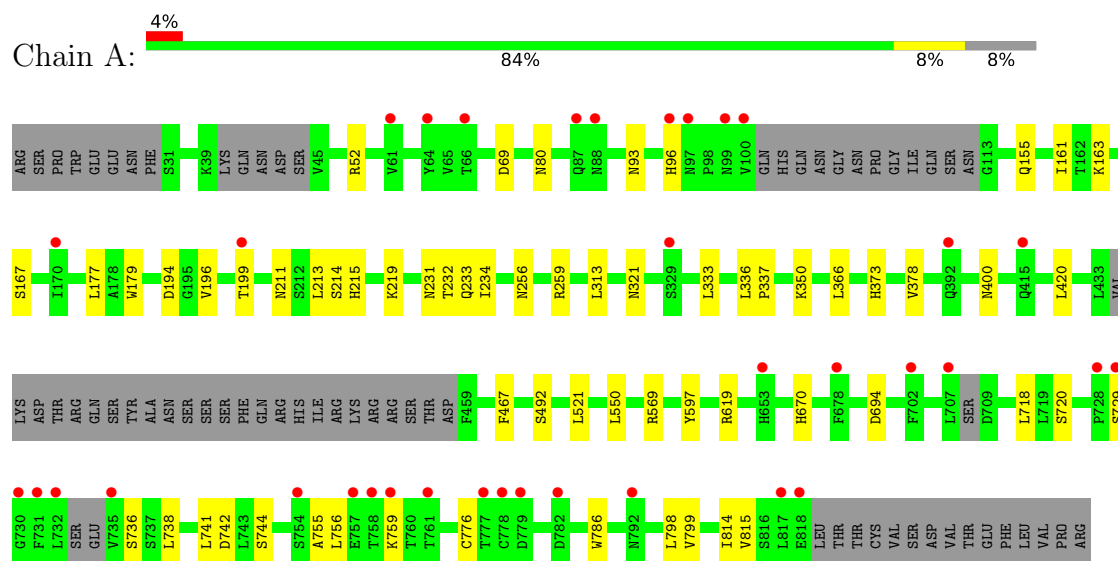
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	87	Total	O	0	0
			87	87		
10	D	72	Total	O	0	0
			72	72		

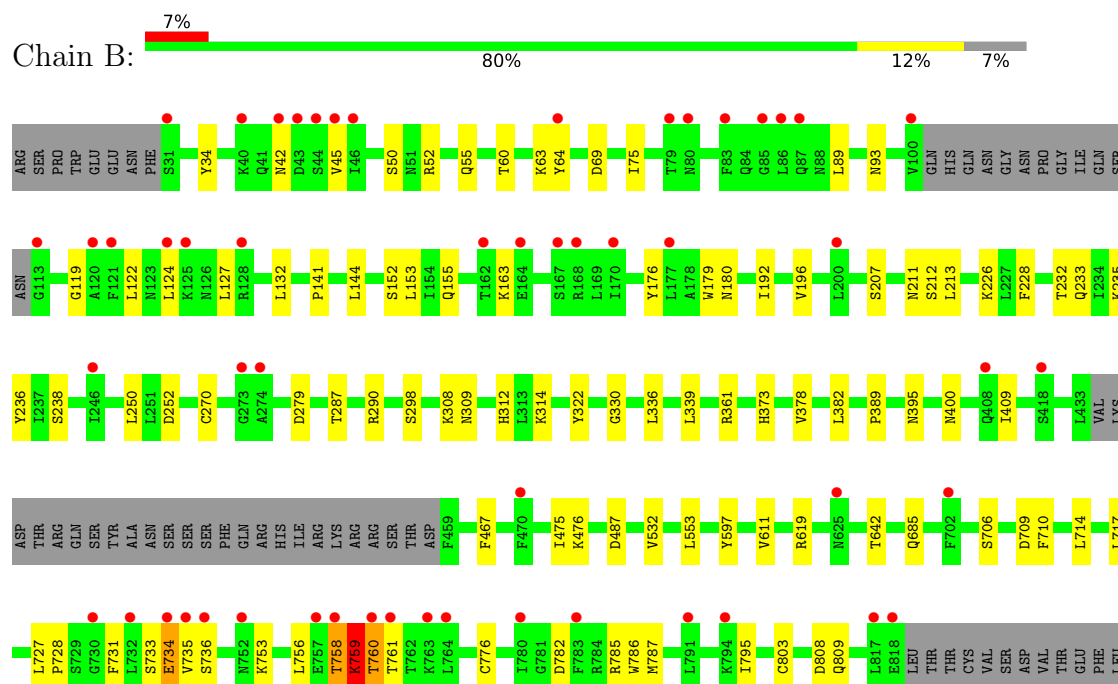
3 Residue-property plots [i](#)

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



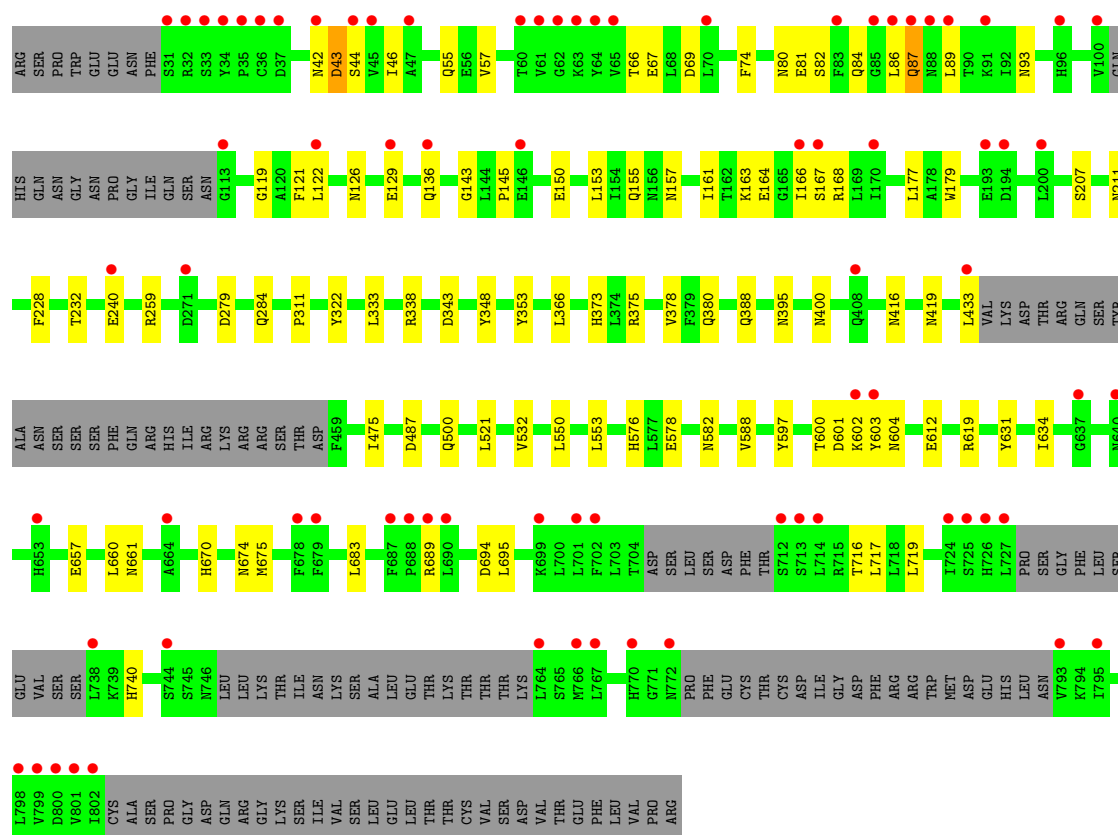
• Molecule 1: Toll-like receptor 8



VAL
PRO
ARG

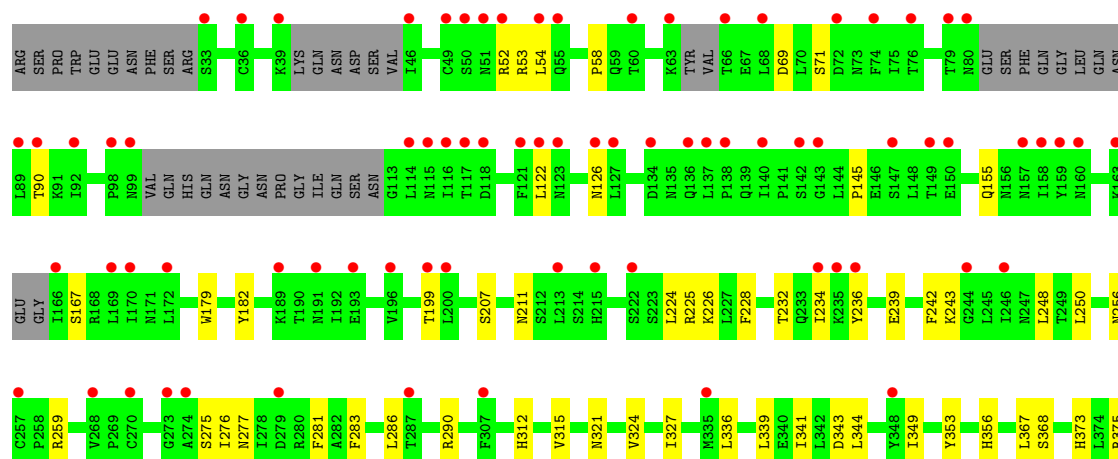
• Molecule 1: Toll-like receptor 8

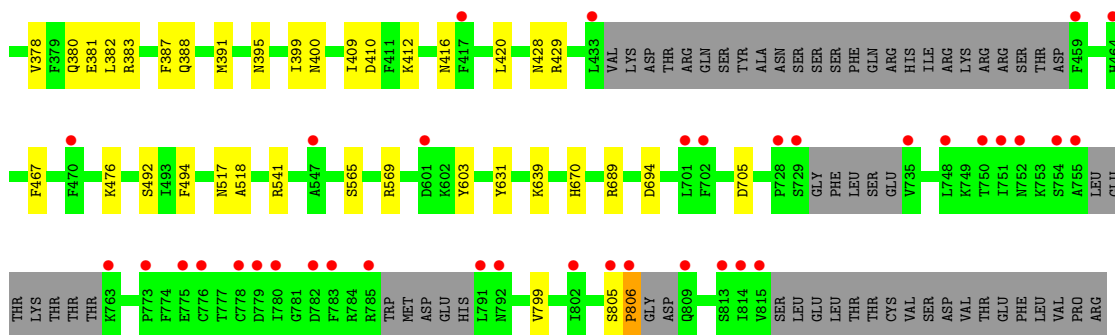
Chain C: 



• Molecule 1: Toll-like receptor 8

Chain D: 





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

Chain E:  50%



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

Chain F:  100%

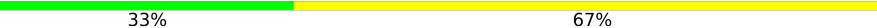


- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  67%

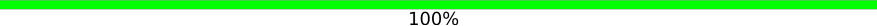


- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  33%



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

Chain I:  100%



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

Chain J:  100%

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 M:  67% 33%

MAG1
MAG2
BMA3

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

Chain O:  67% 33%

MAG1
MAG2
BMA3

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

Chain K:  50% 50%

MAG1
MAG2
BMA3
MAN4

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

Chain P:  75% 25%

MAG1
MAG2
BMA3
MAN4

- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  40% 60%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.82Å 141.57Å 171.26Å 90.00° 90.41° 90.00°	Depositor
Resolution (Å)	47.86 – 2.50 47.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.8 (47.86-2.50) 88.6 (47.86-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.211 , 0.255 0.212 , 0.256	Depositor DCC
R_{free} test set	1982 reflections (0.71%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23787	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: U57, BMA, MAN, 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	0.10	0/5844	0.30	0/7973
1	B	0.13	0/6140	0.34	1/8332 (0.0%)
1	C	0.11	0/5501	0.32	0/7470
1	D	0.14	0/5417	0.34	0/7375
All	All	0.12	0/22902	0.33	1/31150 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3
1	C	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	308	LYS	CD-CE-NZ	-6.33	91.63	111.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	758	THR	Peptide
1	B	759	LYS	Peptide
1	B	760	THR	Peptide

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Mol	Chain	Res	Type	Group
1	C	87	GLN	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	5716	0	5411	33	0
1	B	6015	0	5956	60	0
1	C	5393	0	5236	70	1
1	D	5312	0	4887	67	0
2	E	50	0	42	1	0
3	F	25	0	22	0	0
4	G	39	0	33	2	0
4	H	39	0	32	3	0
4	I	39	0	34	0	0
4	J	39	0	32	0	0
4	L	39	0	34	0	0
4	M	39	0	32	3	0
4	O	39	0	34	1	0
5	K	50	0	42	3	0
5	P	50	0	42	0	0
6	N	61	0	52	1	0
7	A	22	0	20	2	0
7	B	44	0	40	2	0
7	C	33	0	30	7	0
7	D	11	0	10	0	0
8	A	70	0	64	0	0
8	B	56	0	52	3	0
8	C	42	0	39	0	0
8	D	56	0	52	6	1
9	A	21	0	0	0	0
9	B	21	0	0	0	0
9	C	21	0	0	0	0
9	D	21	0	0	0	0
10	A	155	0	0	5	0
10	B	110	0	0	1	0
10	C	87	0	0	7	0
10	D	72	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	23787	0	22228	240	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (240) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:1004:MAN:C1	4:H:3:BMA:O3	1.64	1.42
7:C:913:MAN:C1	4:M:3:BMA:O6	1.64	1.41
7:A:1013:MAN:C1	4:G:3:BMA:O6	1.66	1.41
7:C:905:MAN:C1	5:K:3:BMA:O6	1.65	1.40
1:D:395:ASN:HD21	8:D:916:NAG:C1	1.35	1.36
1:D:395:ASN:ND2	8:D:916:NAG:C1	2.03	1.19
1:B:395:ASN:HD21	8:B:1016:NAG:C1	1.68	1.05
1:B:395:ASN:ND2	8:B:1016:NAG:C1	2.20	1.05
1:C:87:GLN:O	1:C:87:GLN:OE1	1.76	1.04
1:C:87:GLN:NE2	1:C:126:ASN:H	1.62	0.96
1:B:395:ASN:HD21	8:B:1016:NAG:C2	1.86	0.88
1:B:124:LEU:HD23	1:B:127:LEU:HB2	1.60	0.83
1:C:87:GLN:HE22	1:C:126:ASN:H	1.26	0.83
1:B:733:SER:HB3	1:B:758:THR:HA	1.64	0.80
1:D:399:ILE:HG13	1:D:420:LEU:HD21	1.65	0.78
1:B:736:SER:OG	1:B:761:THR:O	2.02	0.76
1:B:733:SER:O	1:B:735:VAL:N	2.19	0.74
1:D:242:PHE:H	1:D:243:LYS:HE2	1.51	0.74
7:B:1004:MAN:C1	4:H:3:BMA:C3	2.66	0.74
1:B:279:ASP:OD2	10:B:1101:HOH:O	2.06	0.73
1:D:239:GLU:HG3	1:D:281:PHE:HB2	1.70	0.73
1:B:141:PRO:HB2	1:B:144:LEU:HD21	1.69	0.72
1:C:87:GLN:O	1:C:87:GLN:CD	2.35	0.70
1:D:395:ASN:CG	8:D:916:NAG:C1	2.65	0.70
1:D:167:SER:HA	1:D:199:THR:HG21	1.75	0.69
1:C:119:GLY:HA2	1:C:122:LEU:HD13	1.75	0.67
1:C:87:GLN:HE22	1:C:126:ASN:N	1.92	0.67
1:C:582:ASN:ND2	10:C:1002:HOH:O	2.28	0.66
1:C:475:ILE:HD11	1:C:487:ASP:HB2	1.77	0.66
1:C:388:GLN:NE2	10:C:1003:HOH:O	2.28	0.66
1:C:87:GLN:HE22	1:C:126:ASN:HB2	1.61	0.65
1:B:34:TYR:O	1:B:60:THR:OG1	2.14	0.64
1:C:259:ARG:NH2	1:C:348:TYR:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:ILE:HB	1:C:67:GLU:HB2	1.78	0.64
7:C:905:MAN:C1	5:K:3:BMA:C6	2.74	0.64
1:B:163:LYS:HA	1:B:196:VAL:HG23	1.80	0.64
1:A:52:ARG:HG2	1:A:799:VAL:HG11	1.80	0.63
1:B:759:LYS:HB3	1:B:760:THR:OG1	1.98	0.63
1:C:416:ASN:ND2	10:C:1006:HOH:O	2.33	0.62
1:D:122:LEU:HA	1:D:145:PRO:HG3	1.82	0.60
1:C:240:GLU:OE1	1:C:240:GLU:N	2.33	0.60
1:D:375:ARG:HD2	1:D:400:ASN:HD21	1.67	0.59
1:C:716:THR:HG23	1:C:740:HIS:HB3	1.84	0.58
1:D:242:PHE:N	1:D:243:LYS:HE2	2.17	0.58
1:B:475:ILE:HD11	1:B:487:ASP:HB2	1.86	0.58
1:D:368:SER:HA	1:D:395:ASN:HD22	1.69	0.58
1:C:395:ASN:ND2	10:C:1008:HOH:O	2.35	0.58
1:D:52:ARG:HG2	1:D:799:VAL:HG21	1.86	0.57
1:D:395:ASN:ND2	8:D:916:NAG:O5	2.37	0.57
1:D:167:SER:CA	1:D:199:THR:HG21	2.34	0.57
1:C:602:LYS:HD3	1:C:603:TYR:H	1.69	0.57
1:B:119:GLY:CA	1:B:122:LEU:HD22	2.35	0.57
1:C:211:ASN:O	1:C:232:THR:HA	2.05	0.56
1:B:228:PHE:HA	1:B:252:ASP:HB3	1.87	0.56
1:D:639:LYS:HA	1:D:639:LYS:HE2	1.87	0.56
1:B:753:LYS:HA	1:B:756:LEU:HD12	1.88	0.55
1:B:63:LYS:H	1:B:63:LYS:HE2	1.70	0.55
1:C:80:ASN:O	1:C:84:GLN:NE2	2.39	0.55
1:B:756:LEU:HB3	1:B:786:TRP:CD1	2.41	0.55
1:D:388:GLN:HA	1:D:391:MET:HE3	1.89	0.55
1:C:660:LEU:HD21	1:C:683:LEU:HD22	1.89	0.54
1:D:518:ALA:HB2	1:D:541:ARG:HG3	1.90	0.54
1:C:57:VAL:HG11	1:C:82:SER:HB3	1.90	0.54
1:A:231:ASN:ND2	10:A:1111:HOH:O	2.41	0.54
1:C:69:ASP:HA	1:C:93:ASN:HB3	1.89	0.54
7:C:913:MAN:C1	4:M:3:BMA:C6	2.78	0.54
1:D:356:HIS:CE1	1:D:383:ARG:HH11	2.26	0.54
1:B:192:ILE:HD11	1:B:213:LEU:HD22	1.91	0.53
1:C:42:ASN:O	1:C:43:ASP:HB2	2.08	0.53
1:C:87:GLN:NE2	1:C:126:ASN:N	2.42	0.53
7:C:913:MAN:C2	4:M:3:BMA:O6	2.51	0.53
1:A:161:ILE:HD12	1:A:177:LEU:HD13	1.91	0.53
1:C:521:LEU:HD13	1:C:550:LEU:HD21	1.90	0.53
1:D:476:LYS:HD2	4:O:1:NAG:H83	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ASP:OD2	1:A:219:LYS:NZ	2.35	0.53
1:A:521:LEU:HD13	1:A:550:LEU:HD21	1.91	0.53
1:A:211:ASN:O	1:A:232:THR:HA	2.08	0.52
1:B:611:VAL:HG13	1:B:642:THR:HG22	1.91	0.52
1:D:259:ARG:NH1	1:D:321:ASN:O	2.42	0.52
1:C:129:GLU:HG3	1:C:150:GLU:HB3	1.91	0.52
1:C:419:ASN:O	1:C:419:ASN:ND2	2.43	0.52
1:B:45:VAL:HG11	1:B:64:TYR:HD1	1.74	0.52
1:B:706:SER:HB3	1:B:709:ASP:OD1	2.09	0.52
1:C:375:ARG:NH1	10:C:1016:HOH:O	2.43	0.52
1:D:670:HIS:HA	1:D:694:ASP:HB3	1.92	0.51
1:D:242:PHE:H	1:D:243:LYS:CE	2.21	0.51
1:A:350:LYS:NZ	10:A:1109:HOH:O	2.39	0.51
1:D:234:ILE:O	1:D:256:ASN:HB3	2.11	0.51
1:C:284:GLN:NE2	10:C:1011:HOH:O	2.40	0.50
1:D:399:ILE:HD12	1:D:420:LEU:HD11	1.92	0.50
1:C:717:LEU:CD2	1:C:719:LEU:HG	2.41	0.50
1:D:207:SER:HA	1:D:228:PHE:HB2	1.92	0.50
1:B:212:SER:OG	1:B:233:GLN:OE1	2.24	0.50
1:D:367:LEU:O	1:D:395:ASN:ND2	2.45	0.50
1:D:467:PHE:HB3	6:N:1:NAG:H81	1.93	0.50
1:B:782:ASP:OD1	1:B:785:ARG:NH2	2.43	0.50
1:B:532:VAL:HB	1:B:553:LEU:HD22	1.94	0.50
1:D:69:ASP:OD1	1:D:71:SER:OG	2.27	0.50
1:D:387:PHE:O	1:D:391:MET:HG3	2.11	0.49
1:B:336:LEU:HB3	1:B:339:LEU:HB2	1.95	0.49
1:B:373:HIS:HA	1:B:400:ASN:HB3	1.94	0.49
1:B:597:TYR:HB3	1:B:619:ARG:HB2	1.94	0.49
1:C:136:GLN:HG2	1:C:157:ASN:HD21	1.77	0.49
1:B:207:SER:HA	1:B:228:PHE:HB2	1.94	0.49
1:B:236:TYR:CE2	1:B:238:SER:HB3	2.47	0.49
1:A:569:ARG:NH2	10:A:1121:HOH:O	2.45	0.49
1:C:86:LEU:HB3	1:C:89:LEU:HG	1.95	0.48
1:C:333:LEU:HD22	1:C:366:LEU:HD11	1.96	0.48
1:D:225:ARG:HA	1:D:248:LEU:HA	1.95	0.48
1:D:226:LYS:HG2	1:D:250:LEU:HB3	1.94	0.48
1:B:298:SER:HB3	1:B:322:TYR:HE2	1.78	0.48
1:B:734:GLU:HG2	1:B:735:VAL:H	1.77	0.48
1:D:391:MET:SD	1:D:416:ASN:HB3	2.54	0.48
1:A:729:SER:HA	1:A:755:ALA:HA	1.95	0.48
1:B:180:ASN:HB2	1:B:211:ASN:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:GLN:HA	1:D:179:TRP:O	2.13	0.48
1:B:211:ASN:O	1:B:232:THR:HA	2.14	0.48
1:C:657:GLU:O	1:C:661:ASN:ND2	2.47	0.48
1:A:718:LEU:HA	1:A:742:ASP:HB3	1.96	0.47
1:B:287:THR:HA	1:B:309:ASN:O	2.14	0.47
1:C:87:GLN:NE2	1:C:126:ASN:HB2	2.27	0.47
1:D:290:ARG:HD2	1:D:312:HIS:O	2.14	0.47
1:D:54:LEU:HD13	1:D:58:PRO:HD3	1.97	0.47
1:C:161:ILE:HD12	1:C:177:LEU:HD13	1.96	0.47
1:D:327:ILE:HG12	1:D:344:LEU:HD13	1.96	0.47
1:B:119:GLY:C	1:B:122:LEU:HD22	2.39	0.47
1:A:756:LEU:HD13	1:A:786:TRP:HB2	1.96	0.47
1:C:87:GLN:HE22	1:C:126:ASN:CB	2.28	0.47
1:D:382:LEU:HB3	1:D:409:ILE:HD13	1.96	0.47
1:A:798:LEU:HD22	1:A:815:VAL:HG11	1.97	0.47
1:B:290:ARG:HD2	1:B:312:HIS:O	2.15	0.47
1:D:283:PHE:HA	1:D:286:LEU:HD12	1.96	0.47
1:D:705:ASP:OD1	1:D:705:ASP:N	2.45	0.47
1:D:375:ARG:HD2	1:D:400:ASN:ND2	2.30	0.46
1:C:207:SER:HA	1:C:228:PHE:HB2	1.96	0.46
1:C:532:VAL:HB	1:C:553:LEU:HD22	1.97	0.46
1:D:343:ASP:HA	1:D:373:HIS:HB2	1.96	0.46
1:D:410:ASP:OD1	1:D:412:LYS:HE3	2.16	0.46
1:C:689:ARG:HG2	1:C:689:ARG:HH11	1.80	0.46
1:A:597:TYR:HB3	1:A:619:ARG:HB2	1.98	0.46
1:B:760:THR:HG22	1:B:761:THR:N	2.30	0.46
1:D:53:ARG:HE	1:D:53:ARG:HB2	1.53	0.46
1:A:333:LEU:HD22	1:A:366:LEU:HD11	1.98	0.46
1:A:467:PHE:HB3	2:E:1:NAG:H81	1.97	0.46
1:B:119:GLY:O	1:B:122:LEU:CD2	2.64	0.46
1:A:670:HIS:HA	1:A:694:ASP:HB3	1.98	0.46
1:C:597:TYR:HB3	1:C:619:ARG:HB2	1.99	0.45
1:A:163:LYS:HA	1:A:196:VAL:HG23	1.98	0.45
7:C:905:MAN:C2	5:K:3:BMA:O6	2.56	0.45
1:D:420:LEU:HD23	1:D:420:LEU:HA	1.72	0.45
1:D:211:ASN:O	1:D:232:THR:HA	2.17	0.45
1:B:803:CYS:HB2	1:B:809:GLN:O	2.17	0.45
1:D:90:THR:HA	1:D:126:ASN:O	2.16	0.45
1:D:336:LEU:HD13	1:D:339:LEU:HD22	1.98	0.45
1:D:689:ARG:NH1	10:D:1012:HOH:O	2.50	0.45
1:B:55:GLN:O	1:B:75:ILE:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:685:GLN:HG3	1:B:710:PHE:HA	1.99	0.45
1:C:600:THR:O	1:C:602:LYS:N	2.51	0.45
7:A:1013:MAN:C5	4:G:3:BMA:O6	2.65	0.44
1:A:373:HIS:HA	1:A:400:ASN:HB3	1.98	0.44
1:C:603:TYR:HB3	1:C:631:TYR:CD1	2.53	0.44
1:D:324:VAL:HG11	1:D:349:ILE:HD11	2.00	0.44
1:B:382:LEU:HB3	1:B:409:ILE:HG12	2.00	0.44
1:B:467:PHE:HB3	4:H:1:NAG:H81	2.00	0.44
1:C:259:ARG:HG3	1:C:322:TYR:CZ	2.53	0.44
1:D:429:ARG:NH1	1:D:492:SER:OG	2.49	0.44
1:C:670:HIS:HA	1:C:694:ASP:HB3	2.00	0.44
1:D:315:VAL:HG22	1:D:341:ILE:HB	2.00	0.44
1:D:494:PHE:HA	1:D:517:ASN:HA	2.00	0.43
1:A:80:ASN:ND2	10:A:1126:HOH:O	2.49	0.43
1:B:69:ASP:HA	1:B:93:ASN:HB3	1.99	0.43
1:B:132:LEU:HB2	1:B:153:LEU:HD23	2.00	0.43
1:C:153:LEU:HB2	1:C:177:LEU:HD23	2.00	0.43
1:A:492:SER:OG	10:A:1101:HOH:O	2.21	0.43
1:D:395:ASN:CG	8:D:916:NAG:O5	2.61	0.43
1:A:214:SER:HA	1:A:233:GLN:O	2.19	0.43
1:B:290:ARG:NH2	1:B:314:LYS:HD3	2.34	0.43
1:C:674:ASN:HB3	1:C:675:MET:H	1.63	0.43
1:B:714:LEU:HD21	1:B:717:LEU:HD13	1.99	0.43
1:C:121:PHE:O	1:C:145:PRO:HG3	2.19	0.43
1:B:152:SER:HA	1:B:176:TYR:HB2	1.99	0.43
1:B:727:LEU:HD23	1:B:727:LEU:HA	1.87	0.43
1:C:604:ASN:HA	1:C:634:ILE:HA	2.00	0.43
1:C:163:LYS:HG2	1:C:167:SER:OG	2.18	0.43
1:A:69:ASP:HA	1:A:93:ASN:HB3	2.01	0.43
1:C:375:ARG:HD3	1:C:400:ASN:HD21	1.83	0.43
1:B:235:LYS:HG2	1:B:270:CYS:SG	2.59	0.42
1:B:728:PRO:HG2	1:B:731:PHE:CD1	2.54	0.42
1:B:808:ASP:CG	1:B:809:GLN:HG2	2.43	0.42
1:C:343:ASP:HA	1:C:373:HIS:HB2	2.01	0.42
1:C:576:HIS:ND1	1:C:578:GLU:OE2	2.46	0.42
1:A:720:SER:HA	1:A:744:SER:O	2.20	0.42
1:C:55:GLN:HA	1:C:74:PHE:HB2	2.02	0.42
1:A:155:GLN:HA	1:A:179:TRP:O	2.19	0.42
1:A:167:SER:O	1:A:199:THR:HG21	2.19	0.42
1:D:805:SER:HA	1:D:806:PRO:HA	1.82	0.42
1:C:166:ILE:HD13	1:C:166:ILE:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:603:TYR:HB3	1:D:631:TYR:CD1	2.55	0.42
1:A:738:LEU:HD21	1:A:741:LEU:HD13	2.01	0.42
1:C:81:GLU:HA	1:C:84:GLN:CD	2.44	0.42
1:C:588:VAL:HG13	1:C:612:GLU:HB3	2.01	0.42
1:C:602:LYS:CE	1:C:602:LYS:HA	2.50	0.42
1:D:373:HIS:HA	1:D:400:ASN:HB3	2.01	0.42
1:D:395:ASN:OD1	8:D:916:NAG:C1	2.68	0.42
1:C:164:GLU:HA	1:C:168:ARG:HH12	1.85	0.41
1:B:155:GLN:HA	1:B:179:TRP:O	2.20	0.41
1:D:353:TYR:CZ	1:D:380:GLN:HG2	2.55	0.41
1:D:356:HIS:HE1	1:D:381:GLU:OE1	2.04	0.41
1:A:313:LEU:HD23	1:A:336:LEU:HD22	2.03	0.41
1:A:420:LEU:HD23	1:A:420:LEU:HA	1.90	0.41
1:C:603:TYR:HB3	1:C:631:TYR:CE1	2.54	0.41
1:C:311:PRO:O	1:C:338:ARG:NE	2.48	0.41
1:C:602:LYS:HA	1:C:602:LYS:HE2	2.01	0.41
1:D:428:ASN:O	1:D:429:ARG:HD2	2.20	0.41
1:A:776:CYS:SG	1:A:814:ILE:HG22	2.60	0.41
1:C:155:GLN:HA	1:C:179:TRP:O	2.19	0.41
1:A:259:ARG:NH1	1:A:321:ASN:O	2.52	0.41
1:D:224:LEU:HD23	1:D:224:LEU:HA	1.86	0.41
1:D:242:PHE:HB3	1:D:286:LEU:HD21	2.02	0.41
1:A:337:PRO:HB2	1:C:311:PRO:HB3	2.01	0.41
1:B:226:LYS:HG2	1:B:250:LEU:HB3	2.03	0.41
1:C:87:GLN:HE22	1:C:126:ASN:CA	2.33	0.41
1:C:353:TYR:CZ	1:C:380:GLN:HG2	2.56	0.41
1:B:361:ARG:HA	1:B:389:PRO:HB3	2.03	0.41
1:B:776:CYS:HB2	1:B:803:CYS:HB3	1.99	0.41
1:C:695:LEU:HB2	1:C:719:LEU:HD23	2.02	0.41
1:D:155:GLN:NE2	1:D:182:TYR:OH	2.26	0.41
1:D:236:TYR:HD1	1:D:277:ASN:HB3	1.85	0.41
1:D:275:SER:OG	1:D:276:ILE:N	2.53	0.41
1:C:717:LEU:C	1:C:717:LEU:HD23	2.46	0.41
1:D:565:SER:O	1:D:569:ARG:HG3	2.21	0.41
1:A:234:ILE:O	1:A:256:ASN:HB3	2.20	0.40
1:D:242:PHE:C	1:D:243:LYS:HE2	2.46	0.40
1:A:213:LEU:C	1:A:215:HIS:H	2.30	0.40
1:B:50:SER:O	1:B:52:ARG:NH1	2.55	0.40
1:B:89:LEU:HD23	1:B:89:LEU:HA	1.85	0.40
1:B:787:MET:HE3	1:B:795:ILE:HD12	2.03	0.40
1:C:433:LEU:H	1:C:500:GLN:HE22	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:905:MAN:O3	10:C:1001:HOH:O	2.22	0.40
1:C:44:SER:HB3	1:C:66:THR:OG1	2.22	0.40

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

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	734/811 (90%)	690 (94%)	41 (6%)	3 (0%)	30	49
1	B	745/811 (92%)	695 (93%)	45 (6%)	5 (1%)	18	34
1	C	667/811 (82%)	626 (94%)	37 (6%)	4 (1%)	21	38
1	D	688/811 (85%)	642 (93%)	44 (6%)	2 (0%)	36	55
All	All	2834/3244 (87%)	2653 (94%)	167 (6%)	14 (0%)	24	43

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	734	GLU
1	A	759	LYS
1	B	759	LYS
1	A	736	SER
1	C	43	ASP
1	A	378	VAL
1	B	42	ASN
1	C	601	ASP

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Mol	Chain	Res	Type
1	B	330	GLY
1	B	378	VAL
1	C	143	GLY
1	C	378	VAL
1	D	378	VAL
1	D	806	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	609/755 (81%)	607 (100%)	2 (0%)	86	94
1	B	687/755 (91%)	686 (100%)	1 (0%)	88	96
1	C	597/755 (79%)	597 (100%)	0	100	100
1	D	536/755 (71%)	536 (100%)	0	100	100
All	All	2429/3020 (80%)	2426 (100%)	3 (0%)	88	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96[A]	HIS
1	A	96[B]	HIS
1	B	476	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	184	ASN
1	A	231	ASN
1	A	285	ASN
1	A	539	ASN
1	A	593	HIS
1	A	604	ASN

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Mol	Chain	Res	Type
1	A	721	HIS
1	A	790	HIS
1	B	42	ASN
1	B	59	GLN
1	B	87	GLN
1	B	174	ASN
1	B	184	ASN
1	B	215	HIS
1	B	312	HIS
1	B	388	GLN
1	B	395	ASN
1	B	539	ASN
1	B	582	ASN
1	B	685	GLN
1	B	809	GLN
1	C	41	GLN
1	C	87	GLN
1	C	157	ASN
1	C	184	ASN
1	C	373	HIS
1	C	400	ASN
1	C	408	GLN
1	C	582	ASN
1	C	595	ASN
1	D	184	ASN
1	D	288	GLN
1	D	309	ASN
1	D	356	HIS
1	D	392	GLN
1	D	395	ASN
1	D	400	ASN
1	D	416	ASN
1	D	595	ASN
1	D	661	ASN
1	D	686	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

40 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	E	1	1,2	14,14,15	0.28	0	17,19,21	0.37	0
2	NAG	E	2	2	14,14,15	0.21	0	17,19,21	0.41	0
2	BMA	E	3	2	11,11,12	0.56	0	15,15,17	0.72	0
2	MAN	E	4	2	11,11,12	0.68	0	15,15,17	0.98	2 (13%)
3	NAG	F	1	3	14,14,15	0.25	0	17,19,21	0.40	0
3	BMA	F	2	3	11,11,12	0.68	0	15,15,17	0.76	0
4	NAG	G	1	4,1	14,14,15	0.28	0	17,19,21	0.37	0
4	NAG	G	2	4	14,14,15	0.28	0	17,19,21	0.41	0
4	BMA	G	3	4	11,11,12	0.62	0	15,15,17	0.71	0
4	NAG	H	1	4	14,14,15	0.24	0	17,19,21	0.37	0
4	NAG	H	2	4	14,14,15	0.19	0	17,19,21	0.44	0
4	BMA	H	3	4	11,11,12	0.62	0	15,15,17	0.70	0
4	NAG	I	1	4,1	14,14,15	0.27	0	17,19,21	0.45	0
4	NAG	I	2	4	14,14,15	0.24	0	17,19,21	0.44	0
4	BMA	I	3	4	11,11,12	0.70	0	15,15,17	0.75	0
4	NAG	J	1	4,1	14,14,15	0.29	0	17,19,21	0.37	0
4	NAG	J	2	4	14,14,15	0.28	0	17,19,21	0.38	0
4	BMA	J	3	4	11,11,12	0.58	0	15,15,17	0.72	0
5	NAG	K	1	1,5	14,14,15	0.29	0	17,19,21	0.36	0
5	NAG	K	2	5	14,14,15	0.20	0	17,19,21	0.44	0
5	BMA	K	3	5	11,11,12	0.61	0	15,15,17	0.72	0
5	MAN	K	4	5	11,11,12	0.75	0	15,15,17	0.97	2 (13%)
4	NAG	L	1	4,1	14,14,15	0.25	0	17,19,21	0.41	0
4	NAG	L	2	4	14,14,15	0.28	0	17,19,21	0.38	0
4	BMA	L	3	4	11,11,12	0.68	0	15,15,17	0.75	0
4	NAG	M	1	4	14,14,15	0.26	0	17,19,21	0.39	0
4	NAG	M	2	4	14,14,15	0.23	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMA	M	3	4	11,11,12	0.62	0	15,15,17	0.78	0
6	NAG	N	1	1,6	14,14,15	0.24	0	17,19,21	0.39	0
6	NAG	N	2	6	14,14,15	0.18	0	17,19,21	0.47	0
6	BMA	N	3	6	11,11,12	0.56	0	15,15,17	0.76	0
6	MAN	N	4	6	11,11,12	0.65	0	15,15,17	1.04	2 (13%)
6	MAN	N	5	6	11,11,12	0.66	0	15,15,17	1.03	2 (13%)
4	NAG	O	1	4,1	14,14,15	0.26	0	17,19,21	0.42	0
4	NAG	O	2	4	14,14,15	0.26	0	17,19,21	0.39	0
4	BMA	O	3	4	11,11,12	0.60	0	15,15,17	0.74	0
5	NAG	P	1	1,5	14,14,15	0.23	0	17,19,21	0.40	0
5	NAG	P	2	5	14,14,15	0.26	0	17,19,21	0.39	0
5	BMA	P	3	5	11,11,12	0.61	0	15,15,17	0.71	0
5	MAN	P	4	5	11,11,12	0.66	0	15,15,17	1.01	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	2/2/19/22	0/1/1/1
3	NAG	F	1	3	-	0/6/23/26	0/1/1/1
3	BMA	F	2	3	-	0/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	NAG	H	1	4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1
4	NAG	I	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	BMA	I	3	4	-	2/2/19/22	0/1/1/1
4	NAG	J	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
5	NAG	K	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	4	MAN	C1-O5-C5	2.51	115.55	112.19
5	K	4	MAN	C1-O5-C5	2.43	115.44	112.19
5	P	4	MAN	C1-O5-C5	2.40	115.41	112.19
6	N	5	MAN	C1-O5-C5	2.38	115.38	112.19
2	E	4	MAN	C1-O5-C5	2.35	115.34	112.19
2	E	4	MAN	O2-C2-C3	-2.18	105.63	110.15
5	P	4	MAN	O2-C2-C3	-2.16	105.68	110.15
6	N	5	MAN	O2-C2-C3	-2.15	105.70	110.15
6	N	4	MAN	O2-C2-C3	-2.13	105.74	110.15
5	K	4	MAN	O2-C2-C3	-2.12	105.76	110.15

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	O	3	BMA	O5-C5-C6-O6

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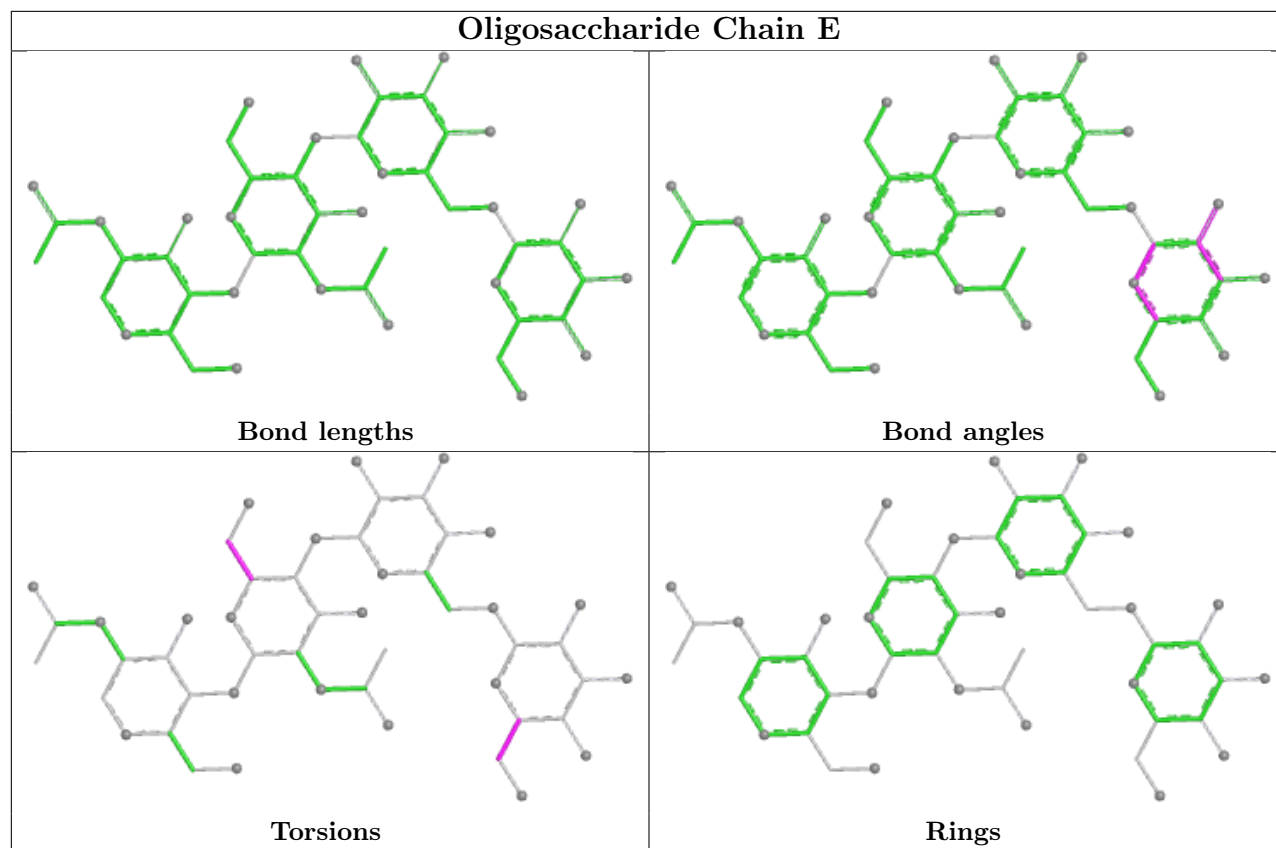
Mol	Chain	Res	Type	Atoms
2	E	4	MAN	O5-C5-C6-O6
6	N	5	MAN	O5-C5-C6-O6
6	N	5	MAN	C4-C5-C6-O6
2	E	4	MAN	C4-C5-C6-O6
4	O	3	BMA	C4-C5-C6-O6
4	I	3	BMA	O5-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
6	N	2	NAG	C4-C5-C6-O6
4	I	3	BMA	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6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

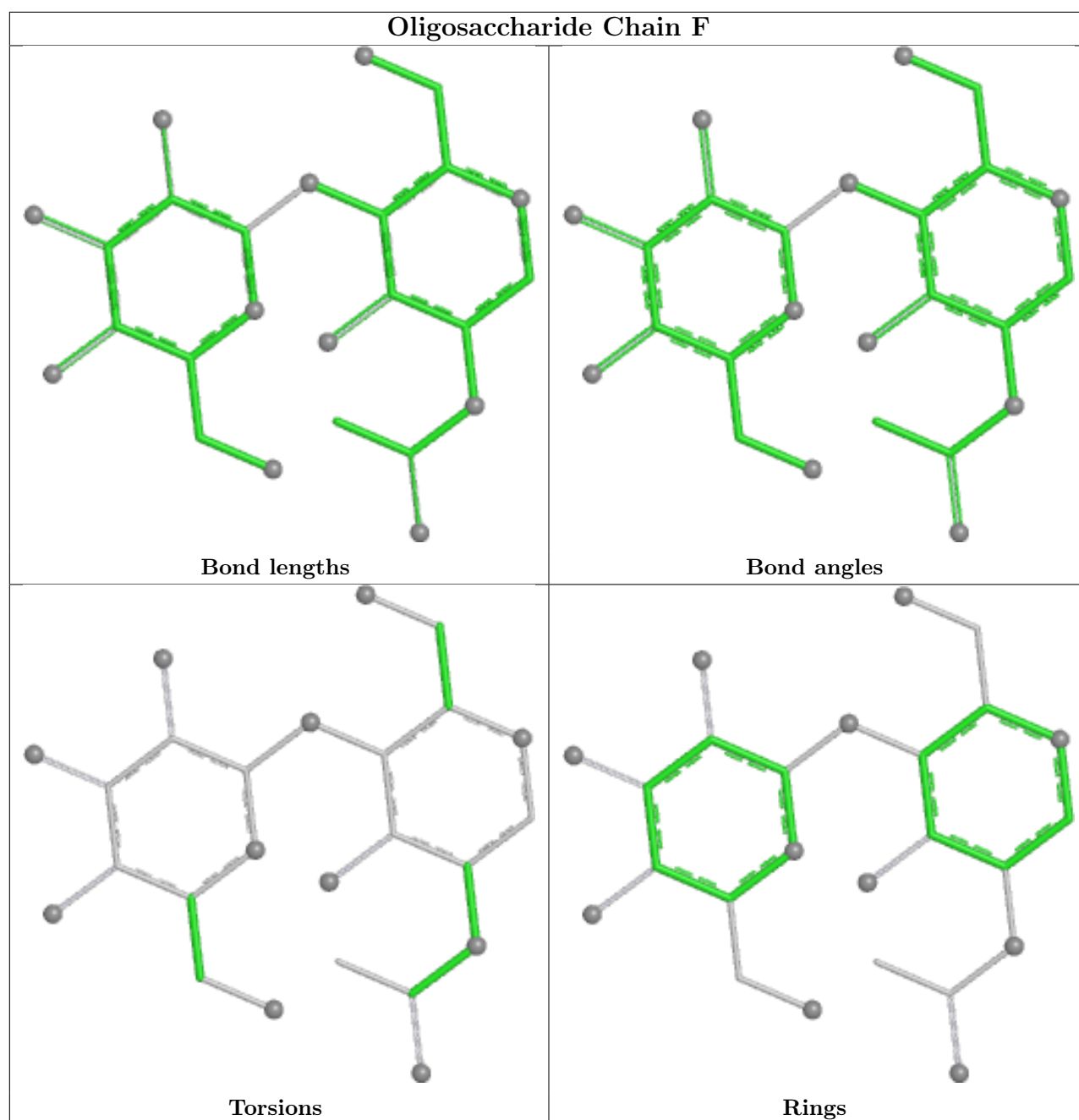
There are no ring outliers.

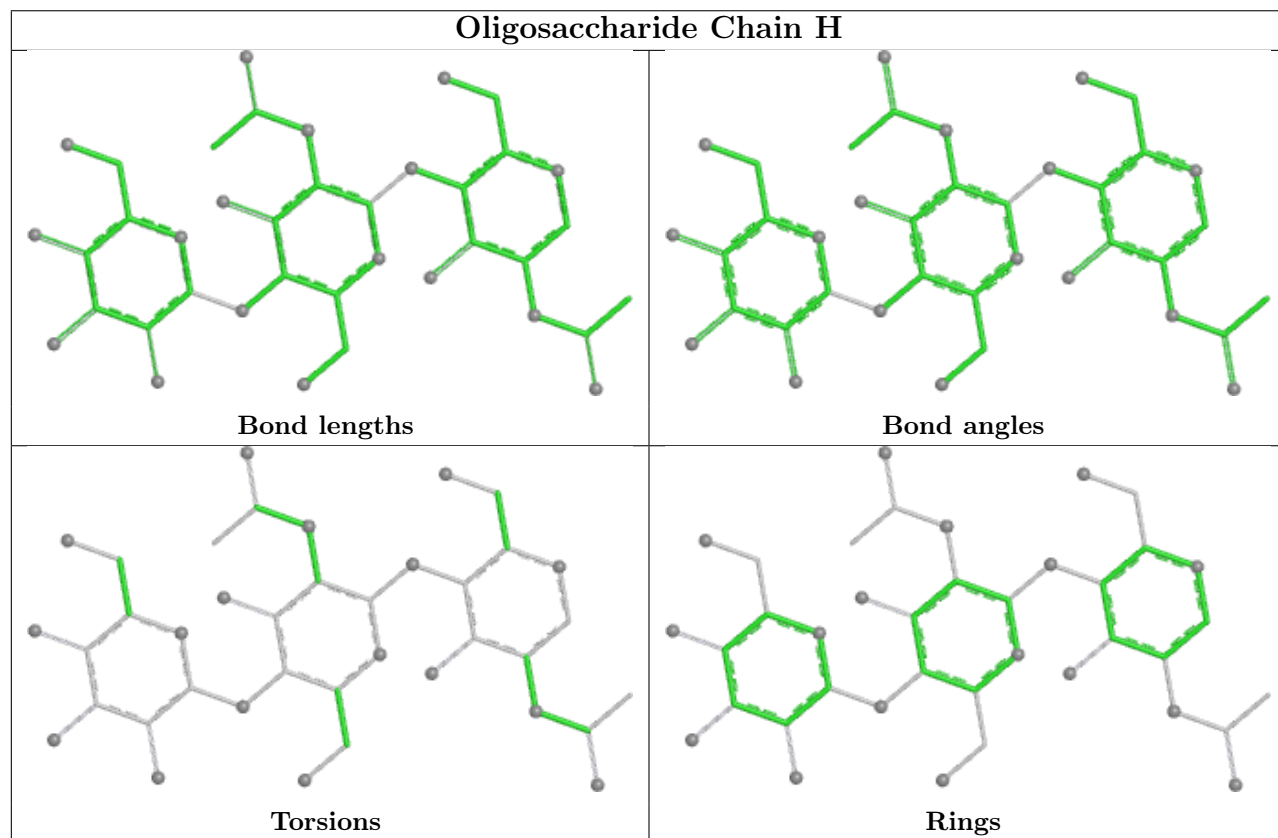
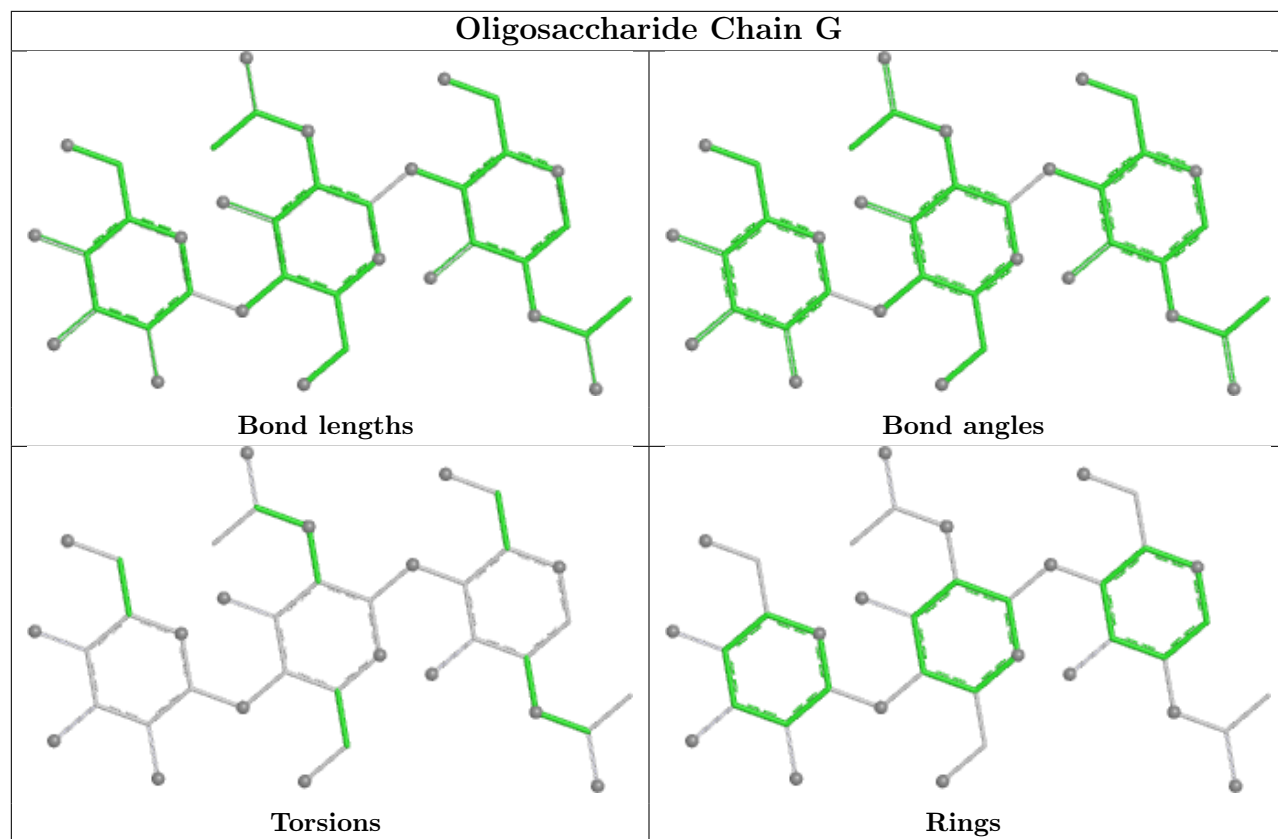
8 monomers are involved in 14 short contacts:

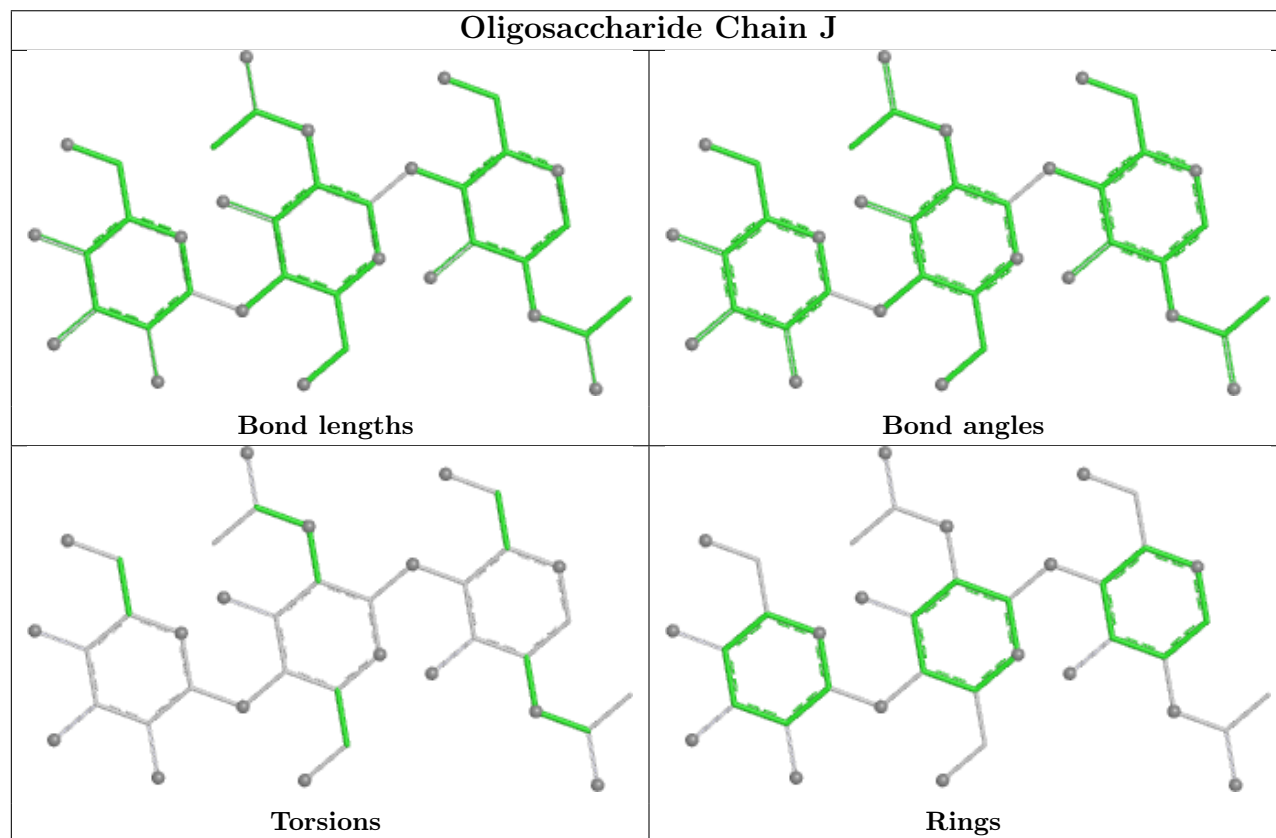
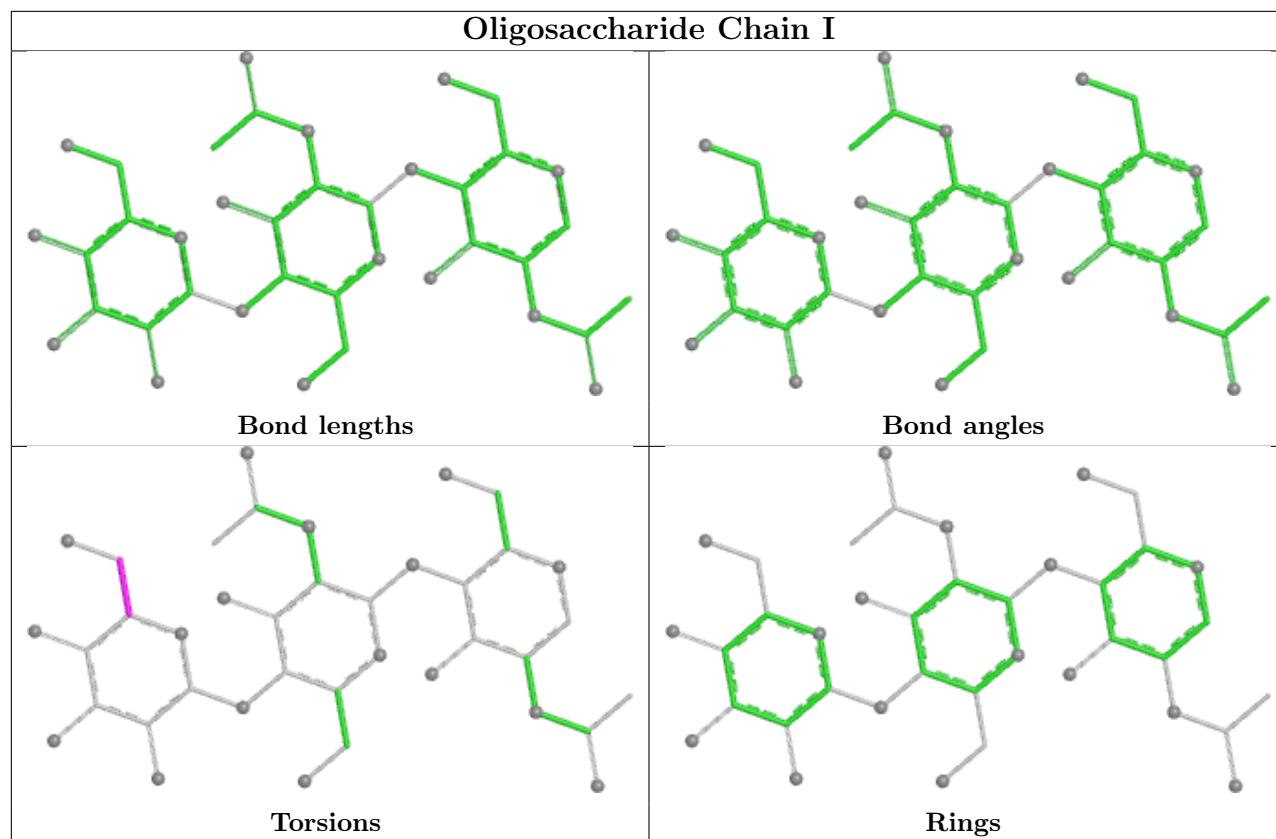
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	3	BMA	3	0
4	H	3	BMA	2	0
4	G	3	BMA	2	0
4	H	1	NAG	1	0
4	O	1	NAG	1	0
2	E	1	NAG	1	0
4	M	3	BMA	3	0
6	N	1	NAG	1	0

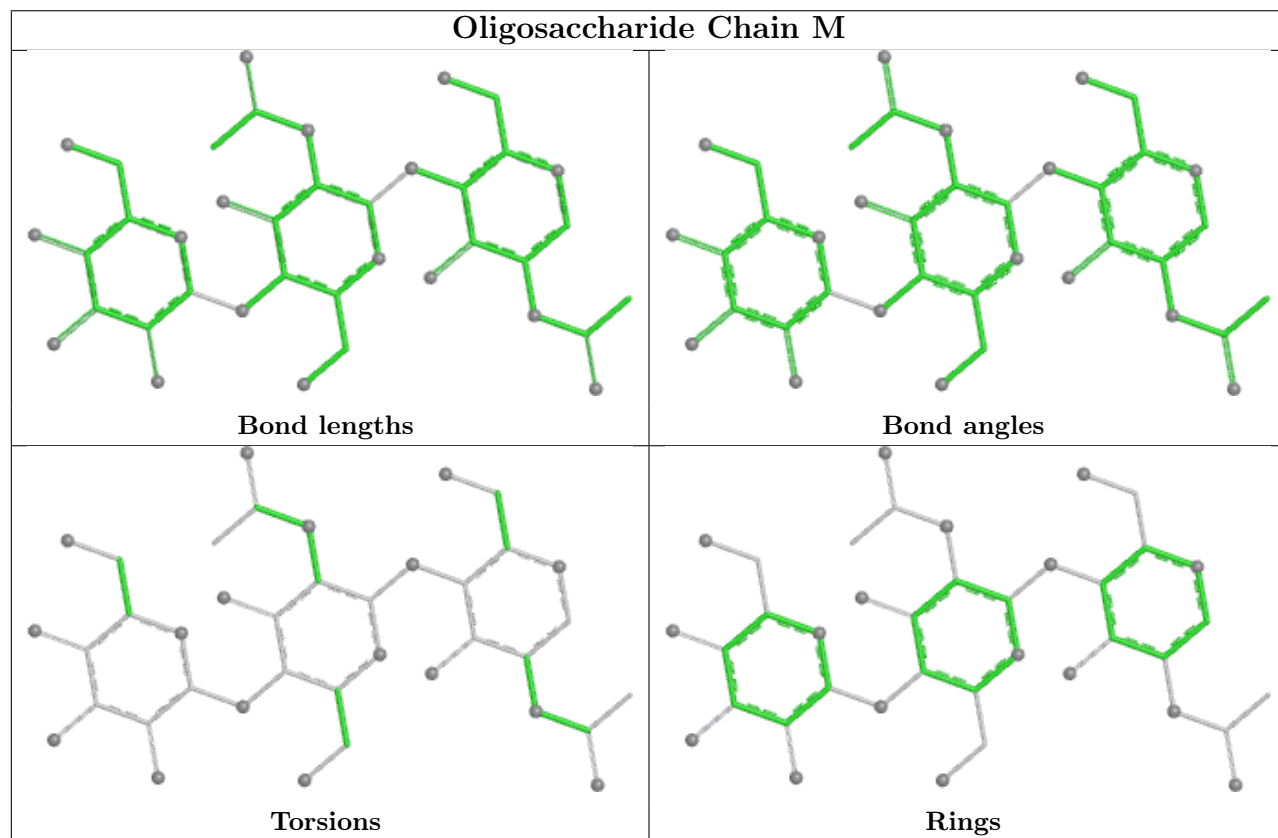
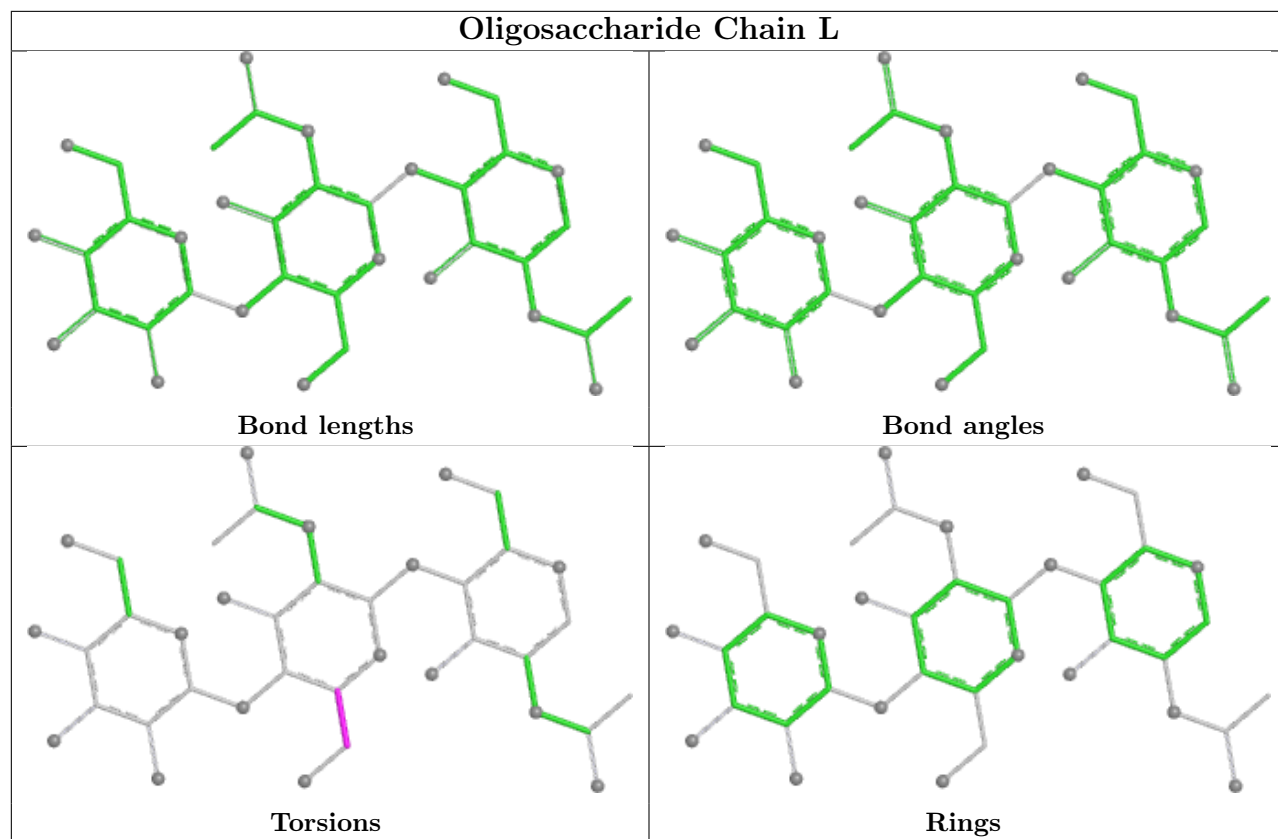
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

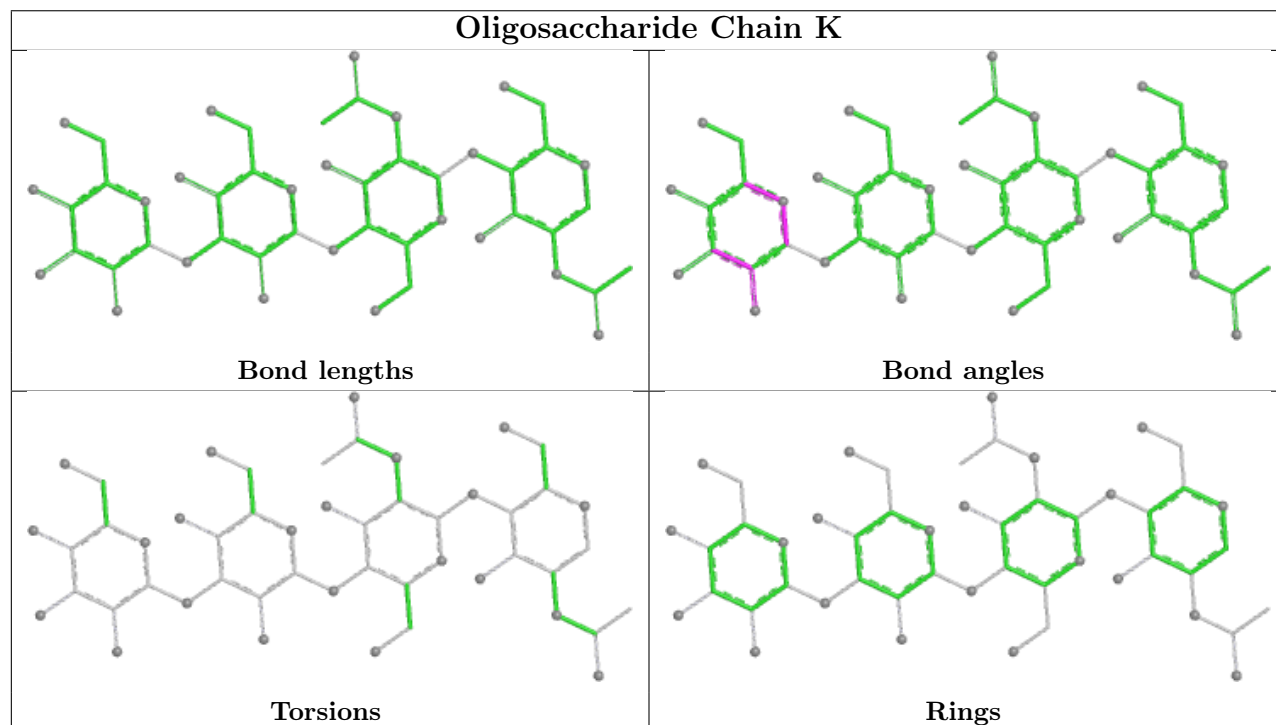
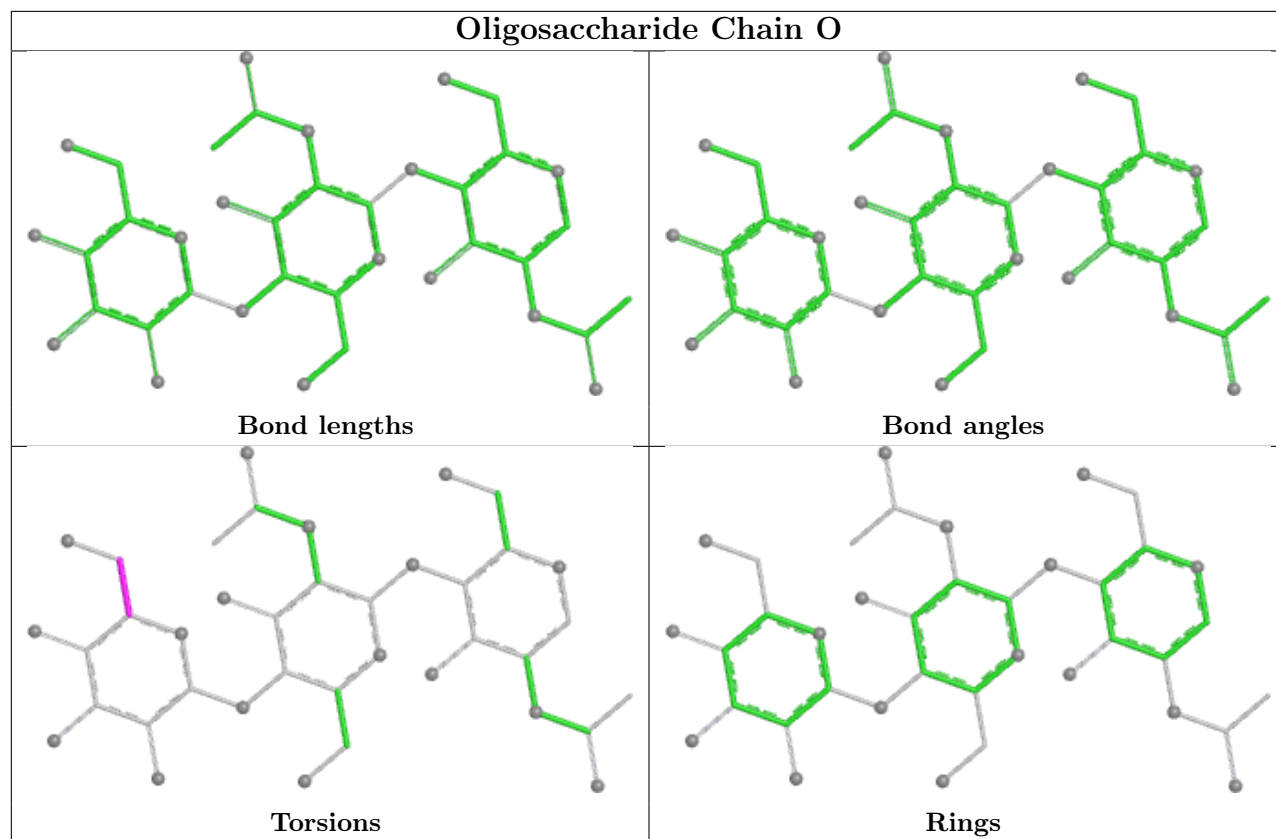


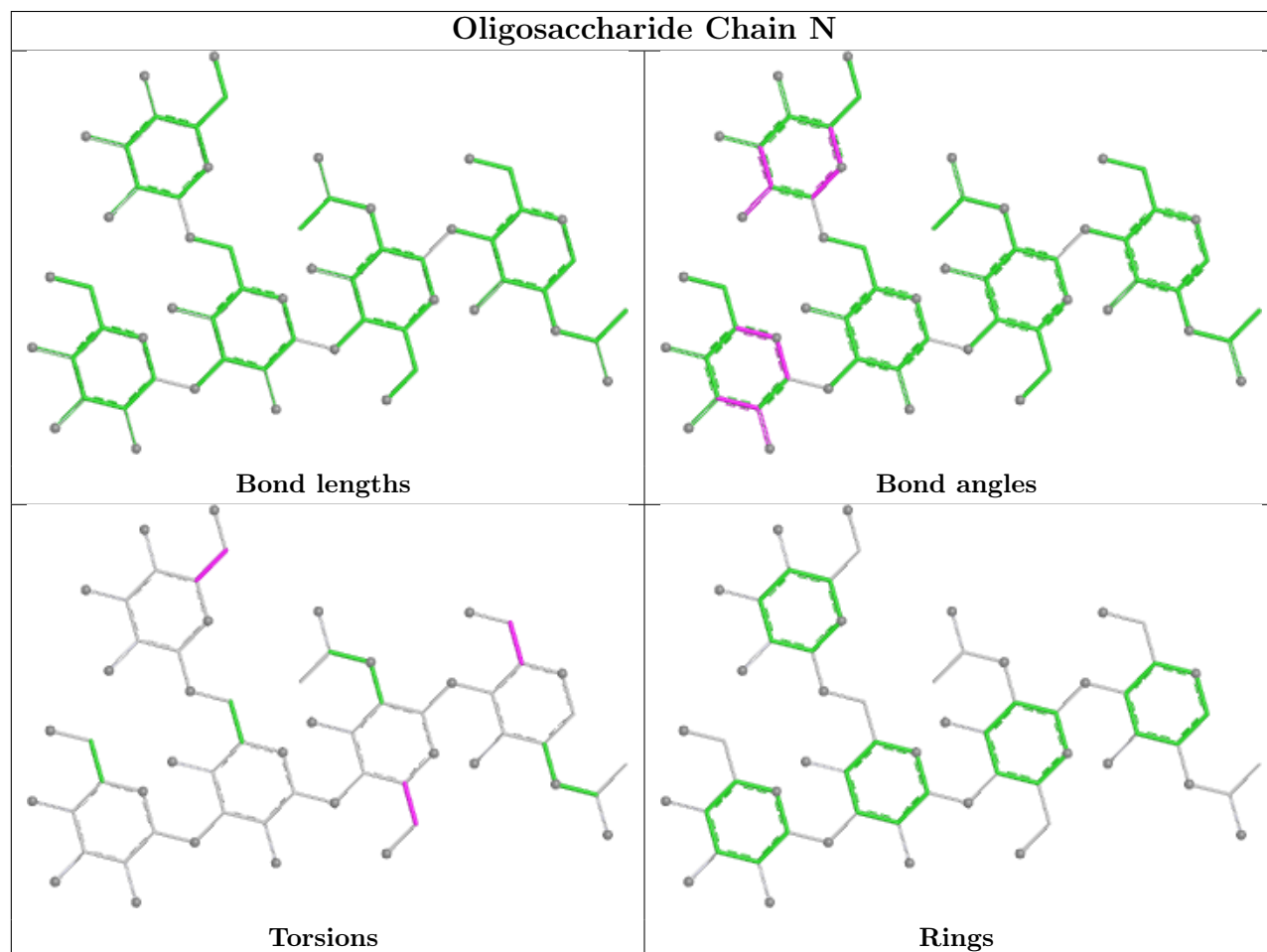
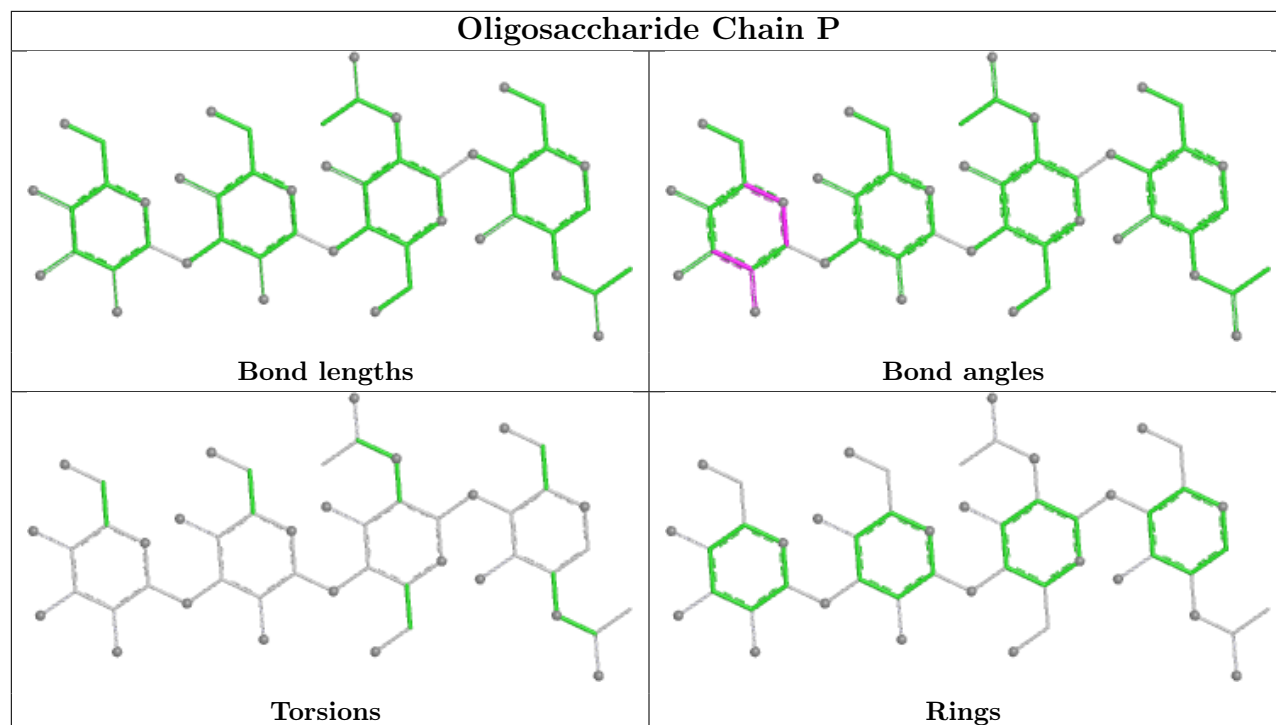












5.6 Ligand geometry

30 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	A	1005	-	11,11,12	0.66	0	15,15,17	0.99	2 (13%)
8	NAG	B	1015	1	14,14,15	0.20	0	17,19,21	0.44	0
8	NAG	D	909	1	14,14,15	0.23	0	17,19,21	0.42	0
7	MAN	C	914	-	11,11,12	0.68	0	15,15,17	0.97	2 (13%)
7	MAN	B	1014	-	11,11,12	0.64	0	15,15,17	1.00	2 (13%)
8	NAG	A	1006	1	14,14,15	0.21	0	17,19,21	0.44	0
9	U57	B	1018	-	20,22,22	1.44	5 (25%)	22,31,31	1.69	5 (22%)
8	NAG	D	915	1	14,14,15	0.21	0	17,19,21	0.43	0
7	MAN	A	1013	-	11,11,12	0.75	0	15,15,17	0.95	2 (13%)
8	NAG	C	916	1	14,14,15	0.20	0	17,19,21	0.45	0
8	NAG	C	909	1	14,14,15	0.22	0	17,19,21	0.43	0
8	NAG	C	915	1	14,14,15	0.24	0	17,19,21	0.41	0
7	MAN	B	1004	-	11,11,12	0.71	0	15,15,17	0.95	2 (13%)
8	NAG	D	917	1	14,14,15	0.19	0	17,19,21	0.46	0
8	NAG	A	1016	1	14,14,15	0.21	0	17,19,21	0.43	0
8	NAG	B	1017	-	14,14,15	0.24	0	17,19,21	0.41	0
7	MAN	B	1013	-	11,11,12	0.71	0	15,15,17	0.96	2 (13%)
8	NAG	A	1009	1	14,14,15	0.24	0	17,19,21	0.41	0
9	U57	A	1017	-	20,22,22	1.45	5 (25%)	22,31,31	1.72	5 (22%)
8	NAG	A	1015	1	14,14,15	0.25	0	17,19,21	0.42	0
8	NAG	B	1016	-	14,14,15	0.21	0	17,19,21	0.44	0
9	U57	C	917	-	20,22,22	1.44	5 (25%)	22,31,31	1.77	6 (27%)
7	MAN	C	913	-	11,11,12	0.70	0	15,15,17	0.96	2 (13%)
7	MAN	C	905	-	11,11,12	0.68	0	15,15,17	0.96	2 (13%)
8	NAG	D	916	-	14,14,15	0.50	0	17,19,21	0.48	0
7	MAN	D	914	-	11,11,12	0.67	0	15,15,17	1.00	2 (13%)
9	U57	D	918	-	20,22,22	1.45	5 (25%)	22,31,31	1.73	6 (27%)
7	MAN	B	1005	-	11,11,12	0.69	0	15,15,17	1.00	2 (13%)
8	NAG	A	1014	1	14,14,15	0.17	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	B	1009	-	14,14,15	0.24	0	17,19,21	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	A	1005	-	-	0/2/19/22	0/1/1/1
8	NAG	B	1015	1	-	2/6/23/26	0/1/1/1
8	NAG	D	909	1	-	2/6/23/26	0/1/1/1
7	MAN	C	914	-	-	0/2/19/22	0/1/1/1
7	MAN	B	1014	-	-	0/2/19/22	0/1/1/1
8	NAG	A	1006	1	-	0/6/23/26	0/1/1/1
9	U57	B	1018	-	-	0/13/13/13	0/2/2/2
8	NAG	D	915	1	-	2/6/23/26	0/1/1/1
7	MAN	A	1013	-	-	0/2/19/22	0/1/1/1
8	NAG	C	916	1	1/1/5/7	1/6/23/26	0/1/1/1
8	NAG	C	909	1	-	4/6/23/26	0/1/1/1
8	NAG	C	915	1	-	0/6/23/26	0/1/1/1
7	MAN	B	1004	-	-	0/2/19/22	0/1/1/1
8	NAG	D	917	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1016	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1017	-	-	0/6/23/26	0/1/1/1
7	MAN	B	1013	-	-	2/2/19/22	0/1/1/1
8	NAG	A	1009	1	-	2/6/23/26	0/1/1/1
9	U57	A	1017	-	-	1/13/13/13	0/2/2/2
8	NAG	A	1015	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1016	-	-	2/6/23/26	0/1/1/1
9	U57	C	917	-	-	2/13/13/13	0/2/2/2
7	MAN	C	913	-	-	0/2/19/22	0/1/1/1
7	MAN	C	905	-	-	2/2/19/22	0/1/1/1
8	NAG	D	916	-	-	2/6/23/26	0/1/1/1
7	MAN	D	914	-	-	0/2/19/22	0/1/1/1
9	U57	D	918	-	-	1/13/13/13	0/2/2/2
7	MAN	B	1005	-	-	2/2/19/22	0/1/1/1
8	NAG	A	1014	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1009	-	-	2/6/23/26	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1017	U57	C03-C02	-3.08	1.40	1.44
9	B	1018	U57	C03-C02	-3.07	1.40	1.44
9	D	918	U57	C03-C02	-3.01	1.40	1.44
9	C	917	U57	C03-C02	-2.90	1.40	1.44
9	A	1017	U57	C03-N05	2.60	1.36	1.33
9	D	918	U57	C03-N05	2.59	1.36	1.33
9	B	1018	U57	C03-N05	2.58	1.36	1.33
9	C	917	U57	C03-N05	2.56	1.36	1.33
9	C	917	U57	C01-N04	-2.39	1.33	1.37
9	D	918	U57	C01-N04	-2.35	1.33	1.37
9	A	1017	U57	C07-N08	2.33	1.38	1.33
9	C	917	U57	C07-N08	2.33	1.38	1.33
9	B	1018	U57	C07-N08	2.32	1.38	1.33
9	D	918	U57	C07-N08	2.32	1.38	1.33
9	B	1018	U57	C01-N04	-2.32	1.34	1.37
9	A	1017	U57	C01-N04	-2.30	1.34	1.37
9	C	917	U57	C18-N17	2.16	1.35	1.31
9	D	918	U57	C18-N17	2.12	1.35	1.31
9	A	1017	U57	C18-N17	2.12	1.35	1.31
9	B	1018	U57	C18-N17	2.11	1.35	1.31

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	917	U57	C03-C02-N17	3.76	124.84	120.41
9	C	917	U57	N04-C07-N05	-3.60	122.63	127.21
9	A	1017	U57	N04-C07-N05	-3.59	122.65	127.21
9	D	918	U57	C03-C02-N17	3.56	124.61	120.41
9	D	918	U57	N04-C07-N05	-3.53	122.72	127.21
9	A	1017	U57	C03-C02-N17	3.50	124.54	120.41
9	B	1018	U57	N04-C07-N05	-3.50	122.77	127.21
9	B	1018	U57	C03-C02-N17	3.40	124.42	120.41
9	C	917	U57	C20-C19-C18	-2.98	118.19	121.93
9	A	1017	U57	C20-C19-C18	-2.89	118.30	121.93
9	D	918	U57	C20-C19-C18	-2.87	118.33	121.93
9	B	1018	U57	C20-C19-C18	-2.86	118.33	121.93
7	B	1014	MAN	C1-O5-C5	2.41	115.42	112.19
7	C	914	MAN	C1-O5-C5	2.39	115.39	112.19
7	B	1013	MAN	C1-O5-C5	2.38	115.37	112.19
7	A	1005	MAN	C1-O5-C5	2.35	115.34	112.19
7	D	914	MAN	C1-O5-C5	2.33	115.31	112.19
9	B	1018	U57	C18-N17-C02	2.32	119.73	116.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1017	U57	C18-N17-C02	2.31	119.72	116.86
7	B	1005	MAN	C1-O5-C5	2.31	115.28	112.19
9	D	918	U57	C18-N17-C02	2.31	119.72	116.86
7	C	905	MAN	C1-O5-C5	2.30	115.27	112.19
7	C	913	MAN	C1-O5-C5	2.30	115.27	112.19
9	C	917	U57	C18-N17-C02	2.29	119.70	116.86
9	C	917	U57	C07-N05-C03	2.27	119.98	114.59
7	B	1004	MAN	C1-O5-C5	2.26	115.22	112.19
7	C	914	MAN	O2-C2-C3	-2.22	105.56	110.15
7	B	1014	MAN	O2-C2-C3	-2.21	105.57	110.15
9	D	918	U57	C07-N05-C03	2.21	119.84	114.59
7	C	905	MAN	O2-C2-C3	-2.21	105.58	110.15
7	B	1013	MAN	O2-C2-C3	-2.19	105.61	110.15
9	A	1017	U57	C07-N05-C03	2.19	119.79	114.59
7	C	913	MAN	O2-C2-C3	-2.18	105.63	110.15
7	B	1004	MAN	O2-C2-C3	-2.18	105.64	110.15
7	A	1005	MAN	O2-C2-C3	-2.16	105.67	110.15
7	B	1005	MAN	O2-C2-C3	-2.15	105.69	110.15
9	B	1018	U57	C07-N05-C03	2.15	119.69	114.59
7	D	914	MAN	O2-C2-C3	-2.14	105.72	110.15
7	A	1013	MAN	C1-O5-C5	2.13	115.04	112.19
7	A	1013	MAN	O2-C2-C3	-2.10	105.81	110.15
9	C	917	U57	C02-C01-N04	2.03	123.59	121.16
9	D	918	U57	C02-C01-N04	2.02	123.58	121.16

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	C	916	NAG	C1

All (33) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
7	B	1005	MAN	C4-C5-C6-O6
8	B	1015	NAG	O5-C5-C6-O6
8	A	1015	NAG	C4-C5-C6-O6
8	B	1016	NAG	C4-C5-C6-O6
8	A	1015	NAG	O5-C5-C6-O6
7	C	905	MAN	O5-C5-C6-O6
8	B	1016	NAG	O5-C5-C6-O6
8	A	1009	NAG	C8-C7-N2-C2
8	A	1009	NAG	O7-C7-N2-C2
8	B	1009	NAG	C8-C7-N2-C2
8	B	1009	NAG	O7-C7-N2-C2
8	C	909	NAG	C8-C7-N2-C2
8	C	909	NAG	O7-C7-N2-C2
8	D	909	NAG	C8-C7-N2-C2
8	D	909	NAG	O7-C7-N2-C2
8	C	909	NAG	O5-C5-C6-O6
8	C	909	NAG	C4-C5-C6-O6
7	B	1013	MAN	O5-C5-C6-O6
7	C	905	MAN	C4-C5-C6-O6
9	C	917	U57	C10-C11-C12-C15
9	D	918	U57	C13-C09-C10-C11
9	C	917	U57	C09-C10-C11-C12
7	B	1013	MAN	C4-C5-C6-O6
8	C	916	NAG	C4-C5-C6-O6

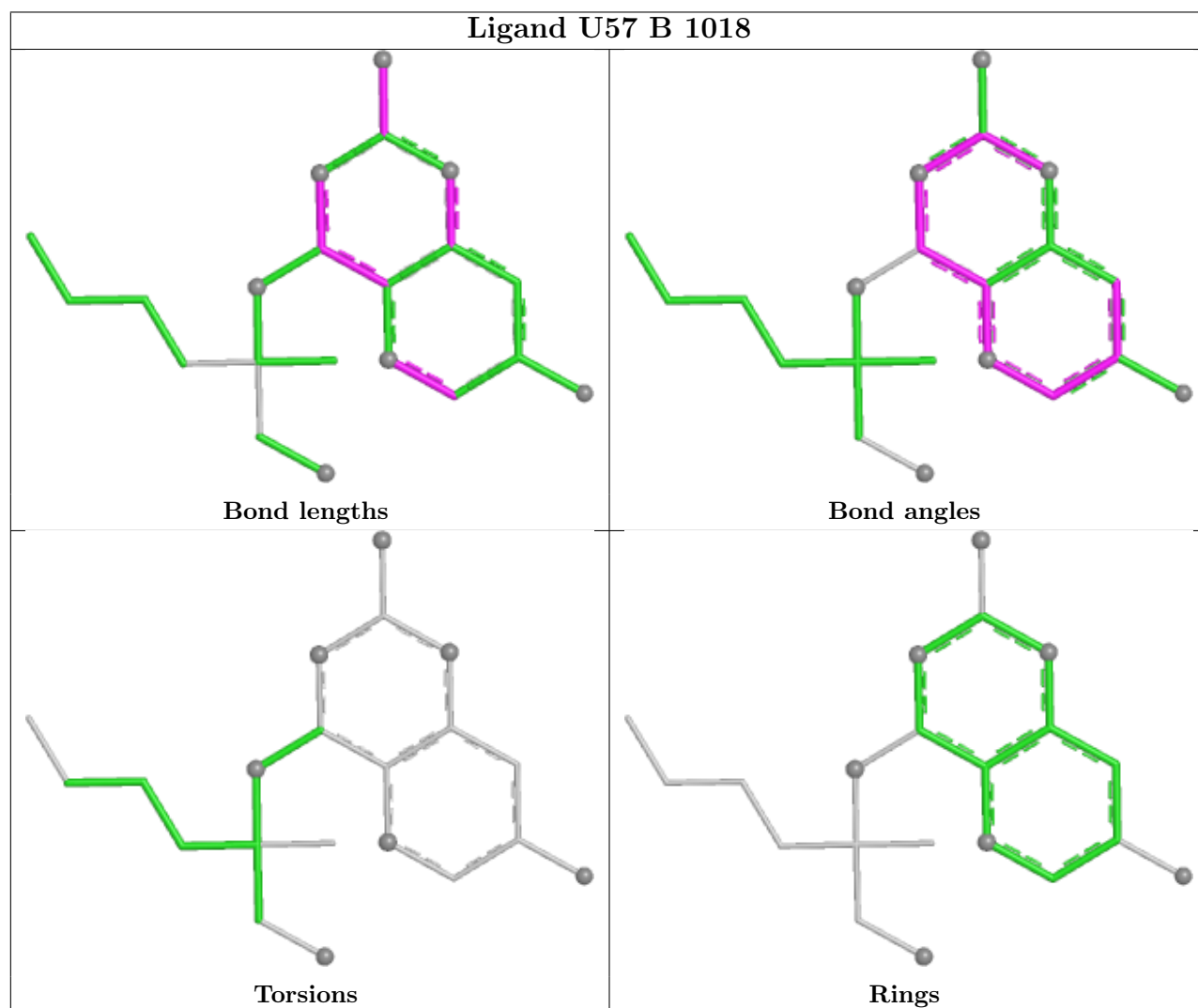
There are no ring outliers.

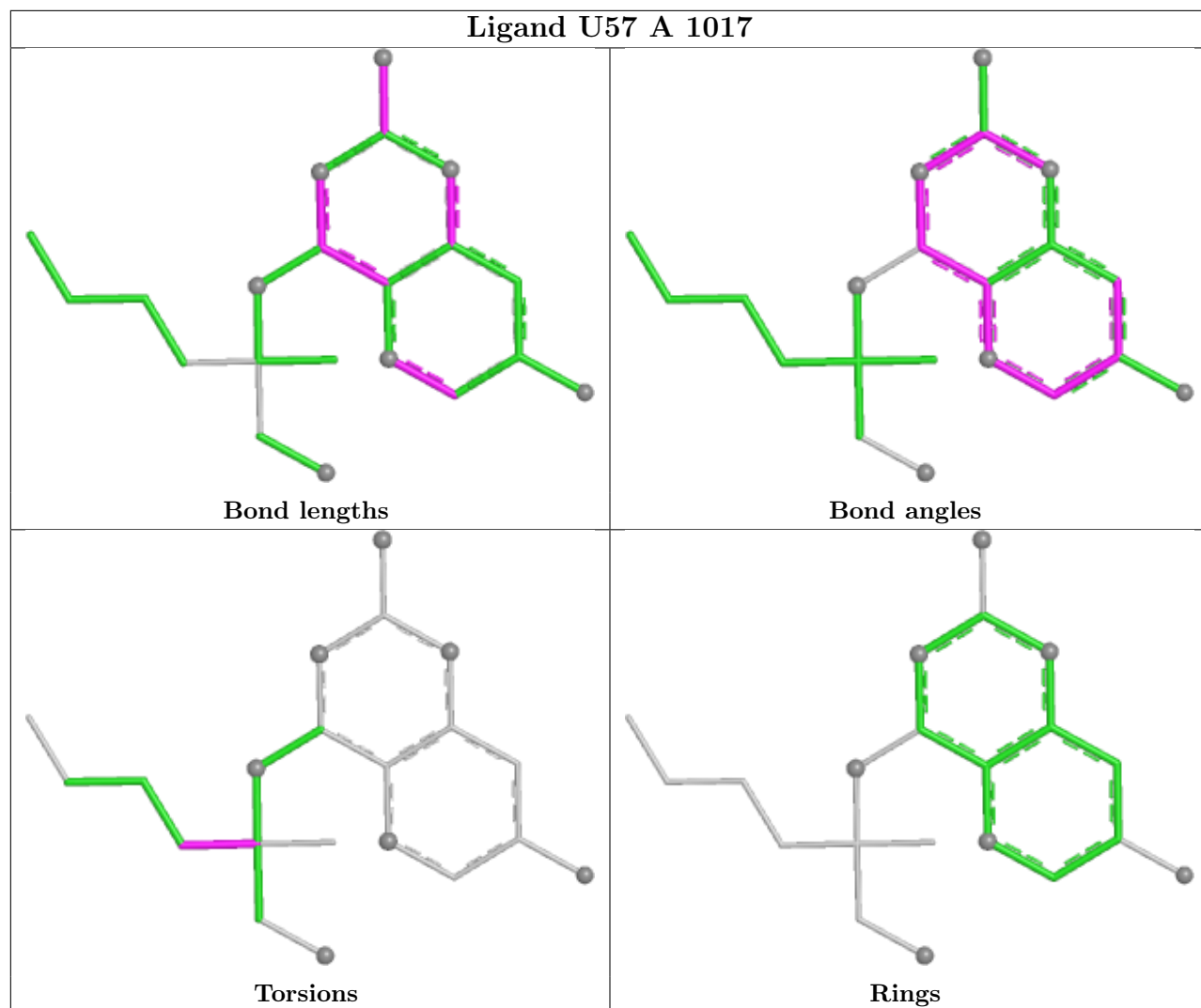
6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1013	MAN	2	0
7	B	1004	MAN	2	0
8	B	1016	NAG	3	0
7	C	913	MAN	3	0
7	C	905	MAN	4	0
8	D	916	NAG	6	1

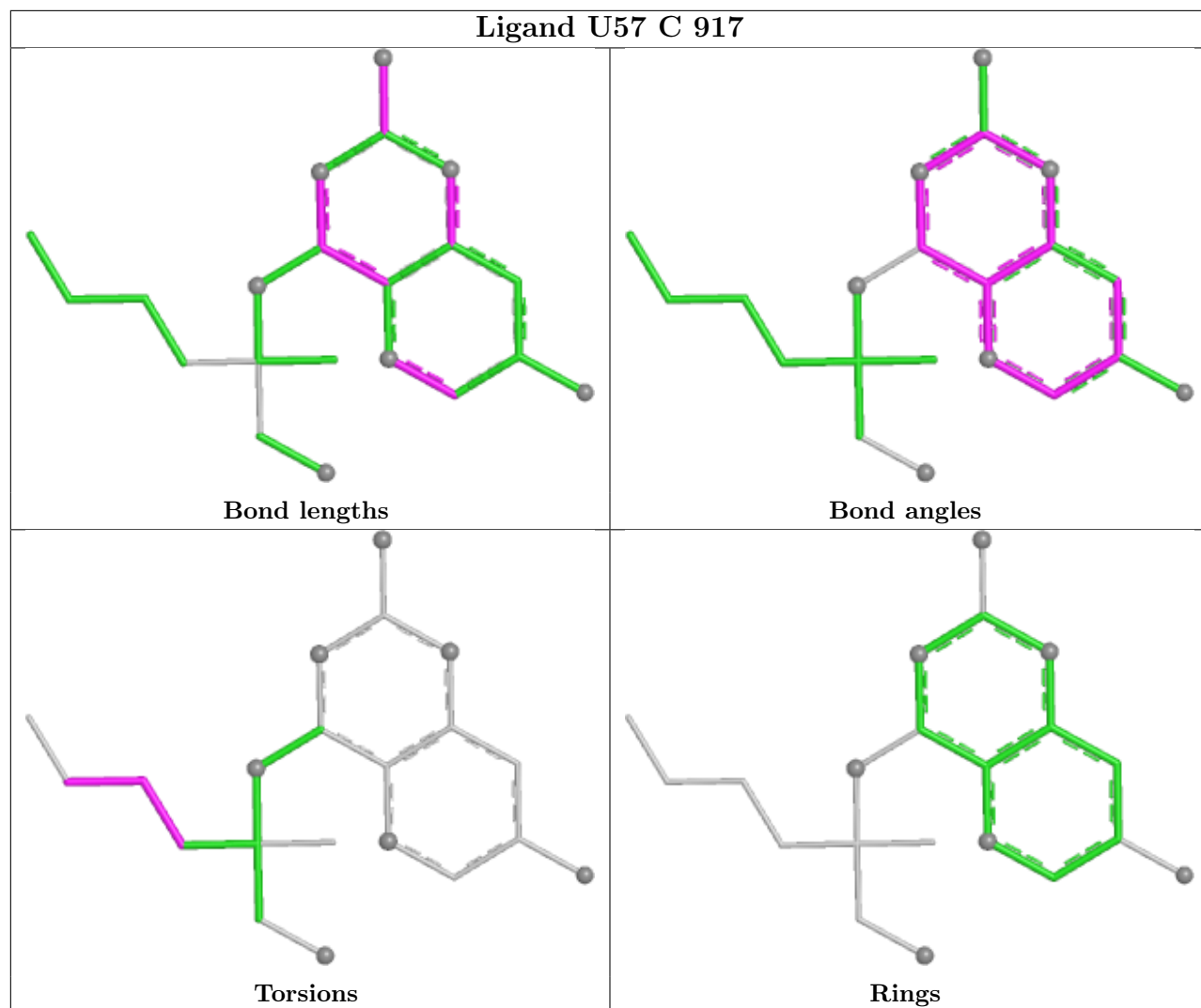
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

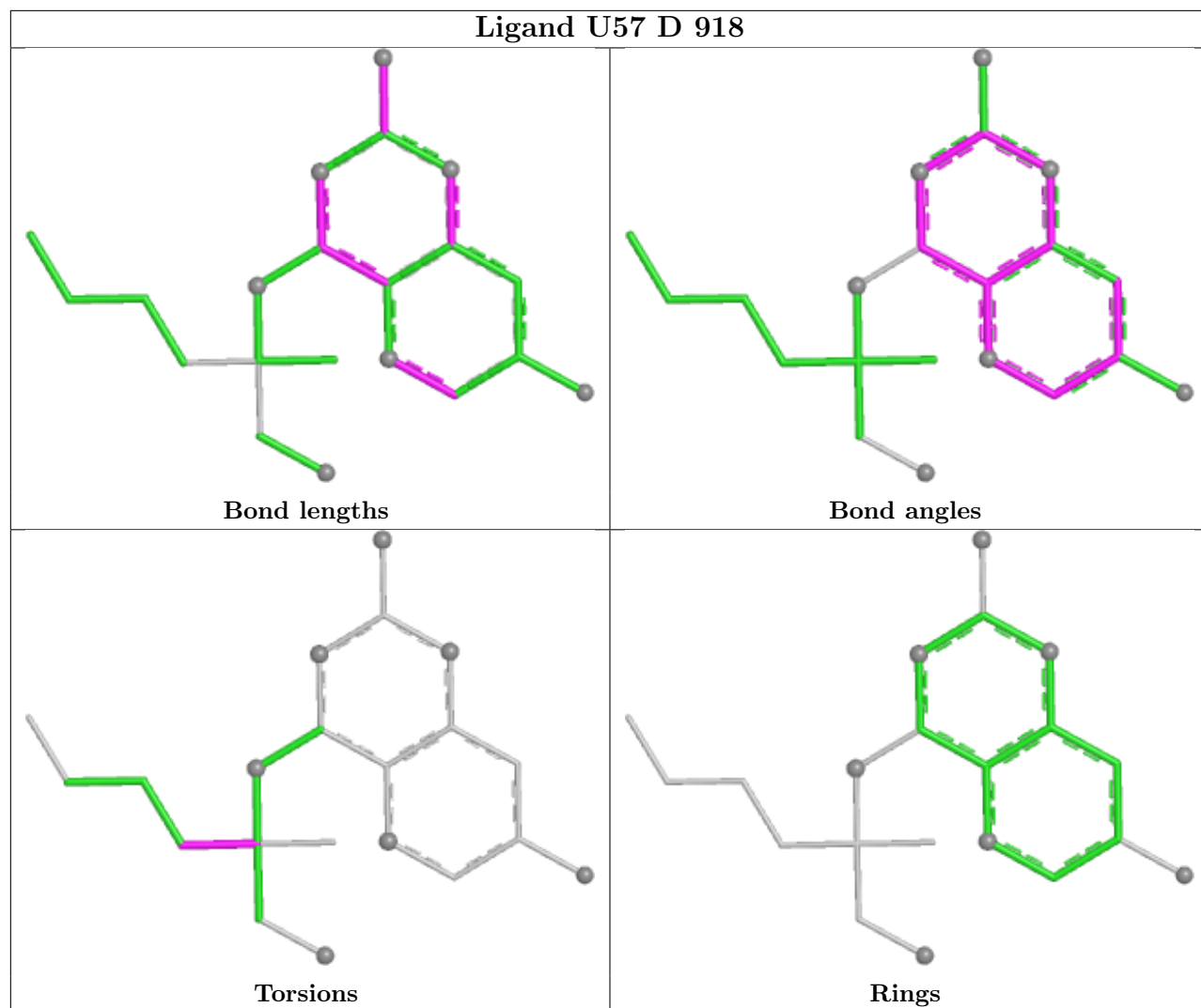
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





Ligand U57 C 917





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.27	36 (4%) 35 31	31, 46, 74, 105	3 (0%)
1	B	751/811 (92%)	0.52	54 (7%) 21 19	31, 52, 91, 125	0
1	C	681/811 (83%)	0.74	78 (11%) 9 8	34, 58, 95, 130	0
1	D	708/811 (87%)	0.90	114 (16%) 4 4	33, 61, 93, 113	0
All	All	2883/3244 (88%)	0.60	282 (9%) 13 11	31, 53, 91, 130	3 (0%)

All (282) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	86	LEU	6.5
1	D	815	VAL	5.6
1	D	80	ASN	5.4
1	D	778	CYS	5.3
1	C	86	LEU	5.3
1	C	690	LEU	5.2
1	D	814	ILE	5.1
1	D	99	ASN	5.0
1	C	87	GLN	5.0
1	D	776	CYS	5.0
1	C	764	LEU	4.8
1	C	727	LEU	4.8
1	B	818	GLU	4.7
1	A	100	VAL	4.6
1	C	802	ILE	4.5
1	C	100	VAL	4.4
1	D	809	GLN	4.3
1	B	735	VAL	4.3
1	D	158	ILE	4.1
1	B	124	LEU	4.1
1	D	775	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	761	THR	4.1
1	D	169	LEU	4.0
1	C	801	VAL	4.0
1	D	33	SER	4.0
1	A	778	CYS	3.9
1	D	735	VAL	3.9
1	D	63	LYS	3.9
1	D	755	ALA	3.9
1	D	74	PHE	3.8
1	B	46	ILE	3.8
1	D	779	ASP	3.8
1	D	729	SER	3.8
1	C	36	CYS	3.8
1	A	702[A]	PHE	3.7
1	D	137	LEU	3.7
1	D	55	GLN	3.7
1	D	46	ILE	3.6
1	D	39	LYS	3.6
1	A	732	LEU	3.6
1	C	433	LEU	3.6
1	D	163	LYS	3.6
1	D	813	SER	3.6
1	C	678	PHE	3.6
1	D	160	ASN	3.5
1	B	780	ILE	3.5
1	D	417	PHE	3.5
1	A	729	SER	3.4
1	D	147	SER	3.4
1	D	702	PHE	3.4
1	B	760	THR	3.4
1	B	752	ASN	3.4
1	D	196	VAL	3.4
1	D	433	LEU	3.4
1	C	688	PRO	3.4
1	B	170	ILE	3.4
1	D	754	SER	3.4
1	A	792	ASN	3.3
1	C	738	LEU	3.3
1	D	783	PHE	3.3
1	C	271	ASP	3.3
1	D	159	TYR	3.3
1	C	772	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	89	LEU	3.3
1	A	730	GLY	3.3
1	B	85	GLY	3.3
1	D	142	SER	3.2
1	D	66	THR	3.2
1	D	118	ASP	3.2
1	C	714	LEU	3.2
1	B	167	SER	3.2
1	C	33	SER	3.2
1	C	702	PHE	3.2
1	B	80	ASN	3.2
1	D	126	ASN	3.2
1	C	166	ILE	3.2
1	D	136	GLN	3.1
1	D	785	ARG	3.1
1	B	164	GLU	3.1
1	D	121	PHE	3.1
1	D	307	PHE	3.1
1	A	97	ASN	3.1
1	A	61	VAL	3.1
1	C	800	ASP	3.1
1	D	166	ILE	3.1
1	D	802	ILE	3.1
1	A	818	GLU	3.1
1	C	712	SER	3.0
1	D	122	LEU	3.0
1	A	759	LYS	3.0
1	D	191	ASN	3.0
1	C	725	SER	3.0
1	D	170	ILE	3.0
1	C	664	ALA	2.9
1	B	732	LEU	2.9
1	C	64	TYR	2.9
1	C	701	LEU	2.9
1	B	734	GLU	2.9
1	D	213	LEU	2.9
1	D	459	PHE	2.9
1	D	782	ASP	2.9
1	B	100	VAL	2.9
1	D	601	ASP	2.9
1	C	167	SER	2.9
1	D	116	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	64	TYR	2.8
1	B	730	GLY	2.8
1	D	115	ASN	2.8
1	D	138	PRO	2.8
1	D	806	PRO	2.8
1	D	117	THR	2.8
1	D	72	ASP	2.8
1	D	244	GLY	2.8
1	C	744	SER	2.8
1	A	735	VAL	2.8
1	C	47	ALA	2.8
1	D	791	LEU	2.8
1	D	189	LYS	2.8
1	B	44	SER	2.8
1	D	51	ASN	2.8
1	C	798	LEU	2.8
1	D	89	LEU	2.8
1	D	193	GLU	2.8
1	D	274	ALA	2.7
1	B	83	PHE	2.7
1	D	234	ILE	2.7
1	A	64	TYR	2.7
1	A	754	SER	2.7
1	A	707	LEU	2.7
1	C	766	MET	2.7
1	C	113	GLY	2.7
1	B	817	LEU	2.7
1	D	76	THR	2.7
1	A	779	ASP	2.7
1	C	31	SER	2.7
1	C	713	SER	2.7
1	D	127	LEU	2.7
1	B	408	GLN	2.7
1	D	157	ASN	2.6
1	C	602	LYS	2.6
1	A	170	ILE	2.6
1	A	731	PHE	2.6
1	C	793	VAL	2.6
1	D	79	THR	2.6
1	A	728	PRO	2.6
1	C	83	PHE	2.6
1	D	50	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	60	THR	2.6
1	B	702	PHE	2.6
1	C	65	VAL	2.6
1	B	162	THR	2.6
1	C	726	HIS	2.6
1	C	699	LYS	2.6
1	D	143	GLY	2.5
1	D	215	HIS	2.5
1	B	418	SER	2.5
1	D	199	THR	2.5
1	C	603	TYR	2.5
1	D	773	PRO	2.5
1	D	751	ILE	2.5
1	A	415	GLN	2.5
1	C	45	VAL	2.5
1	D	752	ASN	2.5
1	A	758	THR	2.5
1	D	149	THR	2.5
1	D	222	SER	2.5
1	C	96	HIS	2.5
1	C	653	HIS	2.5
1	D	268	VAL	2.5
1	B	120	ALA	2.5
1	A	777	THR	2.5
1	C	35	PRO	2.4
1	C	194	ASP	2.4
1	B	87	GLN	2.4
1	B	470	PHE	2.4
1	C	61	VAL	2.4
1	B	736	SER	2.4
1	C	85	GLY	2.4
1	D	270	CYS	2.4
1	B	43	ASP	2.4
1	B	783	PHE	2.4
1	D	90	THR	2.4
1	D	728	PRO	2.4
1	D	763	LYS	2.4
1	D	246	ILE	2.4
1	C	200	LEU	2.4
1	A	96[A]	HIS	2.4
1	B	168	ARG	2.4
1	C	34	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	236	TYR	2.4
1	D	805	SER	2.4
1	A	653	HIS	2.4
1	B	794	LYS	2.4
1	C	689	ARG	2.3
1	B	121	PHE	2.3
1	B	274	ALA	2.3
1	B	273	GLY	2.3
1	B	200	LEU	2.3
1	D	54	LEU	2.3
1	A	88	ASN	2.3
1	D	701	LEU	2.3
1	D	470	PHE	2.3
1	D	348	TYR	2.3
1	C	42	ASN	2.3
1	D	98	PRO	2.3
1	C	60	THR	2.3
1	B	113	GLY	2.3
1	D	114	LEU	2.3
1	C	37	ASP	2.3
1	B	757	GLU	2.3
1	C	679	PHE	2.3
1	C	32	ARG	2.3
1	C	62	GLY	2.2
1	C	408	GLN	2.2
1	C	637	GLY	2.2
1	C	795	ILE	2.2
1	D	140	ILE	2.2
1	D	748	LEU	2.2
1	C	687	PHE	2.2
1	D	335	MET	2.2
1	B	246	ILE	2.2
1	D	92	ILE	2.2
1	D	150	GLU	2.2
1	B	128	ARG	2.2
1	D	68	LEU	2.2
1	C	146	GLU	2.2
1	D	464	HIS	2.2
1	D	547	ALA	2.2
1	D	287	THR	2.2
1	B	177	LEU	2.2
1	B	791	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	52	ARG	2.2
1	A	678	PHE	2.2
1	B	763	LYS	2.2
1	B	625	ASN	2.1
1	B	79	THR	2.1
1	C	70	LEU	2.1
1	C	122	LEU	2.1
1	D	273	GLY	2.1
1	D	750	THR	2.1
1	C	170	ILE	2.1
1	D	780	ILE	2.1
1	D	49	CYS	2.1
1	D	257	CYS	2.1
1	A	757	GLU	2.1
1	A	87	GLN	2.1
1	D	123	ASN	2.1
1	A	66	THR	2.1
1	A	761	THR	2.1
1	C	767	LEU	2.1
1	D	200	LEU	2.1
1	C	129	GLU	2.1
1	D	36	CYS	2.1
1	A	329	SER	2.1
1	B	31	SER	2.1
1	C	44	SER	2.1
1	B	40	LYS	2.1
1	B	125	LYS	2.1
1	C	799	VAL	2.1
1	A	99	ASN	2.1
1	D	172	LEU	2.1
1	C	724	ILE	2.1
1	A	392	GLN	2.1
1	C	136	GLN	2.1
1	B	45	VAL	2.1
1	B	758	THR	2.1
1	C	193	GLU	2.1
1	D	134	ASP	2.1
1	C	770	HIS	2.1
1	B	42	ASN	2.0
1	B	764	LEU	2.0
1	C	88	ASN	2.0
1	C	240	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	91	LYS	2.0
1	D	235	LYS	2.0
1	A	782	ASP	2.0
1	A	817	LEU	2.0
1	C	63	LYS	2.0
1	C	640	ASN	2.0
1	D	792	ASN	2.0
1	A	199	THR	2.0
1	D	279	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	BMA	L	3	11/12	0.73	0.20	83,91,100,102	0
6	MAN	N	5	11/12	0.74	0.14	78,87,95,102	0
4	BMA	I	3	11/12	0.75	0.12	77,87,94,101	0
3	BMA	F	2	11/12	0.77	0.14	72,80,90,92	0
2	MAN	E	4	11/12	0.80	0.14	67,73,85,99	0
5	MAN	P	4	11/12	0.81	0.15	87,95,107,108	0
4	BMA	O	3	11/12	0.83	0.11	93,98,104,104	0
6	MAN	N	4	11/12	0.83	0.11	70,81,89,94	0
5	MAN	K	4	11/12	0.83	0.14	59,77,83,83	0
4	BMA	M	3	11/12	0.85	0.11	76,83,96,101	0
4	BMA	G	3	11/12	0.86	0.12	50,61,71,72	0
5	BMA	K	3	11/12	0.88	0.11	52,62,72,73	0
4	NAG	M	2	14/15	0.88	0.13	46,58,73,84	0
5	BMA	P	3	11/12	0.88	0.12	53,70,79,87	0
4	NAG	O	2	14/15	0.89	0.10	61,71,85,92	0
4	BMA	J	3	11/12	0.90	0.10	56,67,79,83	0
4	NAG	L	2	14/15	0.90	0.11	54,64,82,86	0
2	BMA	E	3	11/12	0.90	0.11	47,59,68,69	0
5	NAG	P	2	14/15	0.90	0.11	36,39,54,62	0

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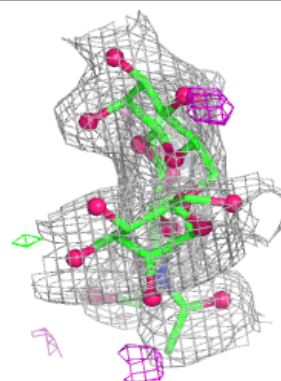
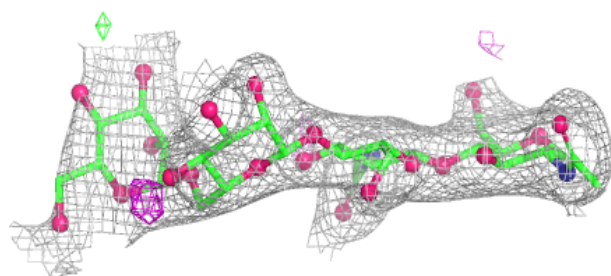
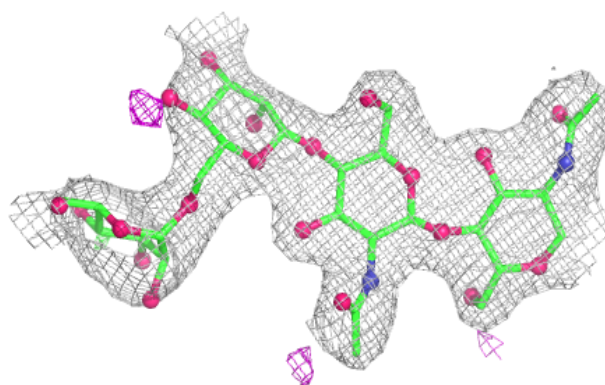
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BMA	H	3	11/12	0.91	0.10	57,63,69,72	0
4	NAG	H	2	14/15	0.91	0.10	35,47,56,60	0
4	NAG	G	2	14/15	0.92	0.08	29,45,53,56	0
6	NAG	N	2	14/15	0.92	0.10	44,58,68,73	0
6	BMA	N	3	11/12	0.92	0.08	67,69,80,83	0
3	NAG	F	1	14/15	0.92	0.07	44,56,68,72	0
4	NAG	I	2	14/15	0.92	0.10	46,56,69,74	0
4	NAG	H	1	14/15	0.93	0.11	35,46,55,56	0
6	NAG	N	1	14/15	0.93	0.10	46,50,58,64	0
4	NAG	G	1	14/15	0.94	0.09	23,37,42,48	0
4	NAG	M	1	14/15	0.94	0.08	40,50,54,54	0
4	NAG	J	2	14/15	0.94	0.08	28,43,51,58	0
5	NAG	K	1	14/15	0.94	0.09	29,41,45,46	0
5	NAG	K	2	14/15	0.94	0.10	41,49,56,56	0
4	NAG	J	1	14/15	0.95	0.06	28,39,41,43	0
4	NAG	L	1	14/15	0.95	0.08	41,48,53,57	0
2	NAG	E	1	14/15	0.95	0.09	30,34,39,48	0
4	NAG	I	1	14/15	0.96	0.08	30,36,45,47	0
5	NAG	P	1	14/15	0.96	0.08	29,35,42,44	0
4	NAG	O	1	14/15	0.97	0.07	36,42,52,52	0
2	NAG	E	2	14/15	0.97	0.07	29,39,51,53	0

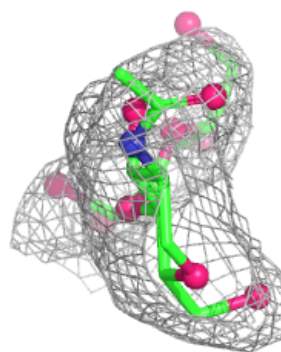
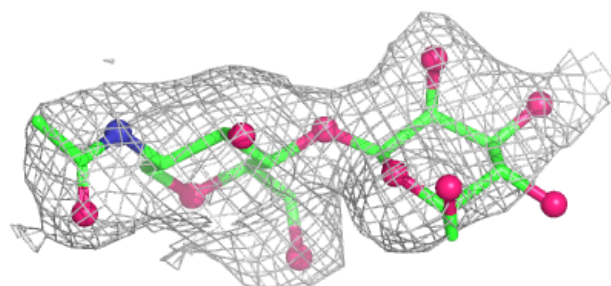
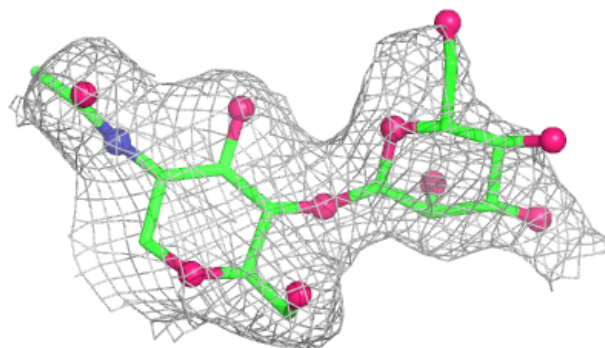
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

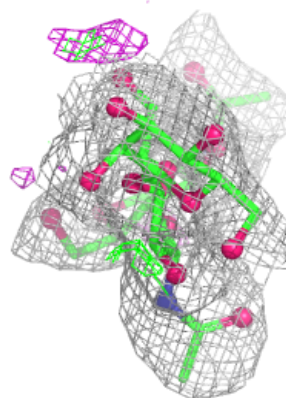
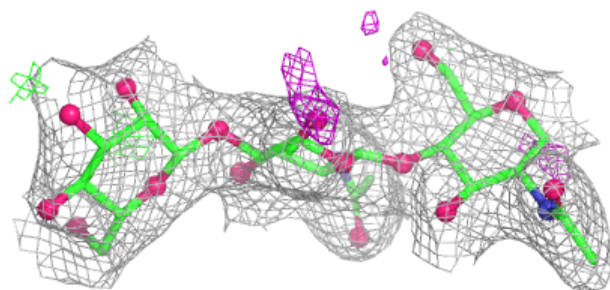
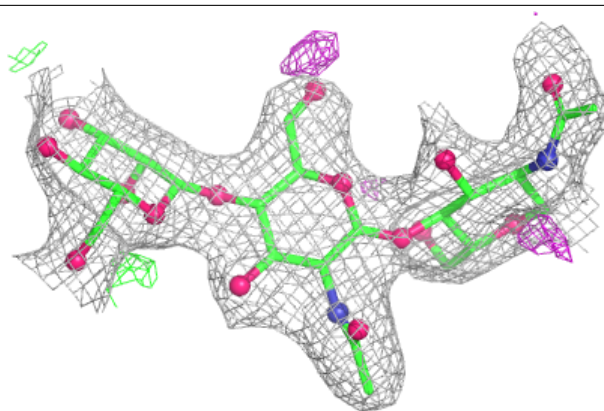
**Electron density around Chain F:**

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

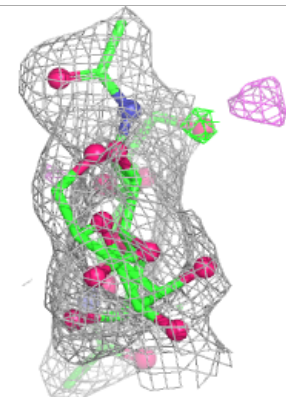
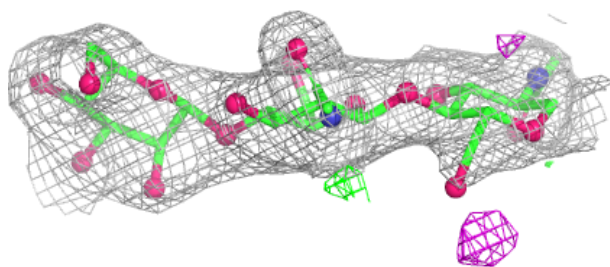
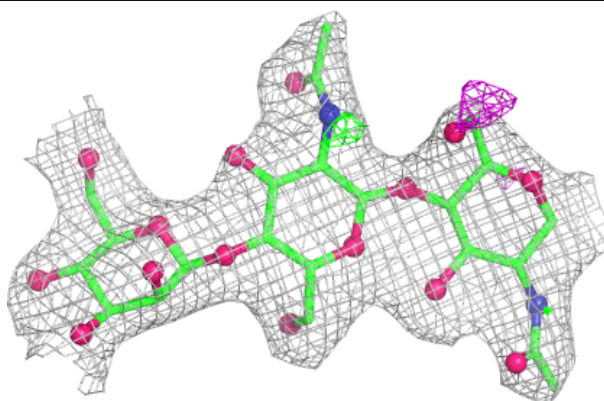


Electron density around Chain G:

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

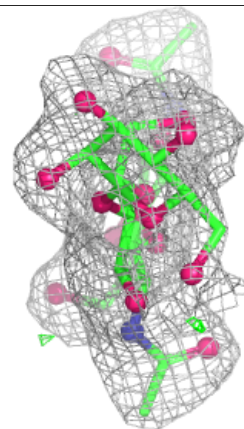
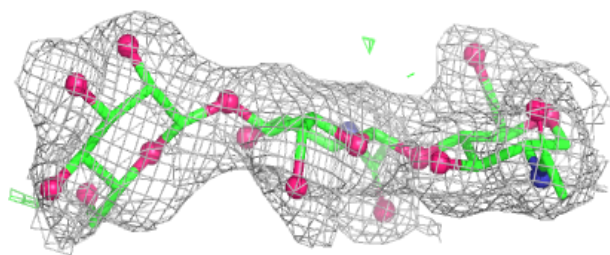
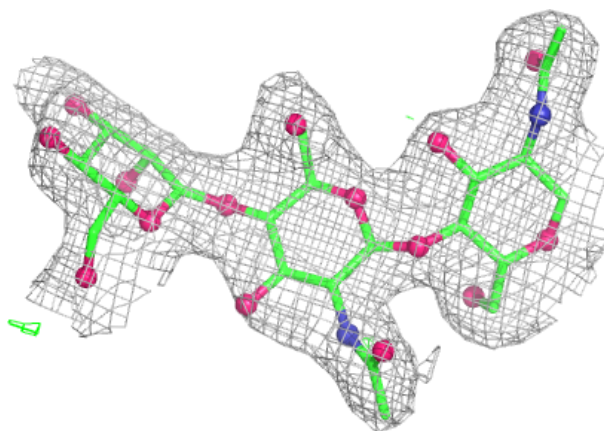
**Electron density around Chain H:**

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



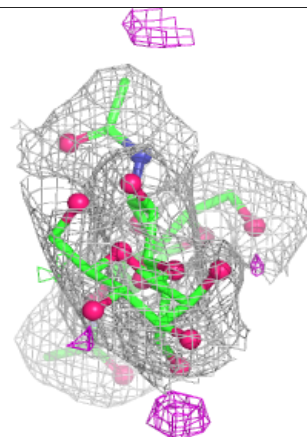
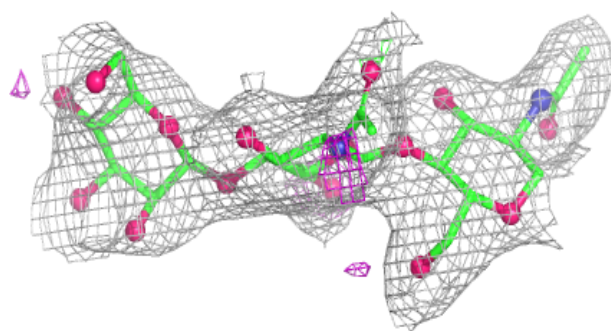
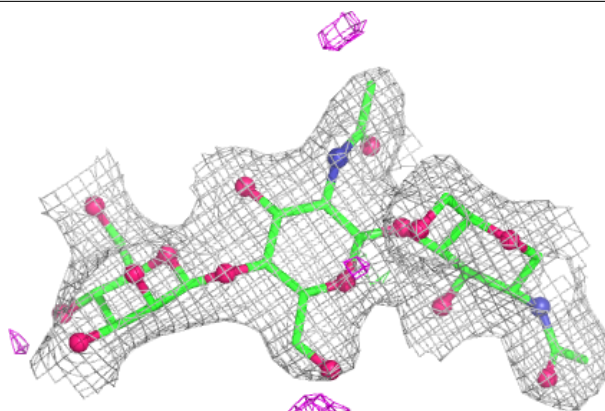
Electron density around Chain I:

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



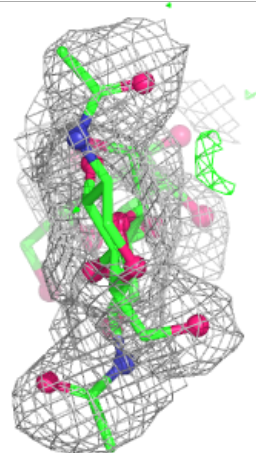
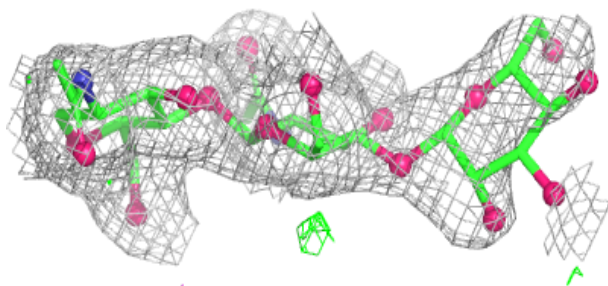
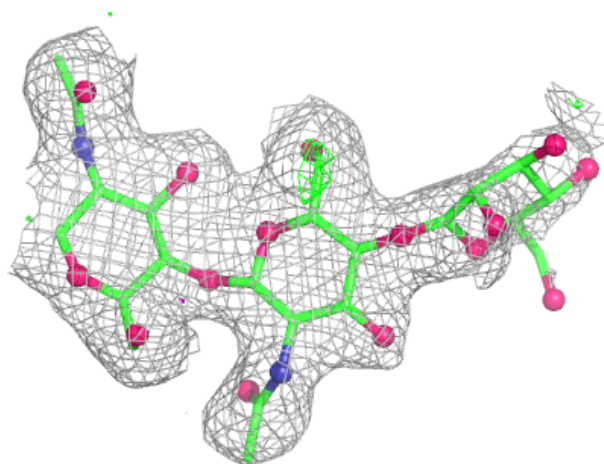
Electron density around Chain J:

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



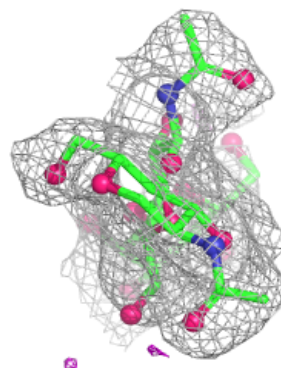
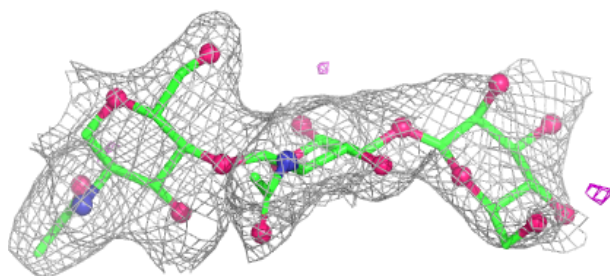
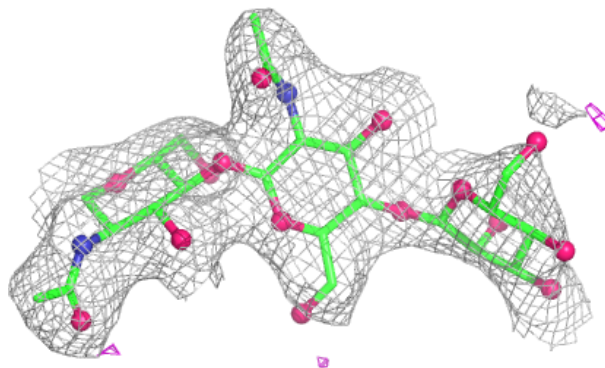
Electron density around Chain L:

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

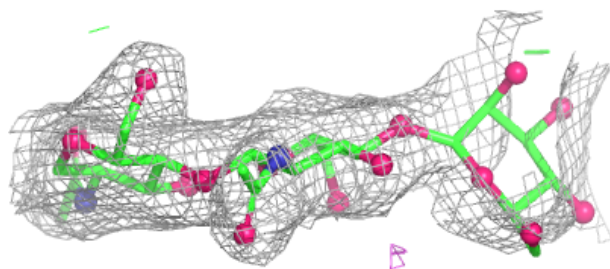
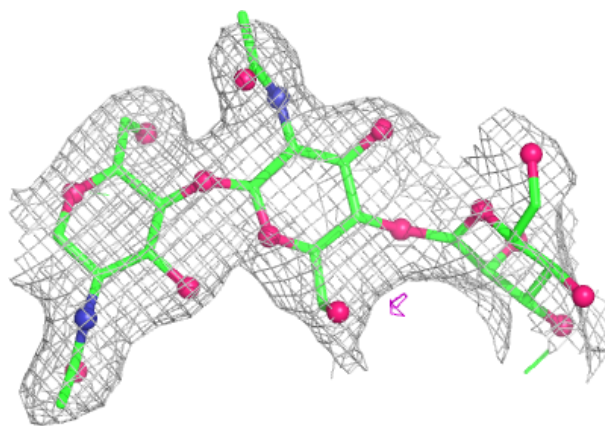


Electron density around Chain M:

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

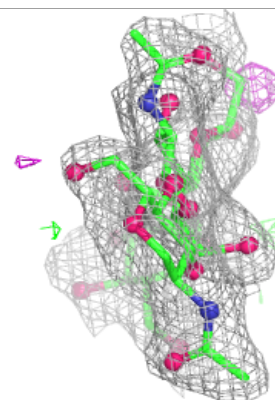
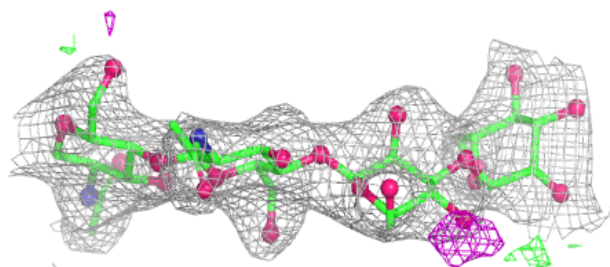
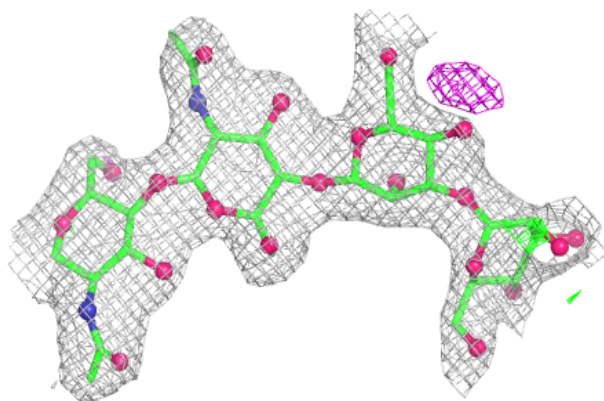
**Electron density around Chain O:**

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

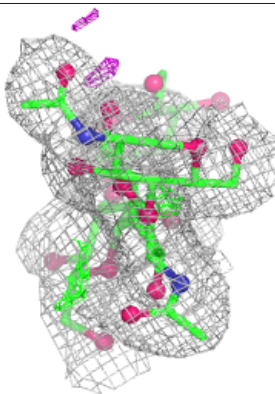
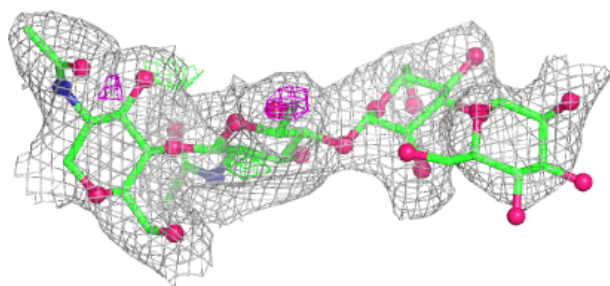
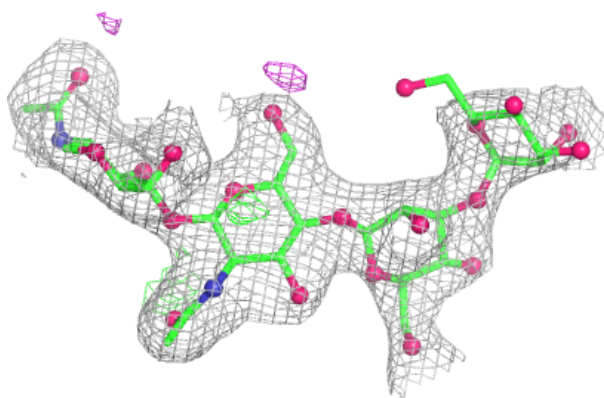


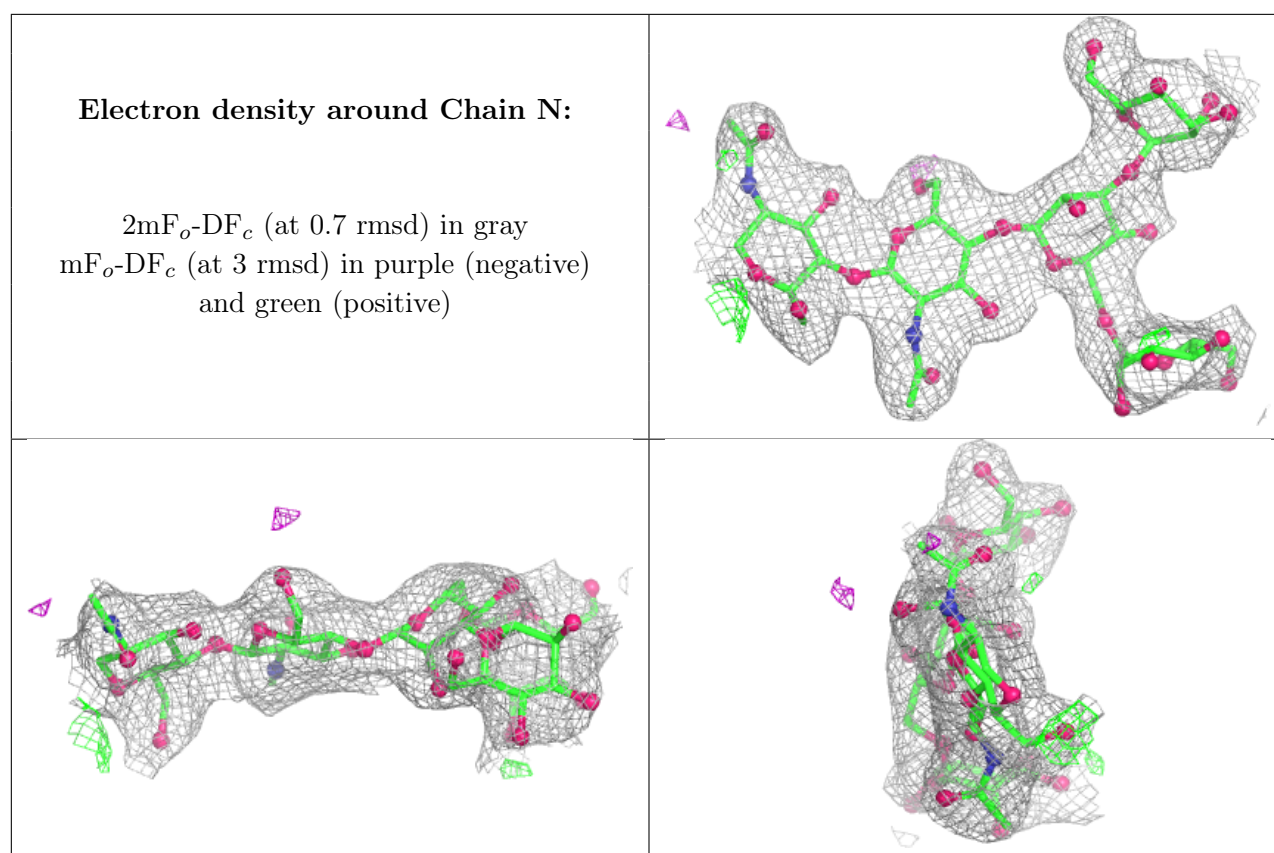
Electron density around Chain K:

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

**Electron density around Chain P:**

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





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($\text{\AA}^2$)	Q<0.9
8	NAG	B	1016	14/15	0.49	0.23	95,104,122,123	0
7	MAN	B	1013	11/12	0.56	0.18	84,97,100,100	0
8	NAG	B	1009	14/15	0.60	0.17	71,76,92,93	0
7	MAN	C	913	11/12	0.61	0.19	81,102,110,110	0
8	NAG	D	916	14/15	0.67	0.28	72,85,103,105	0
7	MAN	C	914	11/12	0.69	0.17	92,107,113,117	0
7	MAN	B	1005	11/12	0.69	0.17	73,81,91,93	0
7	MAN	D	914	11/12	0.74	0.15	78,90,103,111	0
8	NAG	C	915	14/15	0.76	0.13	82,95,104,105	0
7	MAN	A	1013	11/12	0.76	0.14	77,83,90,91	0
7	MAN	B	1014	11/12	0.79	0.15	72,85,90,92	0
8	NAG	A	1014	14/15	0.79	0.14	67,74,83,91	0
8	NAG	D	915	14/15	0.80	0.18	64,79,88,90	0
7	MAN	C	905	11/12	0.80	0.12	81,84,92,96	0

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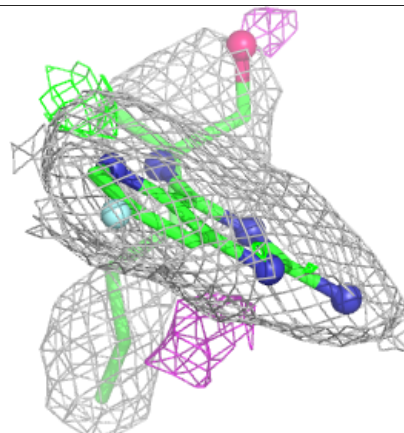
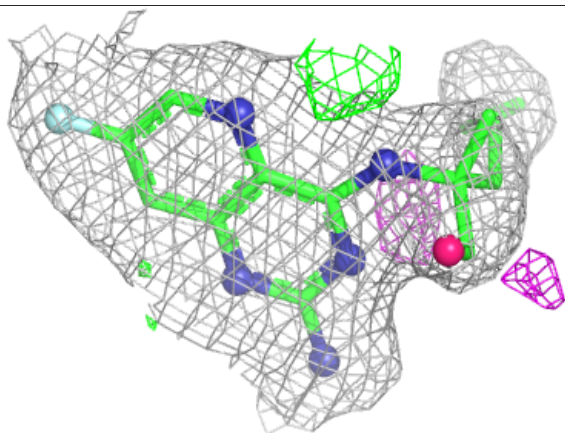
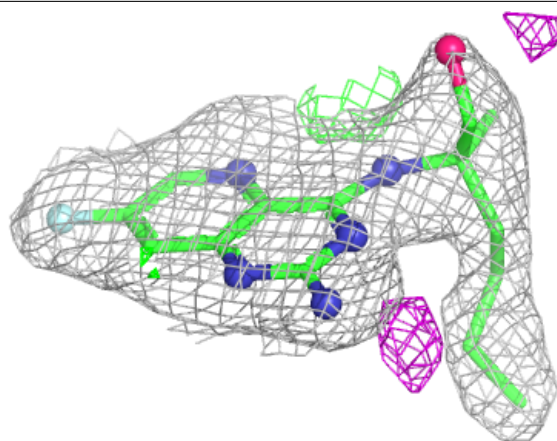
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	NAG	B	1015	14/15	0.81	0.18	49,63,74,85	0
8	NAG	C	916	14/15	0.81	0.14	72,82,91,96	0
8	NAG	C	909	14/15	0.82	0.12	63,71,84,92	0
8	NAG	A	1009	14/15	0.83	0.13	55,68,85,98	0
7	MAN	B	1004	11/12	0.84	0.14	54,67,73,76	0
8	NAG	D	909	14/15	0.85	0.14	56,69,78,93	0
8	NAG	D	917	14/15	0.86	0.12	51,58,72,75	0
8	NAG	A	1015	14/15	0.88	0.12	52,57,66,67	0
8	NAG	A	1016	14/15	0.90	0.10	51,62,67,73	0
7	MAN	A	1005	11/12	0.91	0.10	49,61,67,68	0
9	U57	C	917	21/21	0.91	0.12	41,51,60,76	0
8	NAG	B	1017	14/15	0.92	0.09	47,57,64,66	0
9	U57	A	1017	21/21	0.94	0.09	31,38,47,55	0
9	U57	D	918	21/21	0.95	0.09	33,39,44,53	0
8	NAG	A	1006	14/15	0.96	0.07	34,39,45,45	0
9	U57	B	1018	21/21	0.97	0.07	34,39,45,53	0

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

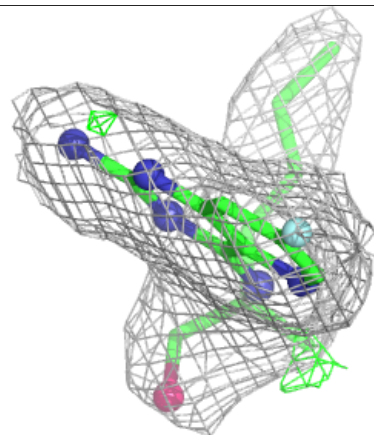
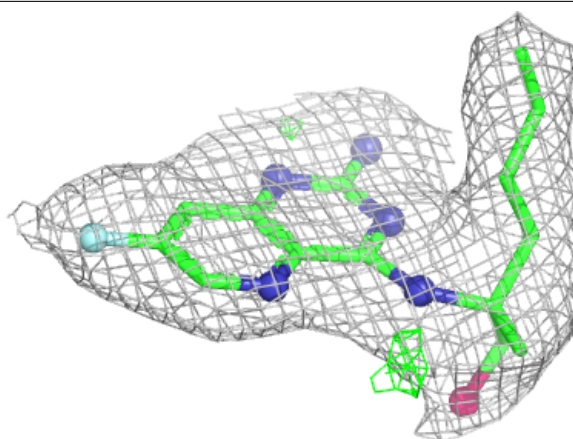
Electron density around U57 C 917:

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



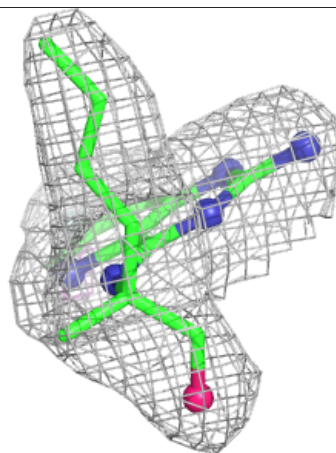
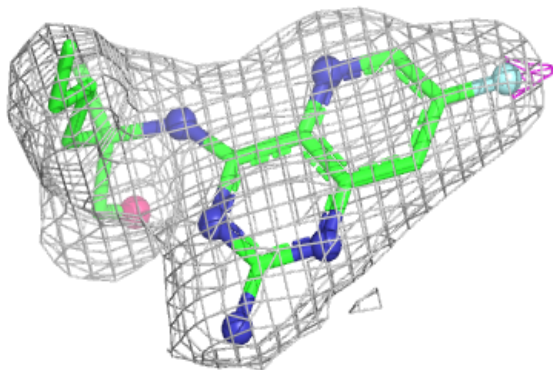
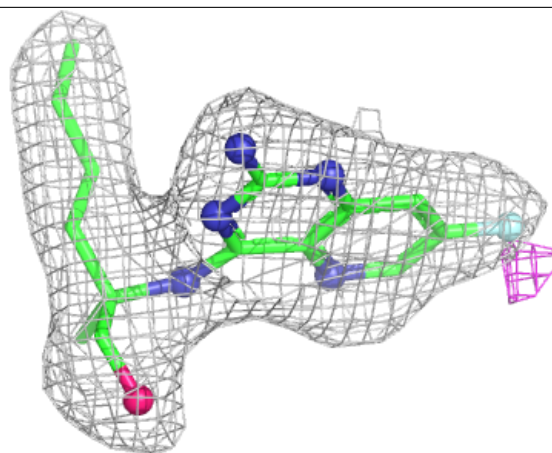
Electron density around U57 A 1017:

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



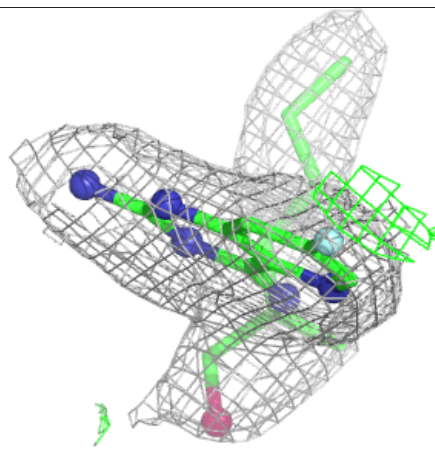
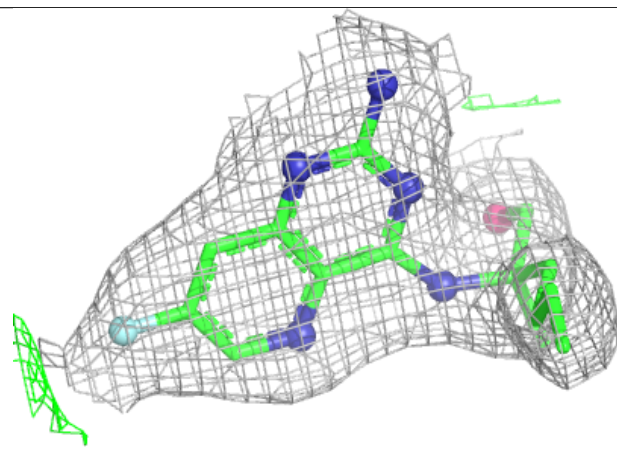
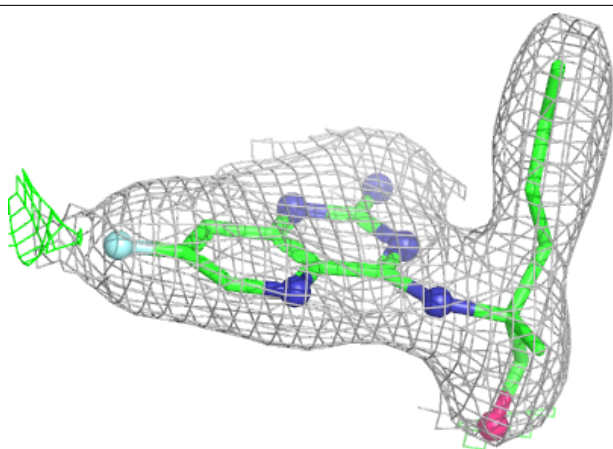
Electron density around U57 D 918:

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



Electron density around U57 B 1018:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.