



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:30 PM UTC

PDB ID : 5AZ5 / pdb_00005az5
Title : Crystal structure of human TLR8 in complex with MB-343
Authors : Tanji, H.; Ohto, U.; Shimizu, T.
Deposited on : 2015-09-27
Resolution : 2.40 Å(reported)

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

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

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:

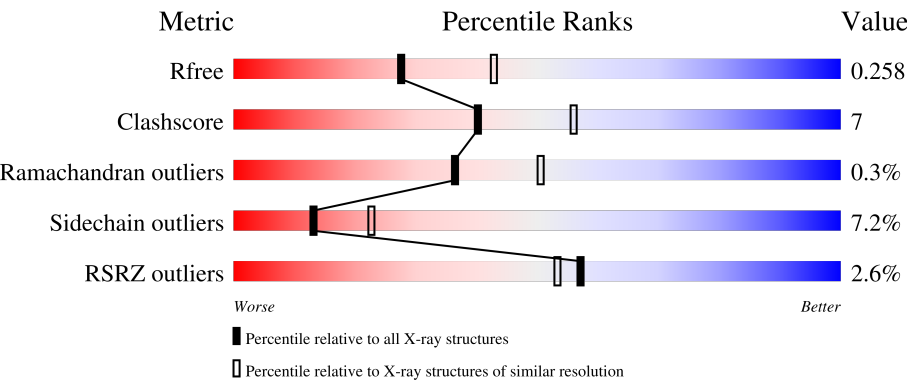
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance 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.



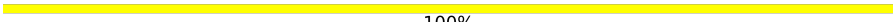
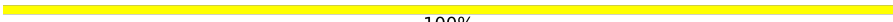
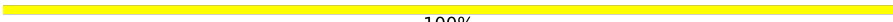
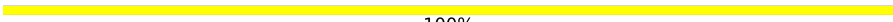
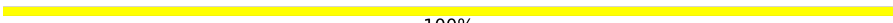
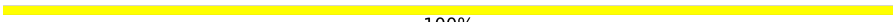
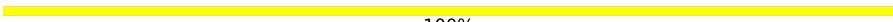
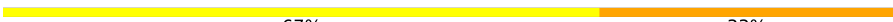
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 $\leq 5\%$. 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	% 77%13%• 8%
1	B	811	2% 76%14%• 8%
1	C	811	4% 74%17%• 8%
1	D	811	3% 72%17%• 8%
2	E	4	100%

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

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 25117 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	748	Total	C	N	O	S	0	0	0
			6029	3857	1023	1130	19			
1	B	749	Total	C	N	O	S	0	0	0
			6033	3859	1024	1131	19			
1	C	748	Total	C	N	O	S	0	0	0
			6024	3854	1023	1128	19			
1	D	746	Total	C	N	O	S	0	0	0
			6008	3844	1019	1126	19			

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



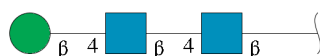
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	G	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	H	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



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

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



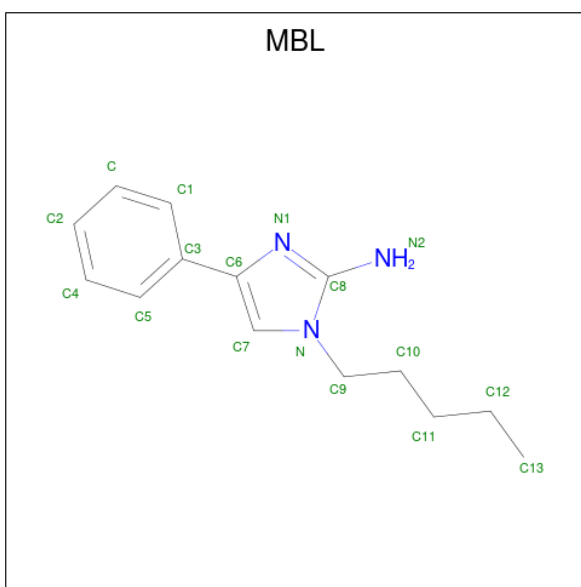
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	N	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	P	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 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.



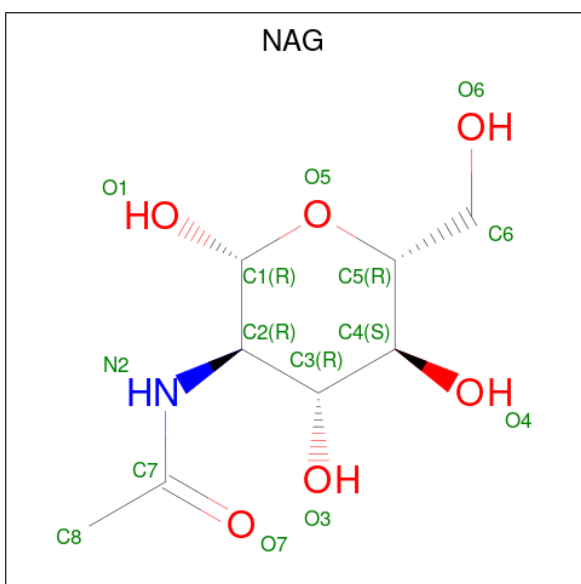
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	M	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 is 1-pentyl-4-phenyl-imidazol-2-amine (CCD ID: MBL) (formula: C₁₄H₁₉N₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			17	14	3		
6	A	1	Total	C	N	0	0
			17	14	3		
6	C	1	Total	C	N	0	0
			17	14	3		
6	C	1	Total	C	N	0	0
			17	14	3		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

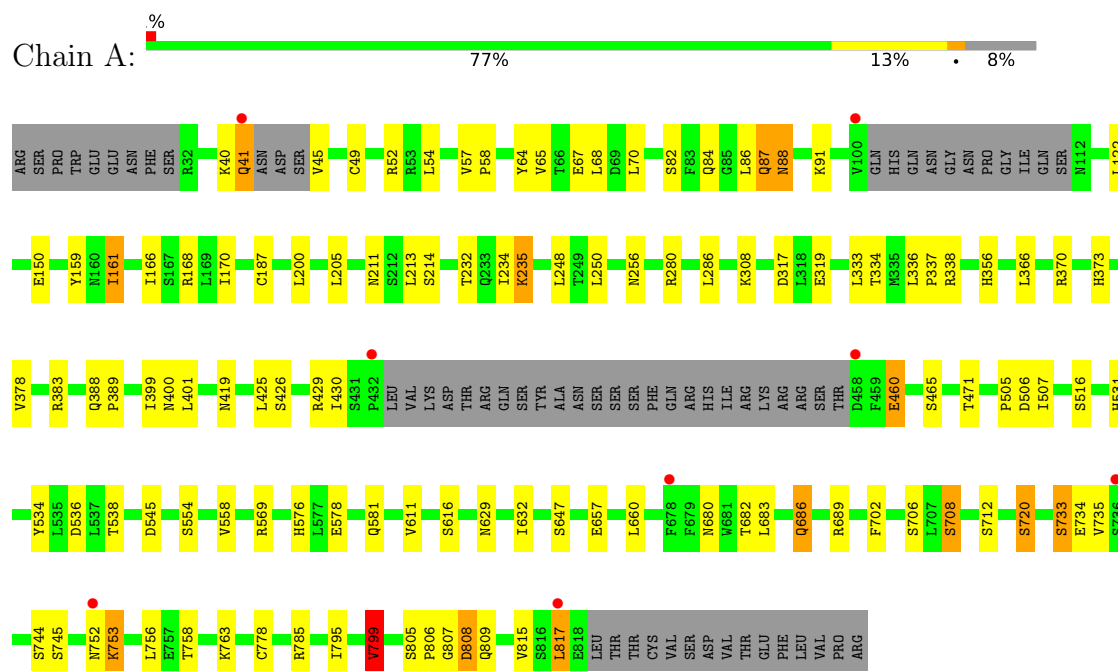
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	98	Total	O	0	0
			98	98		
8	B	83	Total	O	0	0
			83	83		
8	C	57	Total	O	0	0
			57	57		
8	D	53	Total	O	0	0
			53	53		

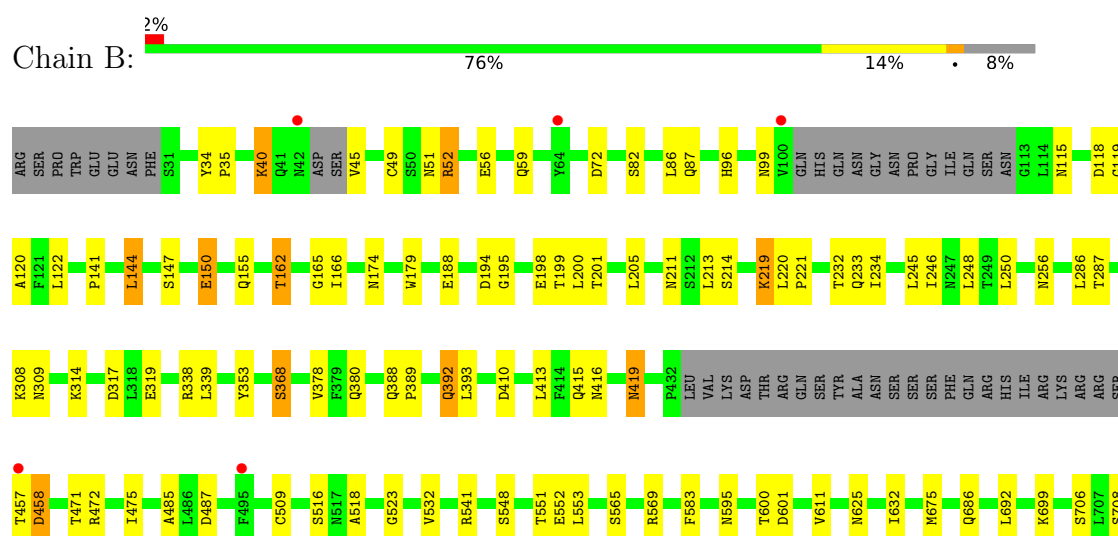
3 Residue-property plots

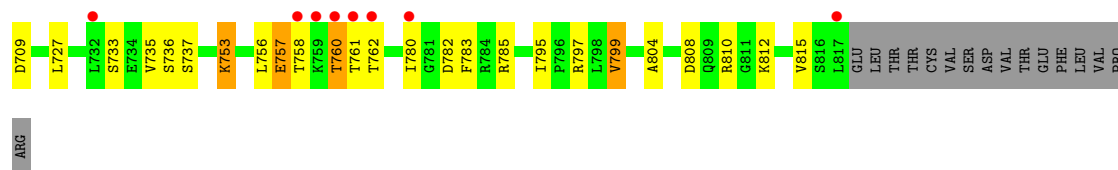
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Toll-like receptor 8

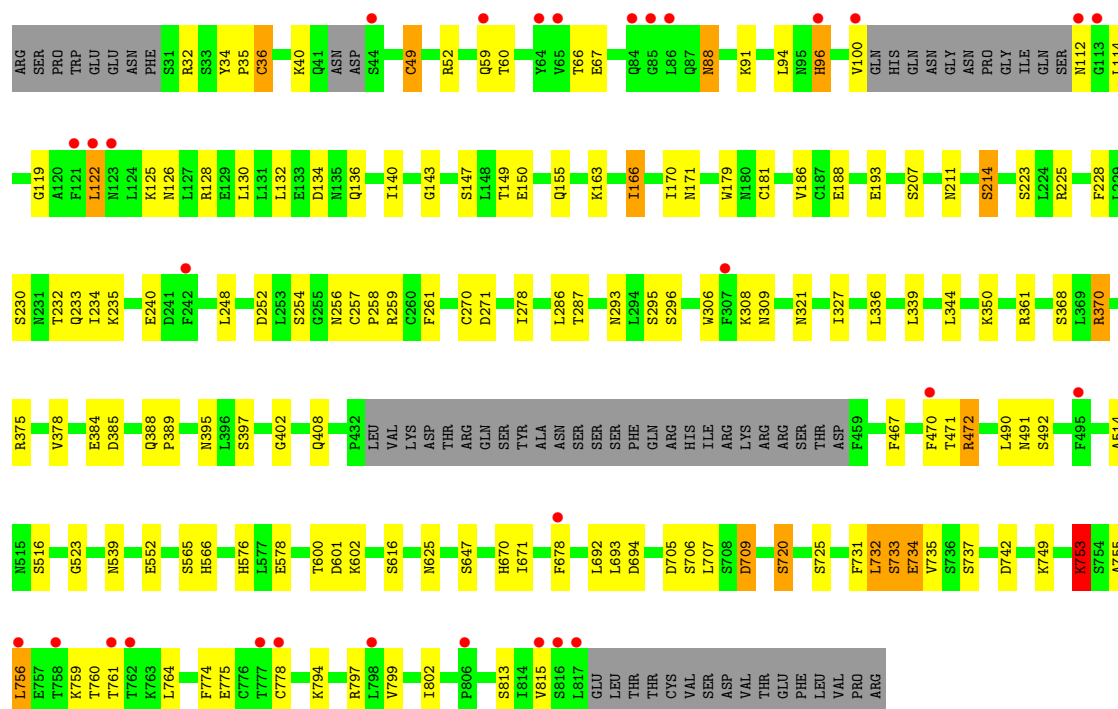
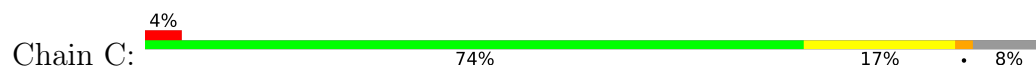


• Molecule 1: Toll-like receptor 8

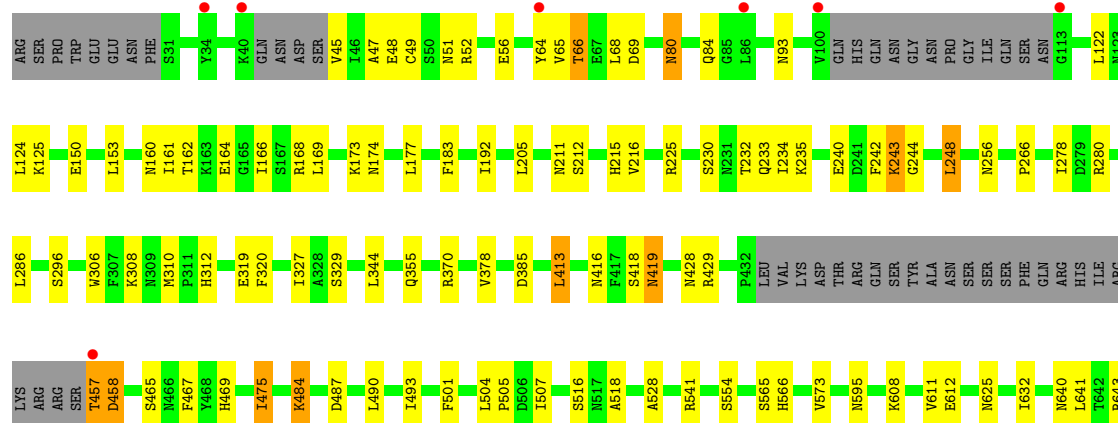


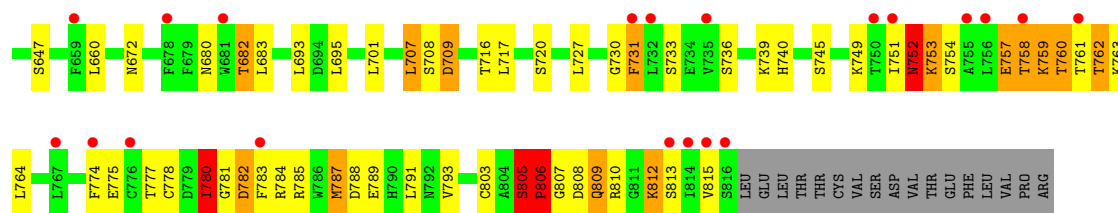


- Molecule 1: Toll-like receptor 8



- Molecule 1: Toll-like receptor 8



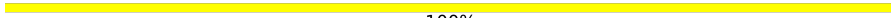


- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

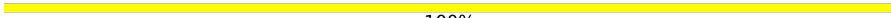


- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

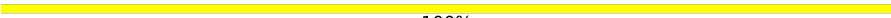


- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%

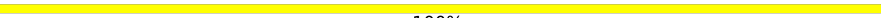


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%



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

Chain I:  100%



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

Chain L:  100%

MAG1
MAG2

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

Chain O:  100%

MAG1
MAG2

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

Chain 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 K:  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 N:  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 P:  100%

MAG1
MAG2
BMA3

- Molecule 5: 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 M:  100%

MAG1
MAG2
BMA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.63Å 141.12Å 170.97Å 90.00° 90.32° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.5 (50.00-2.40) 95.8 (50.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.196 , 0.259 0.200 , 0.258	Depositor DCC
R_{free} test set	7745 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	53.3	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 24.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25117	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: NAG, BMA, MAN, MBL

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	0.87	1/6153 (0.0%)	0.93	4/8343 (0.0%)
1	B	0.79	0/6157	0.90	7/8349 (0.1%)
1	C	0.78	0/6148	0.88	2/8336 (0.0%)
1	D	0.80	1/6132 (0.0%)	0.94	14/8315 (0.2%)
All	All	0.81	2/24590 (0.0%)	0.91	27/33343 (0.1%)

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	1
1	D	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	215	HIS	CG-ND1	-5.44	1.32	1.38
1	A	426	SER	CA-C	-5.01	1.46	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	805	SER	C-N-CD	8.69	139.71	120.60
1	D	760	THR	N-CA-C	8.56	123.02	112.58
1	D	216	VAL	N-CA-C	-6.79	102.70	109.02
1	D	752	ASN	N-CA-C	-6.72	101.66	110.53
1	B	219	LYS	N-CA-C	6.50	120.51	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	310	MET	CA-C-N	6.29	126.41	119.87
1	D	310	MET	C-N-CA	6.29	126.41	119.87
1	A	702	PHE	N-CA-C	5.99	117.64	108.42
1	D	708	SER	N-CA-C	-5.98	100.99	109.96
1	D	709	ASP	N-CA-C	-5.97	98.07	110.80
1	D	65	VAL	N-CA-C	5.71	116.37	108.84
1	A	799	VAL	CB-CA-C	-5.65	103.81	112.05
1	B	757	GLU	N-CA-C	-5.63	102.30	110.24
1	D	806	PRO	CA-N-CD	-5.48	103.83	111.50
1	B	795	ILE	CB-CA-C	-5.44	104.92	111.18
1	D	242	PHE	N-CA-C	5.32	119.46	112.92
1	C	166	ILE	N-CA-C	5.31	116.13	111.56
1	C	737	SER	N-CA-C	5.23	116.98	111.28
1	D	243	LYS	CA-C-N	5.18	131.03	121.70
1	D	243	LYS	C-N-CA	5.18	131.03	121.70
1	A	581	GLN	N-CA-C	5.18	117.67	111.71
1	A	460	GLU	N-CA-C	5.16	116.90	111.28
1	B	393	LEU	CA-C-N	5.15	124.94	119.28
1	B	393	LEU	C-N-CA	5.15	124.94	119.28
1	D	385	ASP	N-CA-C	5.08	117.55	111.71
1	B	144	LEU	CA-C-N	5.02	125.25	119.83
1	B	144	LEU	C-N-CA	5.02	125.25	119.83

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	753	LYS	Peptide
1	D	762	THR	Peptide
1	D	780	ILE	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6029	0	6016	54	0
1	B	6033	0	6021	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	6024	0	6015	85	0
1	D	6008	0	5997	129	0
2	E	50	0	43	0	0
2	G	50	0	43	0	0
2	H	50	0	43	0	0
3	F	28	0	25	0	0
3	I	28	0	25	0	0
3	L	28	0	25	0	0
3	O	28	0	25	0	0
4	J	39	0	34	0	0
4	K	39	0	34	1	0
4	N	39	0	34	2	0
4	P	39	0	34	0	0
5	M	50	0	43	0	0
6	A	34	0	0	0	0
6	C	34	0	0	0	0
7	A	42	0	39	3	0
7	B	56	0	52	0	0
7	C	56	0	52	0	0
7	D	42	0	39	2	0
8	A	98	0	0	2	0
8	B	83	0	0	2	0
8	C	57	0	0	3	0
8	D	53	0	0	3	0
All	All	25117	0	24639	324	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (324) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:LYS:HB3	1:D:244:GLY:HA3	1.20	1.17
1:D:759:LYS:HD2	1:D:760:THR:H	1.09	1.09
1:D:758:THR:HB	1:D:760:THR:HG23	1.32	1.08
1:D:759:LYS:HD2	1:D:760:THR:N	1.79	0.97
1:D:751:ILE:HD12	1:D:783:PHE:CD1	2.01	0.96
1:B:761:THR:HB	1:B:762:THR:O	1.68	0.93
1:D:759:LYS:O	1:D:762:THR:N	2.02	0.92
1:D:780:ILE:CD1	1:D:784:ARG:HG3	2.02	0.90
1:C:732:LEU:HB2	1:C:735:VAL:HG21	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:780:ILE:HD12	1:D:784:ARG:HG3	1.55	0.89
1:B:761:THR:HB	1:B:762:THR:C	1.97	0.88
1:D:758:THR:HB	1:D:760:THR:CG2	2.02	0.88
1:C:732:LEU:HB2	1:C:735:VAL:CG2	2.04	0.88
1:D:751:ILE:HD12	1:D:783:PHE:CG	2.10	0.87
1:A:45:VAL:HG13	1:A:65:VAL:HA	1.59	0.82
1:D:757:GLU:HA	1:D:758:THR:C	2.03	0.82
1:C:813:SER:OG	1:C:815:VAL:HG12	1.80	0.81
1:D:243:LYS:CB	1:D:244:GLY:HA3	2.07	0.81
1:D:457:THR:OG1	1:D:458:ASP:N	2.17	0.78
1:D:808:ASP:HA	1:D:809:GLN:C	2.08	0.77
1:D:777:THR:O	1:D:780:ILE:HG22	1.86	0.76
1:C:733:SER:HA	1:C:735:VAL:H	1.49	0.75
1:C:732:LEU:HD21	1:C:764:LEU:HD22	1.69	0.74
1:A:686:GLN:O	1:A:686:GLN:HG3	1.85	0.74
1:D:243:LYS:HB3	1:D:244:GLY:CA	2.08	0.74
1:D:761:THR:O	1:D:762:THR:OG1	2.05	0.74
1:A:686:GLN:HB2	8:A:1079:HOH:O	1.88	0.73
1:D:759:LYS:O	1:D:760:THR:OG1	2.09	0.70
1:D:751:ILE:CD1	1:D:783:PHE:CD1	2.75	0.70
1:D:780:ILE:C	1:D:780:ILE:HD13	2.17	0.70
1:D:153:LEU:HB2	1:D:177:LEU:HD23	1.73	0.70
1:D:775:GLU:HA	1:D:805:SER:HB2	1.76	0.67
1:C:566:HIS:CE1	1:D:490:LEU:HD22	2.30	0.66
1:D:716:THR:HG23	1:D:740:HIS:HB3	1.78	0.66
1:D:739:LYS:HA	1:D:763:LYS:HG3	1.78	0.65
1:D:205:LEU:HD23	1:D:205:LEU:C	2.22	0.64
1:C:733:SER:OG	1:C:734:GLU:HA	1.98	0.64
1:D:660:LEU:HD21	1:D:683:LEU:HD22	1.79	0.64
1:D:806:PRO:HD2	1:D:807:GLY:H	1.62	0.64
1:A:733:SER:HB2	1:A:758:THR:HG21	1.80	0.64
1:C:278:ILE:HB	1:C:306:TRP:CZ2	2.32	0.64
1:C:755:ALA:HB1	1:C:756:LEU:C	2.22	0.64
1:C:707:LEU:HD23	1:C:735:VAL:HG11	1.79	0.64
1:A:536:ASP:OD1	1:A:538:THR:HG23	1.98	0.63
1:C:467:PHE:HB3	4:K:1:NAG:H81	1.79	0.63
1:C:753:LYS:HD3	1:C:755:ALA:HB2	1.82	0.62
1:C:368:SER:HA	1:C:395:ASN:HD22	1.65	0.62
1:D:680:ASN:OD1	1:D:682:THR:HB	1.99	0.62
1:D:782:ASP:OD2	1:D:782:ASP:N	2.29	0.62
1:D:806:PRO:CD	1:D:807:GLY:H	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:GLU:HG3	1:D:174:ASN:HB2	1.83	0.61
1:D:733:SER:HB3	1:D:759:LYS:HB3	1.82	0.61
1:A:460:GLU:OE1	8:A:1001:HOH:O	2.15	0.60
1:B:735:VAL:HG13	1:B:735:VAL:O	2.00	0.60
1:B:804:ALA:O	1:B:810:ARG:NH1	2.34	0.60
1:D:809:GLN:HA	1:D:810:ARG:C	2.26	0.60
1:D:780:ILE:HD13	1:D:780:ILE:O	2.02	0.60
1:C:731:PHE:O	1:C:756:LEU:N	2.34	0.59
1:C:734:GLU:HB2	1:C:760:THR:HG22	1.84	0.59
1:C:66:THR:HG22	1:C:88:ASN:O	2.02	0.59
1:B:761:THR:N	1:B:762:THR:HA	2.17	0.59
1:D:808:ASP:CA	1:D:809:GLN:C	2.76	0.59
1:D:813:SER:OG	1:D:815:VAL:HG12	2.02	0.59
1:C:735:VAL:HG23	1:C:735:VAL:O	2.01	0.59
1:D:761:THR:O	1:D:761:THR:HG22	2.01	0.58
1:C:370:ARG:HD3	8:C:1021:HOH:O	2.02	0.58
1:C:732:LEU:HD22	8:C:1052:HOH:O	2.04	0.58
1:D:758:THR:OG1	1:D:759:LYS:O	2.20	0.58
7:A:914:NAG:O3	7:A:914:NAG:H82	2.03	0.58
1:D:758:THR:CB	1:D:760:THR:HG23	2.20	0.58
1:D:762:THR:OG1	1:D:763:LYS:O	2.22	0.57
1:C:96:HIS:HD2	1:C:134:ASP:HB3	1.69	0.57
1:D:759:LYS:C	1:D:762:THR:H	2.10	0.57
1:D:124:LEU:HB3	8:D:1110:HOH:O	2.05	0.57
1:B:457:THR:O	1:B:458:ASP:HB2	2.04	0.56
1:D:212:SER:OG	1:D:233:GLN:NE2	2.38	0.56
1:D:762:THR:OG1	1:D:763:LYS:N	2.35	0.56
1:D:806:PRO:HD2	1:D:809:GLN:O	2.04	0.56
1:C:692:LEU:C	1:C:692:LEU:HD23	2.30	0.56
1:C:733:SER:HA	1:C:735:VAL:N	2.20	0.56
1:D:752:ASN:ND2	1:D:753:LYS:H	2.04	0.56
1:D:760:THR:N	1:D:761:THR:HA	2.21	0.56
1:C:235:LYS:HD2	1:C:270:CYS:SG	2.46	0.55
1:A:67:GLU:OE2	1:A:91:LYS:HE2	2.06	0.55
1:A:205:LEU:HD23	1:A:205:LEU:C	2.30	0.55
1:C:732:LEU:C	1:C:735:VAL:HG22	2.32	0.55
1:B:234:ILE:O	1:B:256:ASN:HB3	2.07	0.55
1:C:706:SER:HB2	1:C:709:ASP:HB2	1.89	0.55
1:D:733:SER:CB	1:D:759:LYS:HB3	2.36	0.55
1:A:87:GLN:O	1:A:88:ASN:HB2	2.07	0.54
1:B:753:LYS:HD3	1:B:753:LYS:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:ASP:OD1	1:C:293:ASN:HB3	2.06	0.54
1:D:806:PRO:CG	1:D:807:GLY:H	2.21	0.54
1:B:706:SER:HB3	1:B:709:ASP:OD2	2.07	0.54
1:D:211:ASN:O	1:D:232:THR:HA	2.08	0.54
1:B:675:MET:HG2	1:B:699:LYS:HE3	1.90	0.54
1:B:317:ASP:OD1	1:B:319:GLU:OE1	2.25	0.54
1:D:758:THR:N	1:D:759:LYS:HA	2.22	0.54
1:A:807:GLY:O	1:A:808:ASP:OD2	2.25	0.54
1:A:471:THR:HG22	1:A:471:THR:O	2.08	0.53
1:C:214:SER:HA	1:C:233:GLN:O	2.08	0.53
1:A:52:ARG:HG2	1:A:799:VAL:HG11	1.89	0.53
1:B:194:ASP:OD1	1:B:219:LYS:NZ	2.33	0.53
1:A:52:ARG:HG3	1:A:799:VAL:HG21	1.90	0.53
1:A:250:LEU:C	1:A:250:LEU:HD23	2.34	0.53
1:D:164:GLU:O	1:D:168:ARG:NH1	2.40	0.53
1:D:707:LEU:HD12	1:D:731:PHE:CE1	2.43	0.53
1:D:757:GLU:CA	1:D:758:THR:C	2.76	0.53
1:B:205:LEU:C	1:B:205:LEU:HD23	2.33	0.53
1:C:600:THR:O	1:C:601:ASP:HB2	2.08	0.53
1:C:35:PRO:O	1:C:36:CYS:HB2	2.09	0.53
1:D:48:GLU:O	1:D:52:ARG:NH2	2.42	0.53
1:B:392:GLN:HB2	8:B:1136:HOH:O	2.09	0.52
1:C:490:LEU:HD22	1:D:566:HIS:NE2	2.24	0.52
1:B:523:GLY:O	1:B:552:GLU:HB3	2.09	0.52
1:A:708:SER:OG	1:A:734:GLU:OE1	2.26	0.52
1:D:751:ILE:CD1	1:D:783:PHE:CE1	2.93	0.52
1:A:333:LEU:HD22	1:A:366:LEU:HD11	1.90	0.52
1:B:213:LEU:O	1:B:214:SER:HB2	2.09	0.52
1:D:370:ARG:HH22	7:D:1010:NAG:H81	1.75	0.52
1:B:410:ASP:O	1:B:413:LEU:HD23	2.09	0.52
1:D:493:ILE:O	1:D:493:ILE:HG22	2.10	0.52
1:B:211:ASN:O	1:B:232:THR:HA	2.11	0.52
1:C:35:PRO:O	1:C:36:CYS:CB	2.59	0.51
1:C:207:SER:HA	1:C:228:PHE:HB2	1.91	0.51
1:C:140:ILE:HD13	1:C:166:ILE:HD11	1.92	0.51
1:A:680:ASN:OD1	1:A:682:THR:HB	2.11	0.51
1:B:518:ALA:HB2	1:B:541:ARG:HD2	1.91	0.51
1:B:166:ILE:CG2	1:B:200:LEU:HD11	2.41	0.51
1:C:794:LYS:HD3	1:C:794:LYS:N	2.26	0.51
1:D:759:LYS:N	1:D:759:LYS:CD	2.73	0.51
1:A:161:ILE:N	1:A:161:ILE:HD13	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:GLN:CD	1:C:59:GLN:H	2.18	0.50
1:A:40:LYS:O	1:A:41:GLN:OE1	2.29	0.50
1:D:806:PRO:CG	1:D:807:GLY:N	2.73	0.50
1:D:612:GLU:OE2	1:D:643:ARG:NH1	2.44	0.50
1:D:161:ILE:HD12	1:D:177:LEU:HD13	1.92	0.50
1:D:759:LYS:CD	1:D:759:LYS:H	2.24	0.50
1:C:734:GLU:CB	1:C:760:THR:HG22	2.42	0.50
1:D:428:ASN:O	1:D:429:ARG:HD3	2.11	0.50
1:D:752:ASN:ND2	1:D:753:LYS:N	2.60	0.50
1:D:774:PHE:HB2	1:D:803:CYS:HB3	1.94	0.50
1:C:149:THR:HG22	1:C:171:ASN:O	2.11	0.49
1:D:758:THR:CB	1:D:759:LYS:C	2.85	0.49
1:D:806:PRO:CD	1:D:807:GLY:N	2.73	0.49
1:D:707:LEU:HD12	1:D:731:PHE:HE1	1.76	0.49
1:D:754:SER:O	1:D:754:SER:OG	2.28	0.49
1:D:758:THR:HB	1:D:759:LYS:C	2.37	0.49
1:A:809:GLN:HE22	1:A:817:LEU:HD13	1.77	0.49
1:B:761:THR:N	1:B:762:THR:CA	2.75	0.49
1:C:96:HIS:HD2	1:C:134:ASP:CB	2.25	0.49
7:D:1011:NAG:O3	7:D:1011:NAG:H82	2.13	0.49
1:C:130:LEU:HD21	1:C:132:LEU:HD11	1.95	0.49
1:C:692:LEU:HD23	1:C:693:LEU:N	2.27	0.49
1:C:234:ILE:O	1:C:256:ASN:HB3	2.12	0.49
1:A:430:ILE:HD12	1:A:430:ILE:N	2.27	0.49
1:B:162:THR:HG22	1:B:165:GLY:H	1.78	0.49
1:B:808:ASP:O	1:B:812:LYS:NZ	2.45	0.49
1:D:730:GLY:H	1:D:754:SER:HB2	1.78	0.49
1:D:565:SER:O	1:D:566:HIS:C	2.55	0.48
1:A:516:SER:HB3	1:B:516:SER:OG	2.14	0.48
1:D:80:ASN:OD1	1:D:80:ASN:N	2.45	0.48
1:C:88:ASN:HA	1:C:126:ASN:HD22	1.78	0.48
1:A:86:LEU:C	1:A:87:GLN:O	2.54	0.48
1:B:115:ASN:OD1	1:B:115:ASN:C	2.56	0.48
1:C:52:ARG:HG3	1:C:799:VAL:HG11	1.96	0.48
1:B:692:LEU:HD23	1:B:692:LEU:C	2.39	0.48
1:A:752:ASN:OD1	1:A:753:LYS:N	2.46	0.48
1:B:195:GLY:O	1:B:198:GLU:HG2	2.14	0.48
1:C:34:TYR:CD1	1:C:815:VAL:HG11	2.49	0.48
1:D:693:LEU:HD23	1:D:717:LEU:CD1	2.44	0.48
1:D:736:SER:HA	1:D:762:THR:HB	1.95	0.48
1:B:761:THR:CB	1:B:762:THR:C	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:780:ILE:CD1	1:D:784:ARG:CG	2.83	0.48
1:A:534:TYR:CE2	1:A:558:VAL:HG11	2.50	0.47
1:D:780:ILE:CD1	1:D:780:ILE:C	2.85	0.47
1:A:54:LEU:HD13	1:A:58:PRO:HG3	1.95	0.47
1:A:234:ILE:O	1:A:256:ASN:HB3	2.14	0.47
1:D:278:ILE:HB	1:D:306:TRP:CZ2	2.49	0.47
1:A:506:ASP:OD1	1:A:531:HIS:HD2	1.97	0.47
1:A:660:LEU:HD21	1:A:683:LEU:HD22	1.96	0.47
1:B:141:PRO:HB2	1:B:144:LEU:HD21	1.97	0.47
1:A:807:GLY:O	1:A:808:ASP:CG	2.58	0.47
1:B:548:SER:O	1:B:551:THR:OG1	2.21	0.47
1:C:67:GLU:OE2	1:C:91:LYS:CE	2.63	0.47
1:D:225:ARG:O	1:D:248:LEU:HD22	2.14	0.47
1:D:759:LYS:HD2	1:D:759:LYS:N	2.29	0.47
1:B:72:ASP:O	1:B:99:ASN:ND2	2.48	0.47
1:C:223:SER:O	1:C:225:ARG:NH1	2.48	0.47
1:C:670:HIS:HA	1:C:694:ASP:HB3	1.95	0.47
1:C:149:THR:HA	1:C:171:ASN:O	2.15	0.47
1:A:166:ILE:CG2	1:A:200:LEU:HD11	2.45	0.46
1:A:576:HIS:HB3	1:A:578:GLU:OE1	2.15	0.46
1:C:516:SER:OG	1:D:516:SER:HB3	2.14	0.46
1:B:40:LYS:HA	1:B:45:VAL:HA	1.97	0.46
1:C:616:SER:HA	1:C:647:SER:O	2.16	0.46
1:D:775:GLU:HA	1:D:805:SER:CB	2.41	0.46
1:D:806:PRO:HG2	1:D:807:GLY:H	1.81	0.46
1:D:809:GLN:HG3	1:D:812:LYS:HD2	1.97	0.46
1:B:52:ARG:HG2	1:B:799:VAL:HG11	1.97	0.46
1:B:760:THR:HA	1:B:761:THR:C	2.40	0.46
1:C:385:ASP:HA	1:C:388:GLN:HG2	1.97	0.46
1:D:467:PHE:HB3	4:N:1:NAG:H81	1.97	0.46
1:D:753:LYS:HG2	1:D:782:ASP:OD1	2.16	0.46
1:C:88:ASN:N	1:C:88:ASN:HD22	2.14	0.46
1:C:720:SER:OG	1:C:742:ASP:OD2	2.25	0.46
1:B:200:LEU:O	1:B:221:PRO:HG3	2.16	0.46
1:B:250:LEU:HD23	1:B:250:LEU:C	2.40	0.46
1:C:67:GLU:OE2	1:C:91:LYS:HE3	2.15	0.46
1:D:484:LYS:HE2	1:D:505:PRO:HB2	1.97	0.46
1:B:314:LYS:C	1:B:339:LEU:HD12	2.41	0.46
1:D:518:ALA:HB2	1:D:541:ARG:HD2	1.98	0.46
1:A:57:VAL:HG21	1:A:82:SER:HB3	1.98	0.46
1:C:211:ASN:O	1:C:232:THR:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:GLY:HA3	1:C:122:LEU:HD23	1.99	0.45
1:D:759:LYS:H	1:D:759:LYS:HE3	1.81	0.45
1:A:370:ARG:NH2	7:A:913:NAG:H81	2.31	0.45
1:C:388:GLN:N	1:C:389:PRO:CD	2.80	0.45
1:A:211:ASN:O	1:A:232:THR:HA	2.16	0.45
1:C:733:SER:CB	1:C:734:GLU:HA	2.47	0.45
1:C:755:ALA:HA	1:C:756:LEU:CB	2.46	0.45
1:C:602:LYS:NZ	8:C:1006:HOH:O	2.45	0.45
1:C:259:ARG:NH1	1:C:321:ASN:O	2.50	0.45
1:D:413:LEU:C	1:D:413:LEU:HD12	2.41	0.45
1:D:693:LEU:HD21	1:D:695:LEU:HD11	1.99	0.45
1:D:809:GLN:HA	1:D:810:ARG:O	2.16	0.45
1:A:52:ARG:HB3	1:A:54:LEU:HG	1.99	0.45
1:A:401:LEU:HB2	1:A:425:LEU:HD23	1.98	0.45
1:A:616:SER:HA	1:A:647:SER:O	2.17	0.45
1:A:720:SER:HA	1:A:744:SER:O	2.17	0.45
1:D:183:PHE:HB3	1:D:266:PRO:HG2	1.99	0.45
1:D:475:ILE:HD13	1:D:487:ASP:HB2	1.99	0.45
1:D:780:ILE:HG23	1:D:781:GLY:N	2.32	0.45
1:A:505:PRO:O	1:A:507:ILE:HG12	2.17	0.44
1:B:150:GLU:HG2	1:B:174:ASN:HB2	1.99	0.44
1:B:287:THR:HA	1:B:309:ASN:O	2.17	0.44
1:B:338:ARG:HA	1:B:368:SER:OG	2.18	0.44
1:D:166:ILE:HA	1:D:169:LEU:HD12	1.98	0.44
1:D:312:HIS:HE1	8:D:1127:HOH:O	1.99	0.44
1:B:475:ILE:CD1	1:B:487:ASP:HB2	2.47	0.44
1:D:327:ILE:HG12	1:D:344:LEU:HD13	2.00	0.44
1:B:457:THR:O	1:B:458:ASP:CB	2.65	0.44
1:D:501:PHE:HB2	1:D:528:ALA:HB3	1.99	0.44
1:D:757:GLU:HA	1:D:758:THR:O	2.18	0.44
1:D:124:LEU:C	8:D:1110:HOH:O	2.60	0.44
1:A:213:LEU:O	1:A:214:SER:HB2	2.17	0.43
1:D:808:ASP:N	1:D:808:ASP:OD1	2.50	0.43
1:B:388:GLN:N	1:B:389:PRO:CD	2.81	0.43
1:C:49:CYS:C	1:C:52:ARG:HD3	2.43	0.43
1:C:128:ARG:HG2	1:C:147:SER:O	2.19	0.43
1:C:230:SER:HA	1:C:254:SER:O	2.19	0.43
1:C:287:THR:HA	1:C:309:ASN:O	2.18	0.43
1:A:805:SER:HB2	1:A:806:PRO:HA	2.01	0.43
1:C:336:LEU:HD13	1:C:339:LEU:HD22	2.01	0.43
1:C:753:LYS:HD2	1:C:753:LYS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:759:LYS:C	1:D:762:THR:N	2.72	0.43
1:A:317:ASP:OD1	1:A:319:GLU:OE1	2.37	0.43
1:B:34:TYR:CG	1:B:35:PRO:HA	2.54	0.43
1:A:373:HIS:HA	1:A:400:ASN:HB3	2.01	0.42
1:A:471:THR:O	1:A:471:THR:CG2	2.66	0.42
1:C:327:ILE:HG12	1:C:344:LEU:HD13	2.00	0.42
1:D:504:LEU:HD23	1:D:504:LEU:HA	1.87	0.42
1:A:68:LEU:HD21	1:A:70:LEU:HD11	2.01	0.42
1:A:370:ARG:HH22	7:A:913:NAG:H81	1.84	0.42
1:B:782:ASP:HA	1:B:785:ARG:NH1	2.34	0.42
1:D:467:PHE:CB	4:N:1:NAG:H81	2.49	0.42
1:D:758:THR:HB	1:D:760:THR:CB	2.48	0.42
1:C:565:SER:O	1:C:566:HIS:C	2.62	0.42
1:A:545:ASP:O	1:A:545:ASP:CG	2.63	0.42
1:C:155:GLN:HA	1:C:179:TRP:O	2.20	0.42
1:C:181:CYS:O	1:C:211:ASN:HA	2.19	0.42
1:C:472:ARG:HH11	1:C:472:ARG:CG	2.32	0.42
1:C:753:LYS:C	1:C:755:ALA:N	2.74	0.42
1:A:159:TYR:CE1	1:A:187:CYS:HB2	2.54	0.42
1:B:583:PHE:HB3	8:B:1142:HOH:O	2.19	0.42
1:C:732:LEU:O	1:C:735:VAL:HG13	2.20	0.42
1:D:419:ASN:N	1:D:419:ASN:OD1	2.53	0.42
1:D:760:THR:HG1	1:D:762:THR:H	1.67	0.42
1:C:576:HIS:HB3	1:C:578:GLU:OE1	2.20	0.42
1:B:155:GLN:HA	1:B:179:TRP:O	2.20	0.42
1:B:353:TYR:CZ	1:B:380:GLN:HG2	2.55	0.42
1:D:230:SER:O	1:D:232:THR:HG23	2.20	0.42
1:D:234:ILE:O	1:D:256:ASN:HB3	2.19	0.42
1:C:375:ARG:HA	1:C:402:GLY:O	2.20	0.42
1:D:296:SER:HA	1:D:320:PHE:O	2.19	0.42
1:B:119:GLY:O	1:B:120:ALA:C	2.62	0.41
1:D:783:PHE:CE2	1:D:787:MET:SD	3.13	0.41
1:B:600:THR:O	1:B:601:ASP:HB2	2.20	0.41
1:D:505:PRO:O	1:D:507:ILE:HG12	2.20	0.41
1:D:47:ALA:HB3	1:D:68:LEU:HA	2.03	0.41
1:B:532:VAL:HB	1:B:553:LEU:HD22	2.01	0.41
1:C:295:SER:O	1:C:296:SER:C	2.63	0.41
1:D:69:ASP:HA	1:D:93:ASN:HB3	2.02	0.41
1:A:430:ILE:HD12	1:A:430:ILE:H	1.84	0.41
1:B:214:SER:HA	1:B:233:GLN:O	2.20	0.41
1:B:565:SER:OG	1:B:569:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:491:ASN:HB3	1:C:492:SER:H	1.71	0.41
1:D:205:LEU:C	1:D:205:LEU:CD2	2.93	0.41
1:D:788:ASP:HA	1:D:791:LEU:HD21	2.02	0.41
1:A:388:GLN:N	1:A:389:PRO:CD	2.84	0.41
1:D:45:VAL:N	1:D:66:THR:HG1	2.19	0.41
1:B:419:ASN:HD22	1:B:419:ASN:HA	1.72	0.41
1:C:235:LYS:HD3	1:C:235:LYS:N	2.35	0.41
1:D:647:SER:HA	1:D:672:ASN:O	2.20	0.41
1:A:235:LYS:HE2	1:A:235:LYS:HB2	1.87	0.41
1:B:220:LEU:HB2	1:B:245:LEU:HD21	2.03	0.41
1:B:780:ILE:O	1:B:783:PHE:N	2.54	0.41
1:C:514:ALA:HA	1:C:539:ASN:O	2.19	0.41
1:D:319:GLU:OE1	1:D:469:HIS:HD2	2.04	0.41
1:A:356:HIS:CD2	1:A:383:ARG:HE	2.39	0.41
1:C:257:CYS:N	1:C:258:PRO:CD	2.84	0.40
1:C:523:GLY:O	1:C:552:GLU:HB3	2.22	0.40
1:C:749:LYS:O	1:C:774:PHE:HA	2.21	0.40
1:D:764:LEU:O	1:D:793:VAL:HG22	2.21	0.40
1:C:261:PHE:CZ	1:C:350:LYS:HD2	2.57	0.40
1:D:611:VAL:C	1:D:641:LEU:HD12	2.47	0.40
1:B:485:ALA:HA	1:B:509:CYS:O	2.22	0.40
1:D:608:LYS:O	1:D:640:ASN:HB2	2.21	0.40
1:D:707:LEU:CD1	1:D:731:PHE:HE1	2.35	0.40
1:D:758:THR:CB	1:D:760:THR:CG2	2.85	0.40
1:A:336:LEU:N	1:A:337:PRO:CD	2.84	0.40
1:B:756:LEU:O	1:B:757:GLU:C	2.64	0.40
1:C:119:GLY:HA2	1:C:143:GLY:HA3	2.03	0.40
1:D:806:PRO:HD2	1:D:807:GLY:N	2.32	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/811 (91%)	692 (94%)	47 (6%)	1 (0%)	48	64
1	B	741/811 (91%)	694 (94%)	45 (6%)	2 (0%)	36	50
1	C	740/811 (91%)	680 (92%)	56 (8%)	4 (0%)	24	37
1	D	738/811 (91%)	677 (92%)	58 (8%)	3 (0%)	30	43
All	All	2959/3244 (91%)	2743 (93%)	206 (7%)	10 (0%)	36	50

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	806	PRO
1	B	458	ASP
1	D	709	ASP
1	C	378	VAL
1	B	378	VAL
1	C	36	CYS
1	C	60	THR
1	D	378	VAL
1	A	378	VAL
1	C	186	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	695/755 (92%)	648 (93%)	47 (7%)	14	25
1	B	696/755 (92%)	651 (94%)	45 (6%)	15	27
1	C	695/755 (92%)	646 (93%)	49 (7%)	13	23
1	D	693/755 (92%)	635 (92%)	58 (8%)	10	17
All	All	2779/3020 (92%)	2580 (93%)	199 (7%)	13	23

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLN

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Mol	Chain	Res	Type
1	A	49	CYS
1	A	64	TYR
1	A	84	GLN
1	A	87	GLN
1	A	88	ASN
1	A	122	LEU
1	A	150	GLU
1	A	161	ILE
1	A	168	ARG
1	A	170	ILE
1	A	235	LYS
1	A	248	LEU
1	A	280	ARG
1	A	286	LEU
1	A	308	LYS
1	A	334	THR
1	A	338	ARG
1	A	399	ILE
1	A	419	ASN
1	A	429	ARG
1	A	465	SER
1	A	554	SER
1	A	569	ARG
1	A	611	VAL
1	A	629	ASN
1	A	632	ILE
1	A	657	GLU
1	A	686	GLN
1	A	689	ARG
1	A	706	SER
1	A	708	SER
1	A	712	SER
1	A	720	SER
1	A	733	SER
1	A	735	VAL
1	A	745	SER
1	A	753	LYS
1	A	756	LEU
1	A	763	LYS
1	A	778	CYS
1	A	785	ARG
1	A	795	ILE

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Mol	Chain	Res	Type
1	A	799	VAL
1	A	808	ASP
1	A	815	VAL
1	A	817	LEU
1	B	40	LYS
1	B	49	CYS
1	B	51	ASN
1	B	52	ARG
1	B	56	GLU
1	B	59	GLN
1	B	82	SER
1	B	86	LEU
1	B	87	GLN
1	B	96	HIS
1	B	118	ASP
1	B	122	LEU
1	B	147	SER
1	B	150	GLU
1	B	162	THR
1	B	188	GLU
1	B	199	THR
1	B	201	THR
1	B	246	ILE
1	B	248	LEU
1	B	286	LEU
1	B	308	LYS
1	B	368	SER
1	B	392	GLN
1	B	415	GLN
1	B	416	ASN
1	B	419	ASN
1	B	471	THR
1	B	472	ARG
1	B	595	ASN
1	B	611	VAL
1	B	625	ASN
1	B	632	ILE
1	B	686	GLN
1	B	708	SER
1	B	727	LEU
1	B	733	SER
1	B	736	SER

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Mol	Chain	Res	Type
1	B	737	SER
1	B	753	LYS
1	B	758	THR
1	B	760	THR
1	B	797	ARG
1	B	799	VAL
1	B	815	VAL
1	C	32	ARG
1	C	40	LYS
1	C	49	CYS
1	C	88	ASN
1	C	94	LEU
1	C	96	HIS
1	C	100	VAL
1	C	112	ASN
1	C	114	LEU
1	C	122	LEU
1	C	125	LYS
1	C	136	GLN
1	C	150	GLU
1	C	163	LYS
1	C	170	ILE
1	C	188	GLU
1	C	193	GLU
1	C	214	SER
1	C	240	GLU
1	C	248	LEU
1	C	271	ASP
1	C	286	LEU
1	C	308	LYS
1	C	361	ARG
1	C	370	ARG
1	C	384	GLU
1	C	397	SER
1	C	408	GLN
1	C	470	PHE
1	C	471	THR
1	C	472	ARG
1	C	625	ASN
1	C	671	ILE
1	C	678	PHE
1	C	705	ASP

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Mol	Chain	Res	Type
1	C	709	ASP
1	C	720	SER
1	C	725	SER
1	C	732	LEU
1	C	733	SER
1	C	734	GLU
1	C	753	LYS
1	C	756	LEU
1	C	759	LYS
1	C	761	THR
1	C	775	GLU
1	C	778	CYS
1	C	797	ARG
1	C	802	ILE
1	D	49	CYS
1	D	51	ASN
1	D	56	GLU
1	D	64	TYR
1	D	66	THR
1	D	80	ASN
1	D	84	GLN
1	D	122	LEU
1	D	125	LYS
1	D	160	ASN
1	D	162	THR
1	D	173	LYS
1	D	192	ILE
1	D	235	LYS
1	D	240	GLU
1	D	248	LEU
1	D	280	ARG
1	D	286	LEU
1	D	308	LYS
1	D	329	SER
1	D	355	GLN
1	D	413	LEU
1	D	416	ASN
1	D	418	SER
1	D	419	ASN
1	D	457	THR
1	D	458	ASP
1	D	465	SER

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Mol	Chain	Res	Type
1	D	475	ILE
1	D	484	LYS
1	D	554	SER
1	D	573	VAL
1	D	595	ASN
1	D	625	ASN
1	D	632	ILE
1	D	682	THR
1	D	701	LEU
1	D	707	LEU
1	D	720	SER
1	D	727	LEU
1	D	731	PHE
1	D	745	SER
1	D	749	LYS
1	D	752	ASN
1	D	753	LYS
1	D	757	GLU
1	D	758	THR
1	D	759	LYS
1	D	778	CYS
1	D	780	ILE
1	D	782	ASP
1	D	785	ARG
1	D	787	MET
1	D	789	GLU
1	D	805	SER
1	D	806	PRO
1	D	809	GLN
1	D	812	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	88	ASN
1	A	96	HIS
1	A	112	ASN
1	A	160	ASN
1	A	215	HIS
1	A	285	ASN
1	A	312	HIS

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Mol	Chain	Res	Type
1	A	356	HIS
1	A	416	ASN
1	A	419	ASN
1	A	531	HIS
1	A	585	ASN
1	A	629	ASN
1	A	686	GLN
1	A	809	GLN
1	B	51	ASN
1	B	55	GLN
1	B	87	GLN
1	B	136	GLN
1	B	312	HIS
1	B	408	GLN
1	B	419	ASN
1	B	499	ASN
1	B	503	ASN
1	B	581	GLN
1	B	721	HIS
1	B	790	HIS
1	C	88	ASN
1	C	96	HIS
1	C	126	ASN
1	C	184	ASN
1	C	233	GLN
1	C	355	GLN
1	C	388	GLN
1	C	392	GLN
1	C	415	GLN
1	C	539	ASN
1	C	566	HIS
1	C	593	HIS
1	C	604	ASN
1	D	55	GLN
1	D	84	GLN
1	D	123	ASN
1	D	233	GLN
1	D	285	ASN
1	D	312	HIS
1	D	355	GLN
1	D	358	ASN
1	D	380	GLN

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Mol	Chain	Res	Type
1	D	469	HIS
1	D	582	ASN
1	D	593	HIS
1	D	726	HIS
1	D	740	HIS
1	D	752	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

42 non-standard protein/DNA/RNA residues 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	NAG	B	1013	1	14,14,15	0.73	0	17,19,21	1.78	5 (29%)
2	NAG	E	2	2	14,14,15	0.84	0	17,19,21	1.65	6 (35%)
4	NAG	N	2	4	14,14,15	0.58	0	17,19,21	1.42	2 (11%)
4	NAG	K	2	4	14,14,15	0.67	0	17,19,21	2.09	9 (52%)
2	NAG	H	2	2	14,14,15	0.53	0	17,19,21	1.32	3 (17%)
7	NAG	B	1010	1	14,14,15	0.76	1 (7%)	17,19,21	1.78	4 (23%)
3	NAG	O	1	3,1	14,14,15	0.70	1 (7%)	17,19,21	1.63	2 (11%)
2	MAN	G	4	2	11,11,12	0.53	0	15,15,17	1.21	2 (13%)
7	NAG	D	1006	1	14,14,15	0.53	0	17,19,21	1.60	3 (17%)
5	NAG	M	1	1,5	14,14,15	0.54	0	17,19,21	1.21	3 (17%)
4	NAG	J	2	4	14,14,15	1.12	2 (14%)	17,19,21	1.77	5 (29%)
4	NAG	P	1	4,1	14,14,15	0.64	0	17,19,21	1.42	1 (5%)
2	NAG	H	1	1,2	14,14,15	0.78	0	17,19,21	1.72	4 (23%)
3	NAG	L	2	3	14,14,15	0.60	0	17,19,21	1.37	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	F	1	3,1	14,14,15	0.63	0	17,19,21	1.54	4 (23%)
3	NAG	F	2	3	14,14,15	0.82	1 (7%)	17,19,21	1.71	4 (23%)
7	NAG	A	912	1	14,14,15	0.58	0	17,19,21	2.45	4 (23%)
3	NAG	L	1	3,1	14,14,15	0.67	0	17,19,21	1.53	2 (11%)
7	NAG	C	914	1	14,14,15	0.89	1 (7%)	17,19,21	0.94	1 (5%)
7	NAG	A	913	1	14,14,15	0.76	0	17,19,21	1.47	2 (11%)
4	NAG	J	1	4,1	14,14,15	0.91	0	17,19,21	1.25	2 (11%)
2	MAN	H	4	2	11,11,12	0.84	0	15,15,17	1.70	5 (33%)
2	NAG	E	1	1,2	14,14,15	0.90	1 (7%)	17,19,21	1.36	3 (17%)
4	NAG	K	1	4,1	14,14,15	0.73	0	17,19,21	1.47	4 (23%)
7	NAG	B	1012	1	14,14,15	0.89	1 (7%)	17,19,21	1.42	2 (11%)
3	NAG	I	2	3	14,14,15	0.88	1 (7%)	17,19,21	1.82	5 (29%)
2	MAN	E	4	2	11,11,12	0.77	0	15,15,17	1.23	3 (20%)
4	NAG	P	2	4	14,14,15	0.73	0	17,19,21	1.27	2 (11%)
7	NAG	D	1011	1	14,14,15	0.65	0	17,19,21	1.91	5 (29%)
3	NAG	I	1	3,1	14,14,15	0.89	0	17,19,21	1.61	3 (17%)
4	NAG	N	1	4,1	14,14,15	0.94	1 (7%)	17,19,21	1.51	2 (11%)
7	NAG	B	1011	1	14,14,15	0.68	0	17,19,21	1.02	0
7	NAG	C	912	1	14,14,15	0.69	0	17,19,21	1.71	2 (11%)
2	NAG	G	1	1,2	14,14,15	0.63	0	17,19,21	1.48	3 (17%)
5	MAN	M	4	5	11,11,12	0.95	1 (9%)	15,15,17	1.36	3 (20%)
5	NAG	M	2	5	14,14,15	0.91	1 (7%)	17,19,21	0.94	1 (5%)
7	NAG	D	1010	1	14,14,15	0.74	0	17,19,21	1.20	3 (17%)
7	NAG	A	914	1	14,14,15	0.72	0	17,19,21	2.21	6 (35%)
7	NAG	C	913	1	14,14,15	0.94	1 (7%)	17,19,21	1.30	3 (17%)
2	NAG	G	2	2	14,14,15	1.04	1 (7%)	17,19,21	1.25	2 (11%)
7	NAG	C	907	1	14,14,15	0.86	0	17,19,21	1.52	3 (17%)
3	NAG	O	2	3	14,14,15	0.75	0	17,19,21	1.51	4 (23%)

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	NAG	B	1013	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
7	NAG	B	1010	1	-	0/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	2/6/23/26	0/1/1/1
2	MAN	G	4	2	-	0/2/19/22	0/1/1/1
7	NAG	D	1006	1	-	4/6/23/26	0/1/1/1
5	NAG	M	1	1,5	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	NAG	P	1	4,1	-	0/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
7	NAG	A	912	1	-	0/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	0/6/23/26	0/1/1/1
7	NAG	C	914	1	-	2/6/23/26	0/1/1/1
7	NAG	A	913	1	-	2/6/23/26	0/1/1/1
4	NAG	J	1	4,1	-	0/6/23/26	0/1/1/1
2	MAN	H	4	2	-	0/2/19/22	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	0/6/23/26	0/1/1/1
7	NAG	B	1012	1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
4	NAG	P	2	4	-	1/6/23/26	0/1/1/1
7	NAG	D	1011	1	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	0/6/23/26	0/1/1/1
7	NAG	B	1011	1	-	0/6/23/26	0/1/1/1
7	NAG	C	912	1	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
5	MAN	M	4	5	-	2/2/19/22	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
7	NAG	D	1010	1	-	0/6/23/26	0/1/1/1
7	NAG	A	914	1	-	2/6/23/26	0/1/1/1
7	NAG	C	913	1	-	3/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	907	1	-	4/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	2	NAG	O5-C1	-3.03	1.38	1.43
2	G	2	NAG	O5-C1	-2.81	1.39	1.43
4	N	1	NAG	O5-C1	-2.57	1.39	1.43
5	M	2	NAG	O5-C1	-2.57	1.39	1.43
5	M	4	MAN	C2-C3	2.48	1.56	1.52
7	B	1012	NAG	O5-C1	-2.46	1.39	1.43
3	F	2	NAG	O5-C1	-2.34	1.39	1.43
7	C	914	NAG	C1-C2	2.30	1.55	1.52
3	I	2	NAG	O5-C1	-2.26	1.39	1.43
4	J	2	NAG	C2-N2	-2.11	1.42	1.46
3	O	1	NAG	O5-C1	-2.10	1.40	1.43
2	E	1	NAG	C2-N2	-2.02	1.42	1.46
7	C	913	NAG	O5-C1	-2.02	1.40	1.43
7	B	1010	NAG	O5-C1	-2.02	1.40	1.43

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	912	NAG	O5-C1-C2	5.86	120.35	111.29
7	C	912	NAG	C1-O5-C5	5.60	119.70	112.19
7	A	914	NAG	O5-C1-C2	-5.49	102.80	111.29
7	A	912	NAG	C1-O5-C5	5.14	119.07	112.19
7	B	1010	NAG	C1-O5-C5	4.84	118.68	112.19
4	P	1	NAG	C1-O5-C5	4.79	118.60	112.19
4	J	2	NAG	O5-C1-C2	-4.63	104.12	111.29
7	A	914	NAG	C8-C7-N2	4.54	123.65	116.12
3	L	1	NAG	C1-C2-N2	-4.35	103.58	110.43
4	N	1	NAG	O5-C1-C2	-4.26	104.70	111.29
7	A	912	NAG	C4-C3-C2	-4.23	104.81	111.02
7	D	1011	NAG	C8-C7-N2	4.09	122.90	116.12
3	I	1	NAG	C3-C4-C5	-4.04	102.91	110.23
3	F	2	NAG	C3-C4-C5	-4.04	102.92	110.23
3	F	2	NAG	O5-C1-C2	-4.00	105.11	111.29
7	A	912	NAG	C1-C2-N2	-3.78	104.47	110.43
7	D	1006	NAG	C8-C7-N2	3.77	122.37	116.12
3	F	1	NAG	C1-C2-N2	-3.76	104.51	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	1	NAG	C1-C2-N2	-3.72	104.58	110.43
4	K	2	NAG	C1-C2-N2	3.68	116.23	110.43
7	B	1013	NAG	C2-N2-C7	3.59	127.71	122.90
2	H	1	NAG	O5-C1-C2	-3.49	105.89	111.29
3	I	2	NAG	C3-C4-C5	-3.46	103.96	110.23
7	C	907	NAG	C1-C2-N2	-3.36	105.15	110.43
4	N	2	NAG	O5-C1-C2	-3.35	106.11	111.29
4	K	2	NAG	C2-N2-C7	-3.27	118.52	122.90
3	O	1	NAG	C1-O5-C5	3.23	116.52	112.19
4	K	2	NAG	C1-O5-C5	-3.22	107.87	112.19
7	D	1011	NAG	C4-C3-C2	-3.20	106.33	111.02
7	A	913	NAG	O5-C1-C2	-3.14	106.43	111.29
4	J	1	NAG	O5-C1-C2	-3.14	106.44	111.29
3	O	2	NAG	O5-C1-C2	-3.11	106.48	111.29
2	E	2	NAG	O7-C7-N2	3.07	127.41	121.98
3	F	1	NAG	C3-C4-C5	-3.03	104.74	110.23
4	P	2	NAG	C4-C3-C2	-3.00	106.62	111.02
7	B	1013	NAG	O5-C5-C6	2.99	113.47	107.66
4	J	2	NAG	C1-C2-N2	-2.98	105.74	110.43
7	A	913	NAG	O4-C4-C3	-2.97	103.36	110.38
2	H	2	NAG	C3-C4-C5	-2.97	104.85	110.23
5	M	4	MAN	O3-C3-C2	2.95	116.08	110.05
7	D	1011	NAG	O5-C1-C2	-2.93	106.76	111.29
3	I	2	NAG	O4-C4-C5	2.91	116.50	109.32
7	A	914	NAG	C4-C3-C2	-2.90	106.76	111.02
2	H	1	NAG	C2-N2-C7	-2.84	119.09	122.90
2	H	4	MAN	C2-C3-C4	2.84	115.85	110.86
7	B	1013	NAG	C1-O5-C5	2.83	115.98	112.19
3	O	2	NAG	O3-C3-C4	-2.83	103.70	110.38
7	D	1011	NAG	C2-N2-C7	2.81	126.66	122.90
7	C	913	NAG	C1-O5-C5	2.79	115.92	112.19
7	A	914	NAG	O7-C7-N2	-2.77	117.08	121.98
4	J	2	NAG	O6-C6-C5	-2.75	101.97	111.33
2	E	2	NAG	C1-O5-C5	-2.74	108.51	112.19
2	H	4	MAN	C3-C4-C5	2.73	115.17	110.23
2	H	1	NAG	C3-C4-C5	-2.72	105.29	110.23
3	I	1	NAG	C1-C2-N2	-2.72	106.14	110.43
2	E	1	NAG	C1-O5-C5	2.69	115.79	112.19
2	H	1	NAG	O5-C5-C6	2.68	112.87	107.66
2	E	2	NAG	O7-C7-C8	-2.65	117.33	122.05
4	K	2	NAG	O5-C1-C2	-2.65	107.19	111.29
7	D	1006	NAG	O7-C7-C8	-2.65	117.34	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	2	NAG	C8-C7-N2	2.64	120.50	116.12
2	G	1	NAG	C2-N2-C7	2.64	126.43	122.90
3	I	1	NAG	O5-C1-C2	-2.62	107.24	111.29
4	K	2	NAG	O3-C3-C4	-2.59	104.26	110.38
4	K	1	NAG	O4-C4-C5	-2.56	103.03	109.32
7	C	912	NAG	O5-C1-C2	-2.53	107.38	111.29
3	L	2	NAG	C1-O5-C5	2.51	115.56	112.19
2	G	2	NAG	C4-C3-C2	-2.51	107.34	111.02
7	D	1011	NAG	O7-C7-N2	-2.48	117.59	121.98
2	G	1	NAG	O7-C7-C8	-2.48	117.64	122.05
7	B	1012	NAG	C1-O5-C5	2.45	115.47	112.19
2	G	4	MAN	C1-O5-C5	2.45	115.47	112.19
7	B	1010	NAG	O7-C7-N2	-2.44	117.68	121.98
3	L	1	NAG	O7-C7-C8	-2.43	117.72	122.05
5	M	1	NAG	O5-C1-C2	-2.43	107.54	111.29
3	L	2	NAG	O5-C1-C2	-2.41	107.57	111.29
7	D	1006	NAG	O5-C1-C2	-2.37	107.62	111.29
2	H	4	MAN	C1-C2-C3	2.36	113.09	109.64
2	E	1	NAG	O7-C7-C8	-2.36	117.85	122.05
2	E	4	MAN	C1-O5-C5	2.35	115.34	112.19
2	H	2	NAG	O5-C1-C2	-2.33	107.69	111.29
2	G	2	NAG	O6-C6-C5	-2.31	103.47	111.33
4	K	1	NAG	C2-N2-C7	-2.31	119.81	122.90
4	P	2	NAG	O7-C7-N2	2.30	126.04	121.98
5	M	1	NAG	O5-C5-C4	-2.29	105.26	110.83
4	N	2	NAG	C1-C2-N2	2.28	114.02	110.43
5	M	4	MAN	O2-C2-C3	2.27	114.86	110.15
2	H	2	NAG	C1-O5-C5	2.27	115.23	112.19
2	G	1	NAG	O7-C7-N2	2.27	125.99	121.98
4	J	2	NAG	O5-C5-C6	-2.27	103.25	107.66
3	L	2	NAG	O4-C4-C5	2.25	114.87	109.32
4	K	1	NAG	C1-C2-N2	2.25	113.98	110.43
2	H	4	MAN	O3-C3-C4	-2.25	105.08	110.38
5	M	1	NAG	C1-O5-C5	2.24	115.19	112.19
5	M	2	NAG	O4-C4-C3	-2.24	105.10	110.38
2	G	4	MAN	C1-C2-C3	-2.23	106.39	109.64
4	K	2	NAG	O4-C4-C5	2.22	114.78	109.32
3	F	1	NAG	O5-C5-C4	2.21	116.21	110.83
4	J	1	NAG	C8-C7-N2	2.20	119.77	116.12
2	E	4	MAN	O2-C2-C1	2.20	114.27	109.22
4	K	2	NAG	C8-C7-N2	2.19	119.76	116.12
2	E	2	NAG	C3-C4-C5	-2.18	106.28	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	913	NAG	O7-C7-C8	-2.17	118.19	122.05
3	O	2	NAG	O4-C4-C5	2.17	114.67	109.32
3	I	2	NAG	C4-C3-C2	-2.16	107.85	111.02
7	D	1010	NAG	O5-C1-C2	-2.15	107.96	111.29
4	J	2	NAG	C4-C3-C2	-2.15	107.87	111.02
7	C	907	NAG	O4-C4-C3	-2.15	105.32	110.38
3	F	2	NAG	C1-O5-C5	2.14	115.05	112.19
2	E	2	NAG	C2-N2-C7	2.13	125.76	122.90
7	A	914	NAG	C1-O5-C5	2.12	115.03	112.19
7	B	1010	NAG	C2-N2-C7	-2.11	120.07	122.90
7	D	1010	NAG	O5-C5-C4	-2.11	105.70	110.83
2	H	4	MAN	C1-O5-C5	2.10	115.00	112.19
3	O	2	NAG	C4-C3-C2	2.10	114.09	111.02
4	K	2	NAG	O6-C6-C5	-2.10	104.20	111.33
7	C	914	NAG	C1-O5-C5	2.09	114.99	112.19
7	B	1010	NAG	O3-C3-C4	-2.09	105.46	110.38
7	B	1013	NAG	C1-C2-N2	2.08	113.72	110.43
7	D	1010	NAG	O3-C3-C4	2.08	115.28	110.38
7	C	913	NAG	O5-C5-C6	-2.08	103.62	107.66
5	M	4	MAN	O3-C3-C4	2.08	115.27	110.38
3	I	2	NAG	O5-C1-C2	-2.07	108.09	111.29
2	E	2	NAG	O6-C6-C5	-2.07	104.29	111.33
3	F	2	NAG	O5-C5-C6	2.06	111.68	107.66
4	K	1	NAG	O3-C3-C4	2.06	115.23	110.38
7	B	1012	NAG	O6-C6-C5	-2.06	104.33	111.33
4	N	1	NAG	C3-C4-C5	-2.05	106.51	110.23
3	F	1	NAG	O3-C3-C4	2.03	115.17	110.38
2	E	4	MAN	O2-C2-C3	2.03	114.36	110.15
4	K	2	NAG	O4-C4-C3	-2.02	105.62	110.38
7	C	907	NAG	C8-C7-N2	2.01	119.46	116.12
7	B	1013	NAG	C4-C3-C2	2.01	113.97	111.02
7	A	914	NAG	C1-C2-N2	2.01	113.60	110.43
2	E	1	NAG	O6-C6-C5	-2.01	104.50	111.33

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1013	NAG	O5-C5-C6-O6
5	M	4	MAN	O5-C5-C6-O6
7	C	907	NAG	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	B	1013	NAG	C4-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
5	M	4	MAN	C4-C5-C6-O6
7	C	907	NAG	C4-C5-C6-O6
7	D	1006	NAG	O5-C5-C6-O6
7	A	914	NAG	C8-C7-N2-C2
7	A	914	NAG	O7-C7-N2-C2
7	B	1013	NAG	C8-C7-N2-C2
7	B	1013	NAG	O7-C7-N2-C2
7	C	907	NAG	C8-C7-N2-C2
7	C	907	NAG	O7-C7-N2-C2
7	D	1006	NAG	C8-C7-N2-C2
7	D	1006	NAG	O7-C7-N2-C2
7	D	1011	NAG	C8-C7-N2-C2
7	D	1011	NAG	O7-C7-N2-C2
7	D	1006	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
7	C	913	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
7	C	914	NAG	C4-C5-C6-O6
7	C	913	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
7	C	914	NAG	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
7	C	913	NAG	C3-C2-N2-C7
3	I	2	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
7	A	913	NAG	C1-C2-N2-C7
4	P	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
7	A	913	NAG	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	913	NAG	2	0
4	K	1	NAG	1	0
7	D	1011	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	1	NAG	2	0
7	D	1010	NAG	1	0
7	A	914	NAG	1	0

5.5 Carbohydrates [i](#)

36 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	0.90	1 (7%)	17,19,21	1.36	3 (17%)
2	NAG	E	2	2	14,14,15	0.84	0	17,19,21	1.65	6 (35%)
2	BMA	E	3	2	11,11,12	0.78	0	15,15,17	1.77	5 (33%)
2	MAN	E	4	2	11,11,12	0.77	0	15,15,17	1.23	3 (20%)
3	NAG	F	1	3,1	14,14,15	0.63	0	17,19,21	1.54	4 (23%)
3	NAG	F	2	3	14,14,15	0.82	1 (7%)	17,19,21	1.71	4 (23%)
2	NAG	G	1	1,2	14,14,15	0.63	0	17,19,21	1.48	3 (17%)
2	NAG	G	2	2	14,14,15	1.04	1 (7%)	17,19,21	1.25	2 (11%)
2	BMA	G	3	2	11,11,12	0.56	0	15,15,17	1.52	3 (20%)
2	MAN	G	4	2	11,11,12	0.53	0	15,15,17	1.21	2 (13%)
2	NAG	H	1	1,2	14,14,15	0.78	0	17,19,21	1.72	4 (23%)
2	NAG	H	2	2	14,14,15	0.53	0	17,19,21	1.32	3 (17%)
2	BMA	H	3	2	11,11,12	0.68	0	15,15,17	1.61	3 (20%)
2	MAN	H	4	2	11,11,12	0.84	0	15,15,17	1.70	5 (33%)
3	NAG	I	1	3,1	14,14,15	0.89	0	17,19,21	1.61	3 (17%)
3	NAG	I	2	3	14,14,15	0.88	1 (7%)	17,19,21	1.82	5 (29%)
4	NAG	J	1	4,1	14,14,15	0.91	0	17,19,21	1.25	2 (11%)
4	NAG	J	2	4	14,14,15	1.12	2 (14%)	17,19,21	1.77	5 (29%)
4	BMA	J	3	4	11,11,12	0.57	0	15,15,17	1.69	3 (20%)
4	NAG	K	1	4,1	14,14,15	0.73	0	17,19,21	1.47	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	K	2	4	14,14,15	0.67	0	17,19,21	2.09	9 (52%)
4	BMA	K	3	4	11,11,12	0.72	0	15,15,17	1.34	3 (20%)
3	NAG	L	1	3,1	14,14,15	0.67	0	17,19,21	1.53	2 (11%)
3	NAG	L	2	3	14,14,15	0.60	0	17,19,21	1.37	3 (17%)
5	NAG	M	1	1,5	14,14,15	0.54	0	17,19,21	1.21	3 (17%)
5	NAG	M	2	5	14,14,15	0.91	1 (7%)	17,19,21	0.94	1 (5%)
5	BMA	M	3	5	11,11,12	0.68	0	15,15,17	1.53	3 (20%)
5	MAN	M	4	5	11,11,12	0.95	1 (9%)	15,15,17	1.36	3 (20%)
4	NAG	N	1	4,1	14,14,15	0.94	1 (7%)	17,19,21	1.51	2 (11%)
4	NAG	N	2	4	14,14,15	0.58	0	17,19,21	1.42	2 (11%)
4	BMA	N	3	4	11,11,12	1.18	1 (9%)	15,15,17	1.77	4 (26%)
3	NAG	O	1	3,1	14,14,15	0.70	1 (7%)	17,19,21	1.63	2 (11%)
3	NAG	O	2	3	14,14,15	0.75	0	17,19,21	1.51	4 (23%)
4	NAG	P	1	4,1	14,14,15	0.64	0	17,19,21	1.42	1 (5%)
4	NAG	P	2	4	14,14,15	0.73	0	17,19,21	1.27	2 (11%)
4	BMA	P	3	4	11,11,12	0.58	0	15,15,17	1.32	1 (6%)

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	–	0/2/19/22	0/1/1/1
3	NAG	F	1	3,1	–	0/6/23/26	0/1/1/1
3	NAG	F	2	3	–	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	–	0/6/23/26	0/1/1/1
2	NAG	G	2	2	–	2/6/23/26	0/1/1/1
2	BMA	G	3	2	–	2/2/19/22	0/1/1/1
2	MAN	G	4	2	–	0/2/19/22	0/1/1/1
2	NAG	H	1	1,2	–	0/6/23/26	0/1/1/1
2	NAG	H	2	2	–	2/6/23/26	0/1/1/1
2	BMA	H	3	2	–	2/2/19/22	0/1/1/1
2	MAN	H	4	2	–	0/2/19/22	0/1/1/1
3	NAG	I	1	3,1	–	0/6/23/26	0/1/1/1

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	2	NAG	O5-C1	-3.03	1.38	1.43
2	G	2	NAG	O5-C1	-2.81	1.39	1.43
4	N	1	NAG	O5-C1	-2.57	1.39	1.43
5	M	2	NAG	O5-C1	-2.57	1.39	1.43
5	M	4	MAN	C2-C3	2.48	1.56	1.52
4	N	3	BMA	O3-C3	2.47	1.49	1.43
3	F	2	NAG	O5-C1	-2.34	1.39	1.43
3	I	2	NAG	O5-C1	-2.26	1.39	1.43
4	J	2	NAG	C2-N2	-2.11	1.42	1.46
3	O	1	NAG	O5-C1	-2.10	1.40	1.43
2	E	1	NAG	C2-N2	-2.02	1.42	1.46

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	1	NAG	C1-O5-C5	4.79	118.60	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	2	NAG	O5-C1-C2	-4.63	104.12	111.29
4	J	3	BMA	C1-O5-C5	4.52	118.24	112.19
3	L	1	NAG	C1-C2-N2	-4.35	103.58	110.43
2	H	3	BMA	C1-C2-C3	4.29	115.90	109.64
4	N	1	NAG	O5-C1-C2	-4.26	104.70	111.29
3	I	1	NAG	C3-C4-C5	-4.04	102.91	110.23
3	F	2	NAG	C3-C4-C5	-4.04	102.92	110.23
5	M	3	BMA	C1-O5-C5	4.03	117.58	112.19
3	F	2	NAG	O5-C1-C2	-4.00	105.11	111.29
4	N	3	BMA	C1-C2-C3	3.87	115.28	109.64
3	F	1	NAG	C1-C2-N2	-3.76	104.51	110.43
3	O	1	NAG	C1-C2-N2	-3.72	104.58	110.43
4	K	2	NAG	C1-C2-N2	3.68	116.23	110.43
2	H	1	NAG	O5-C1-C2	-3.49	105.89	111.29
3	I	2	NAG	C3-C4-C5	-3.46	103.96	110.23
2	E	3	BMA	O4-C4-C3	-3.37	102.44	110.38
4	N	2	NAG	O5-C1-C2	-3.35	106.11	111.29
4	K	2	NAG	C2-N2-C7	-3.27	118.52	122.90
3	O	1	NAG	C1-O5-C5	3.23	116.52	112.19
4	K	2	NAG	C1-O5-C5	-3.22	107.87	112.19
2	E	3	BMA	C1-O5-C5	3.19	116.46	112.19
4	J	1	NAG	O5-C1-C2	-3.14	106.44	111.29
3	O	2	NAG	O5-C1-C2	-3.11	106.48	111.29
2	E	2	NAG	O7-C7-N2	3.07	127.41	121.98
3	F	1	NAG	C3-C4-C5	-3.03	104.74	110.23
2	G	3	BMA	C1-C2-C3	3.02	114.04	109.64
4	P	2	NAG	C4-C3-C2	-3.00	106.62	111.02
4	J	2	NAG	C1-C2-N2	-2.98	105.74	110.43
2	H	2	NAG	C3-C4-C5	-2.97	104.85	110.23
5	M	4	MAN	O3-C3-C2	2.95	116.08	110.05
3	I	2	NAG	O4-C4-C5	2.91	116.50	109.32
2	E	3	BMA	O5-C5-C6	2.91	113.33	107.66
4	K	3	BMA	C1-C2-C3	2.86	113.81	109.64
2	H	1	NAG	C2-N2-C7	-2.84	119.09	122.90
2	H	4	MAN	C2-C3-C4	2.84	115.85	110.86
3	O	2	NAG	O3-C3-C4	-2.83	103.70	110.38
2	E	3	BMA	C3-C4-C5	2.81	115.32	110.23
4	P	3	BMA	O5-C5-C6	2.79	113.10	107.66
4	J	2	NAG	O6-C6-C5	-2.75	101.97	111.33
2	E	2	NAG	C1-O5-C5	-2.74	108.51	112.19
2	H	4	MAN	C3-C4-C5	2.73	115.17	110.23
2	H	1	NAG	C3-C4-C5	-2.72	105.29	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1	NAG	C1-C2-N2	-2.72	106.14	110.43
2	E	1	NAG	C1-O5-C5	2.69	115.79	112.19
2	H	1	NAG	O5-C5-C6	2.68	112.87	107.66
2	E	2	NAG	O7-C7-C8	-2.65	117.33	122.05
4	K	2	NAG	O5-C1-C2	-2.65	107.19	111.29
3	I	2	NAG	C8-C7-N2	2.64	120.50	116.12
2	G	1	NAG	C2-N2-C7	2.64	126.43	122.90
3	I	1	NAG	O5-C1-C2	-2.62	107.24	111.29
4	K	2	NAG	O3-C3-C4	-2.59	104.26	110.38
4	K	1	NAG	O4-C4-C5	-2.56	103.03	109.32
4	J	3	BMA	O4-C4-C3	-2.51	104.45	110.38
3	L	2	NAG	C1-O5-C5	2.51	115.56	112.19
2	G	2	NAG	C4-C3-C2	-2.51	107.34	111.02
2	G	3	BMA	O2-C2-C3	2.49	115.31	110.15
4	N	3	BMA	C2-C3-C4	-2.49	106.49	110.86
2	G	1	NAG	O7-C7-C8	-2.48	117.64	122.05
2	G	4	MAN	C1-O5-C5	2.45	115.47	112.19
3	L	1	NAG	O7-C7-C8	-2.43	117.72	122.05
5	M	1	NAG	O5-C1-C2	-2.43	107.54	111.29
3	L	2	NAG	O5-C1-C2	-2.41	107.57	111.29
2	G	3	BMA	O4-C4-C3	-2.38	104.77	110.38
2	H	4	MAN	C1-C2-C3	2.36	113.09	109.64
2	E	1	NAG	O7-C7-C8	-2.36	117.85	122.05
2	E	4	MAN	C1-O5-C5	2.35	115.34	112.19
2	H	2	NAG	O5-C1-C2	-2.33	107.69	111.29
2	G	2	NAG	O6-C6-C5	-2.31	103.47	111.33
4	K	1	NAG	C2-N2-C7	-2.31	119.81	122.90
4	P	2	NAG	O7-C7-N2	2.30	126.04	121.98
2	E	3	BMA	O6-C6-C5	2.29	119.15	111.33
5	M	1	NAG	O5-C5-C4	-2.29	105.26	110.83
4	N	2	NAG	C1-C2-N2	2.28	114.02	110.43
5	M	4	MAN	O2-C2-C3	2.27	114.86	110.15
2	H	2	NAG	C1-O5-C5	2.27	115.23	112.19
2	G	1	NAG	O7-C7-N2	2.27	125.99	121.98
4	K	3	BMA	C3-C4-C5	2.27	114.35	110.23
4	J	2	NAG	O5-C5-C6	-2.27	103.25	107.66
3	L	2	NAG	O4-C4-C5	2.25	114.87	109.32
4	K	1	NAG	C1-C2-N2	2.25	113.98	110.43
2	H	4	MAN	O3-C3-C4	-2.25	105.08	110.38
5	M	1	NAG	C1-O5-C5	2.24	115.19	112.19
4	N	3	BMA	O3-C3-C2	2.24	114.62	110.05
5	M	2	NAG	O4-C4-C3	-2.24	105.10	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	4	MAN	C1-C2-C3	-2.23	106.39	109.64
4	K	2	NAG	O4-C4-C5	2.22	114.78	109.32
3	F	1	NAG	O5-C5-C4	2.21	116.21	110.83
4	J	3	BMA	O3-C3-C4	2.21	115.59	110.38
4	J	1	NAG	C8-C7-N2	2.20	119.77	116.12
2	E	4	MAN	O2-C2-C1	2.20	114.27	109.22
4	K	2	NAG	C8-C7-N2	2.19	119.76	116.12
2	E	2	NAG	C3-C4-C5	-2.18	106.28	110.23
3	O	2	NAG	O4-C4-C5	2.17	114.67	109.32
4	N	3	BMA	O6-C6-C5	2.16	118.70	111.33
3	I	2	NAG	C4-C3-C2	-2.16	107.85	111.02
2	H	3	BMA	C1-O5-C5	2.16	115.08	112.19
4	J	2	NAG	C4-C3-C2	-2.15	107.87	111.02
3	F	2	NAG	C1-O5-C5	2.14	115.05	112.19
2	E	2	NAG	C2-N2-C7	2.13	125.76	122.90
2	H	3	BMA	O6-C6-C5	2.12	118.56	111.33
5	M	3	BMA	O3-C3-C4	2.11	115.35	110.38
2	H	4	MAN	C1-O5-C5	2.10	115.00	112.19
3	O	2	NAG	C4-C3-C2	2.10	114.09	111.02
4	K	2	NAG	O6-C6-C5	-2.10	104.20	111.33
5	M	4	MAN	O3-C3-C4	2.08	115.27	110.38
3	I	2	NAG	O5-C1-C2	-2.07	108.09	111.29
2	E	2	NAG	O6-C6-C5	-2.07	104.29	111.33
5	M	3	BMA	O4-C4-C5	-2.07	104.23	109.32
3	F	2	NAG	O5-C5-C6	2.06	111.68	107.66
4	K	1	NAG	O3-C3-C4	2.06	115.23	110.38
4	K	3	BMA	O3-C3-C4	2.05	115.22	110.38
4	N	1	NAG	C3-C4-C5	-2.05	106.51	110.23
3	F	1	NAG	O3-C3-C4	2.03	115.17	110.38
2	E	4	MAN	O2-C2-C3	2.03	114.36	110.15
4	K	2	NAG	O4-C4-C3	-2.02	105.62	110.38
2	E	1	NAG	O6-C6-C5	-2.01	104.50	111.33

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	4	MAN	O5-C5-C6-O6
2	G	3	BMA	C4-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
5	M	4	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	G	3	BMA	O5-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	H	3	BMA	O5-C5-C6-O6
2	H	3	BMA	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
4	J	3	BMA	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
4	N	3	BMA	C4-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
4	K	3	BMA	C4-C5-C6-O6

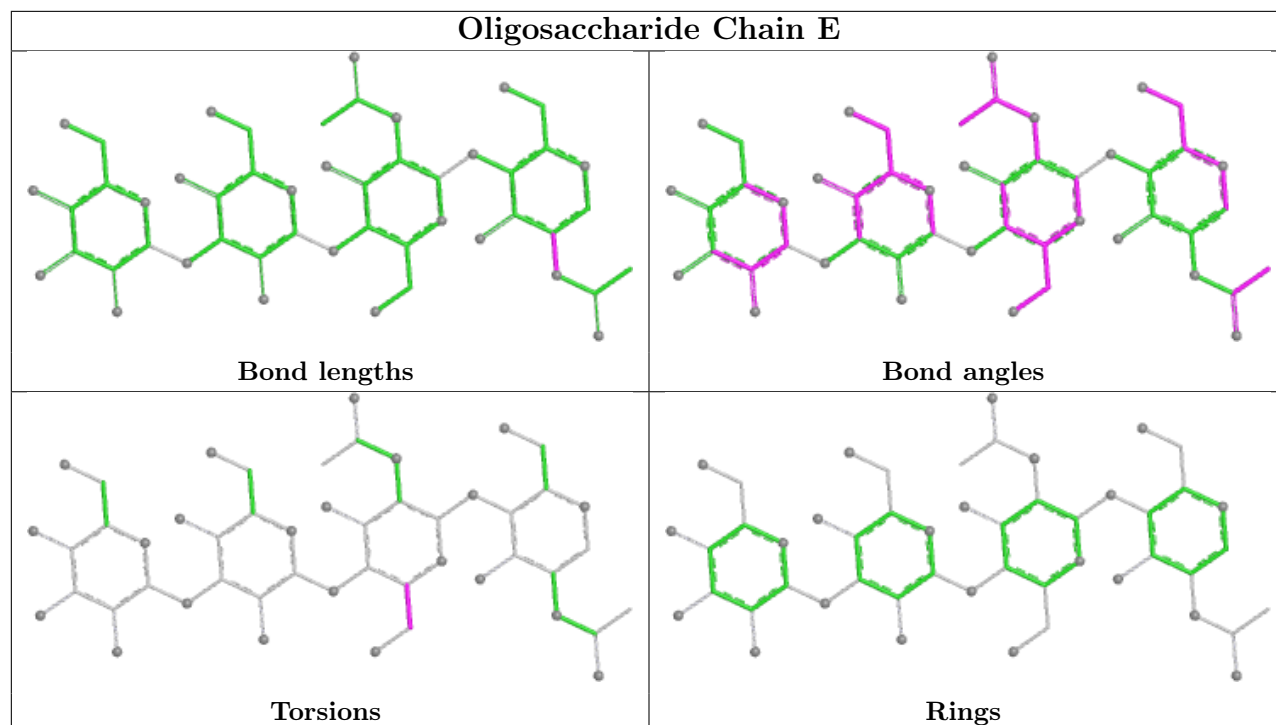
There are no ring outliers.

2 monomers are involved in 3 short contacts:

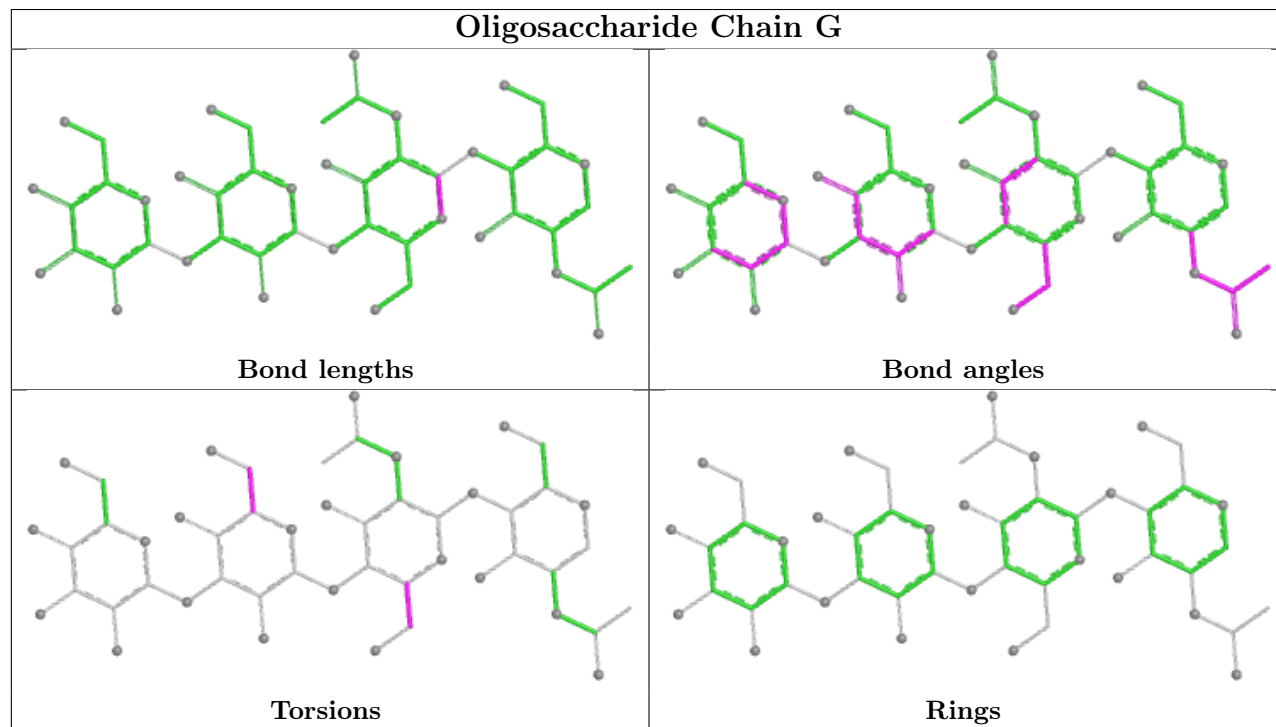
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1	NAG	1	0
4	N	1	NAG	2	0

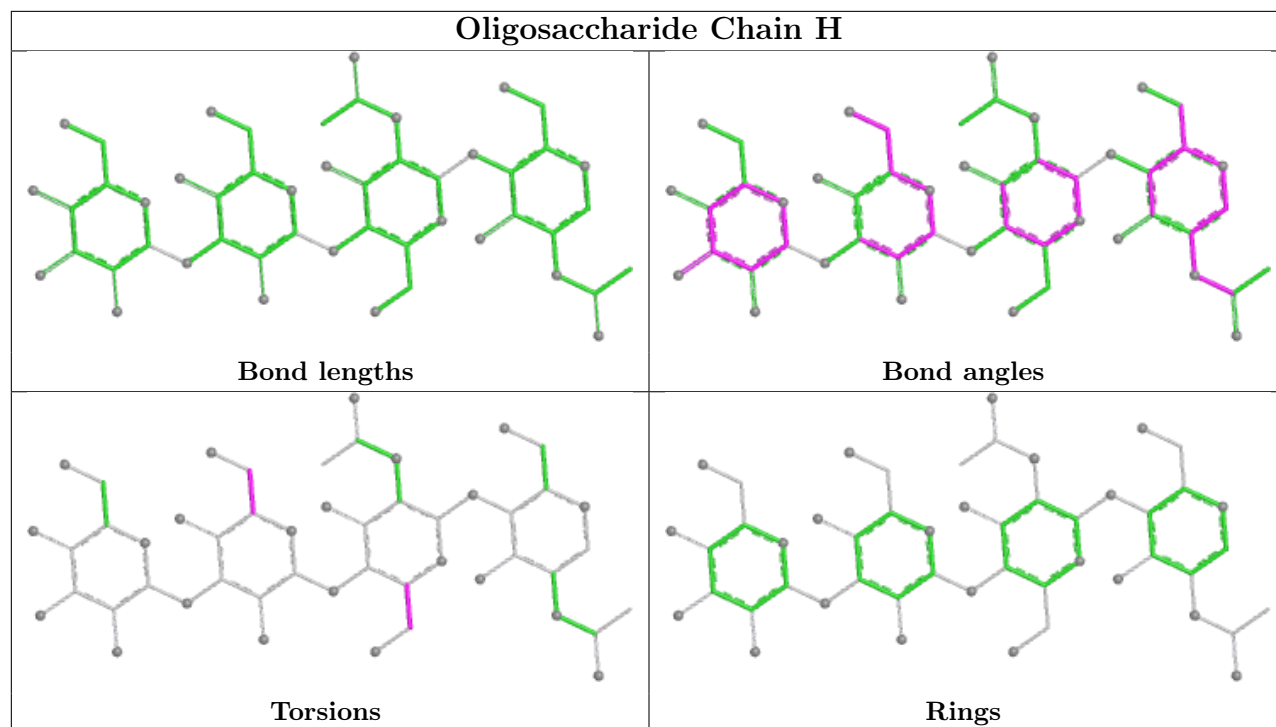
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

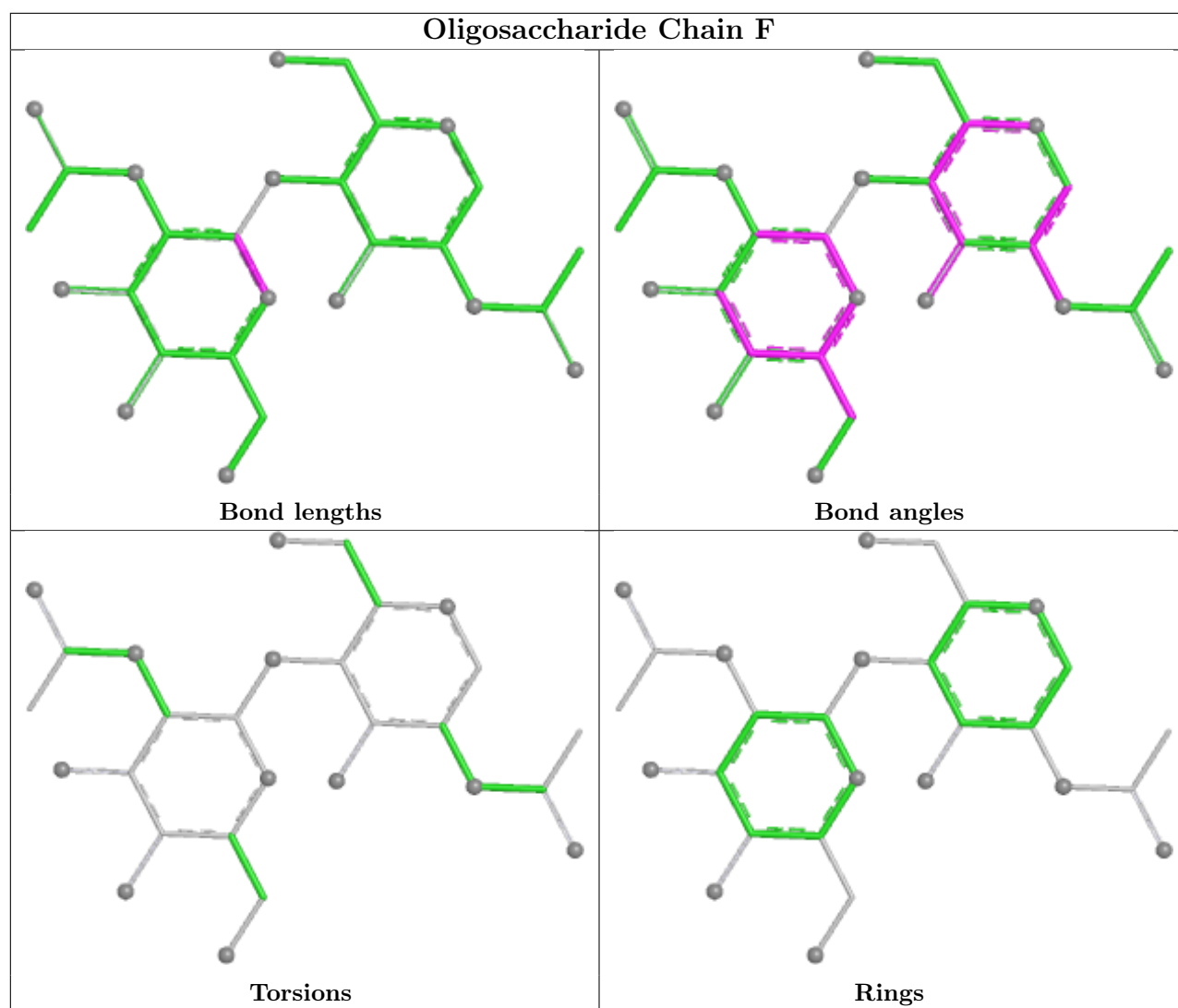
Oligosaccharide Chain E

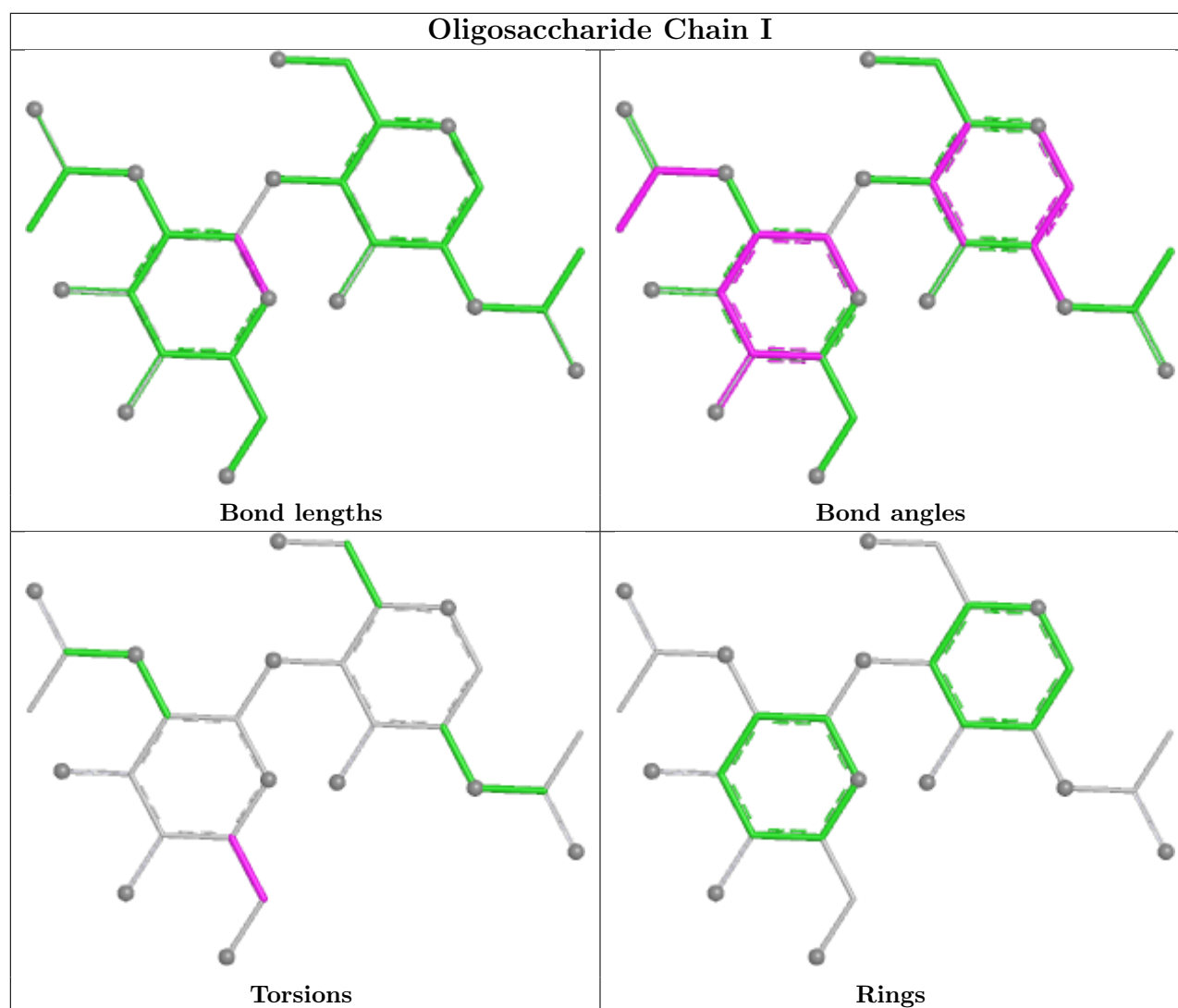


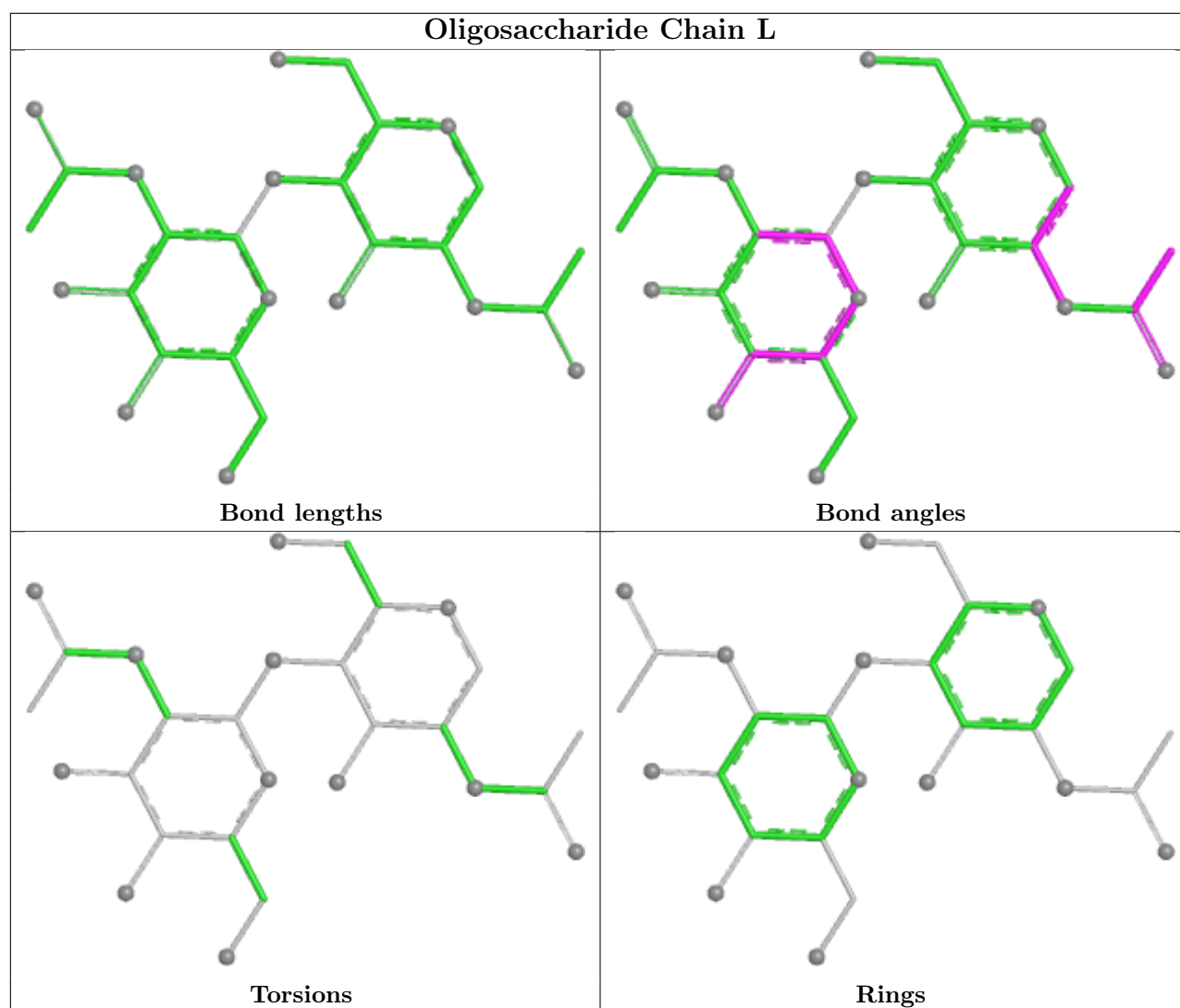
Oligosaccharide Chain G

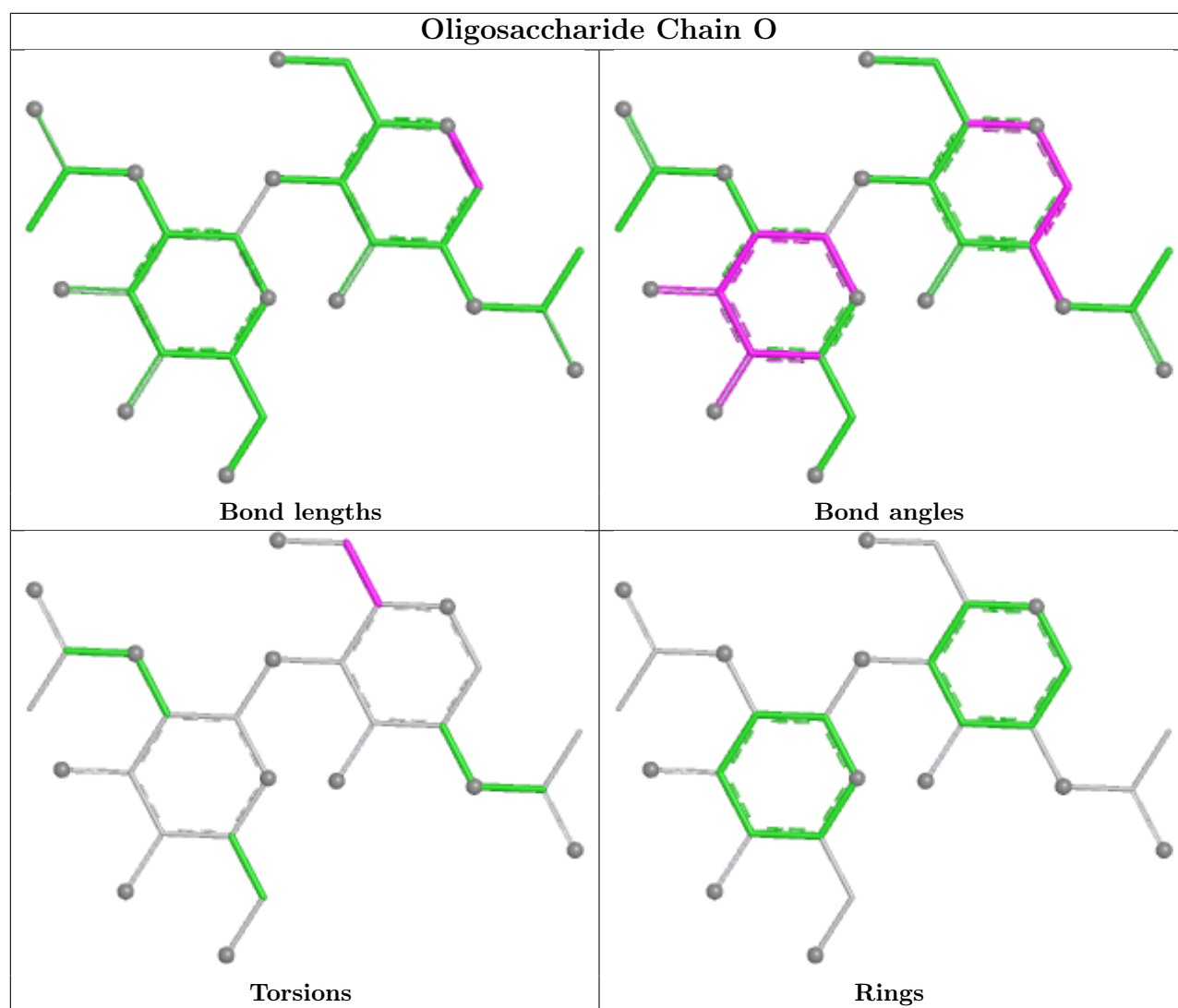


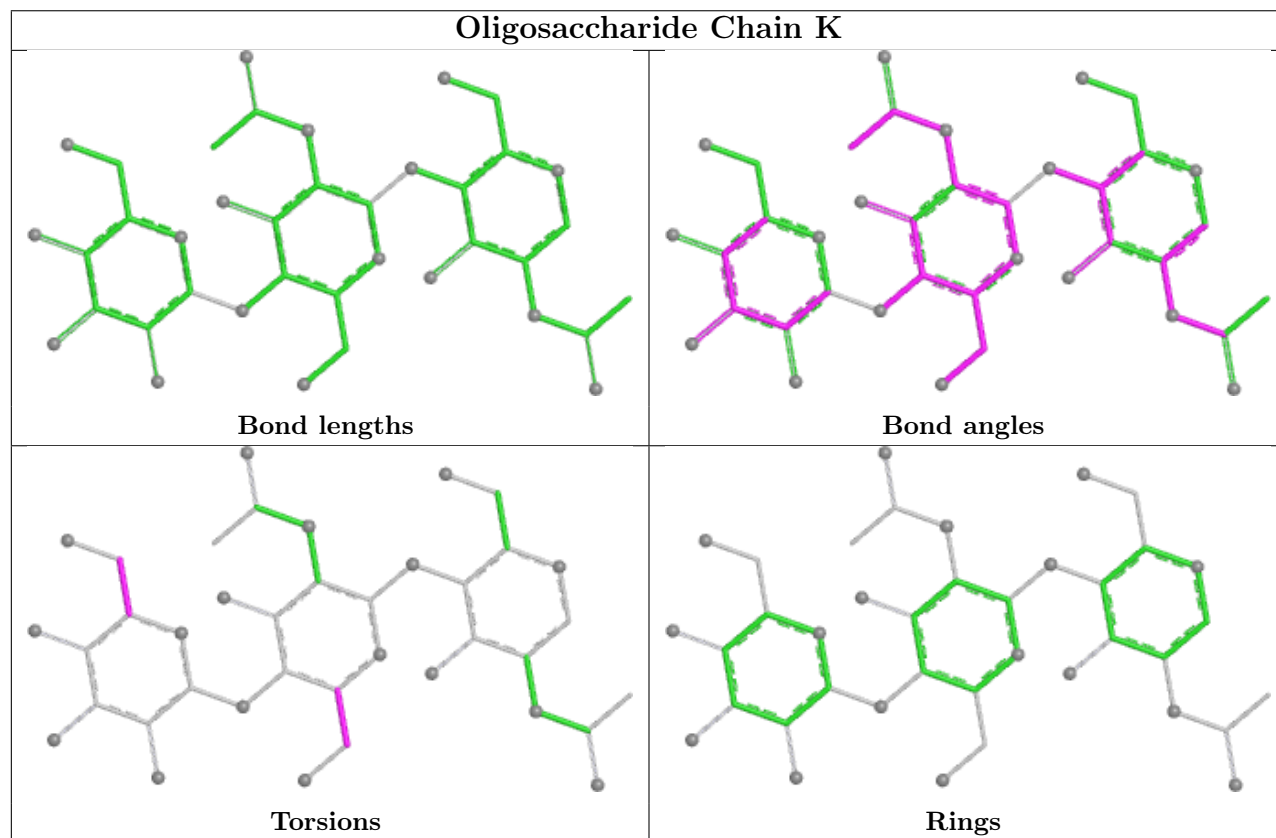
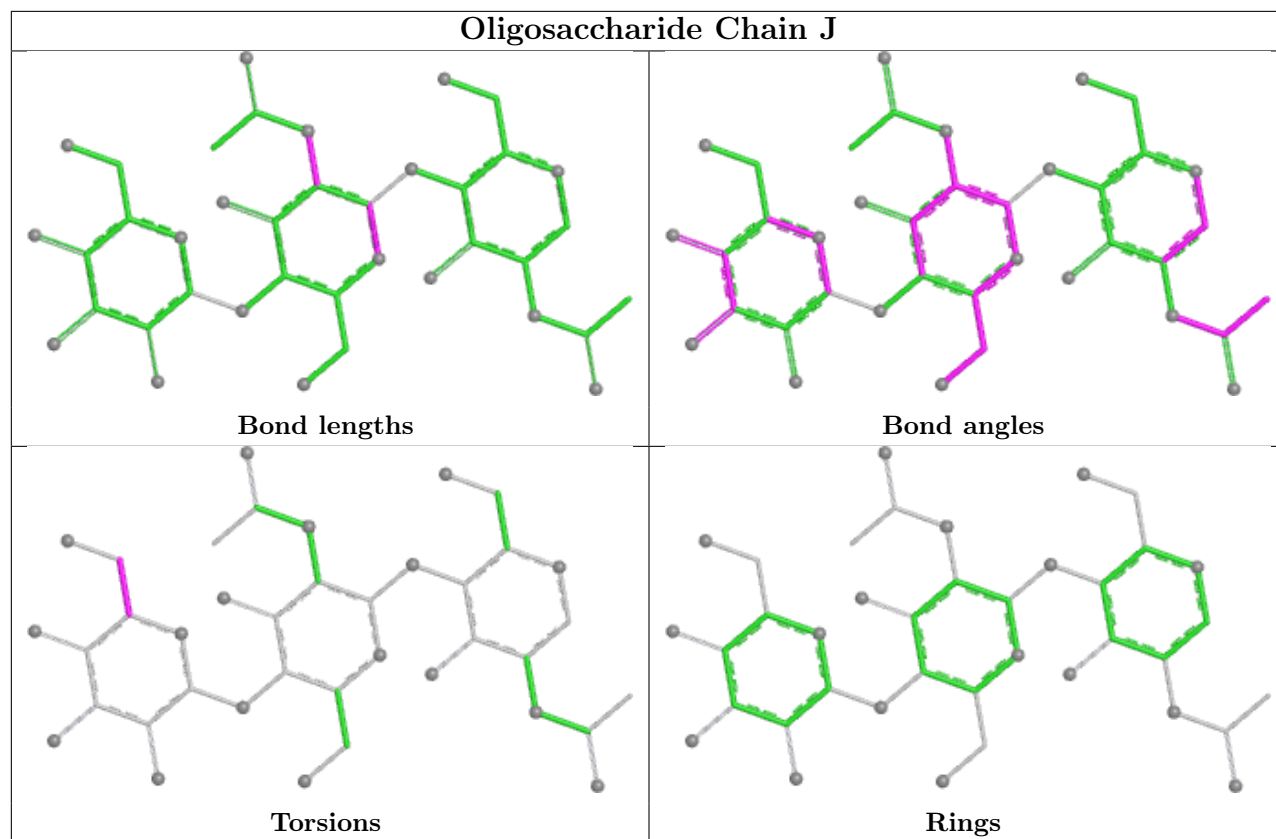


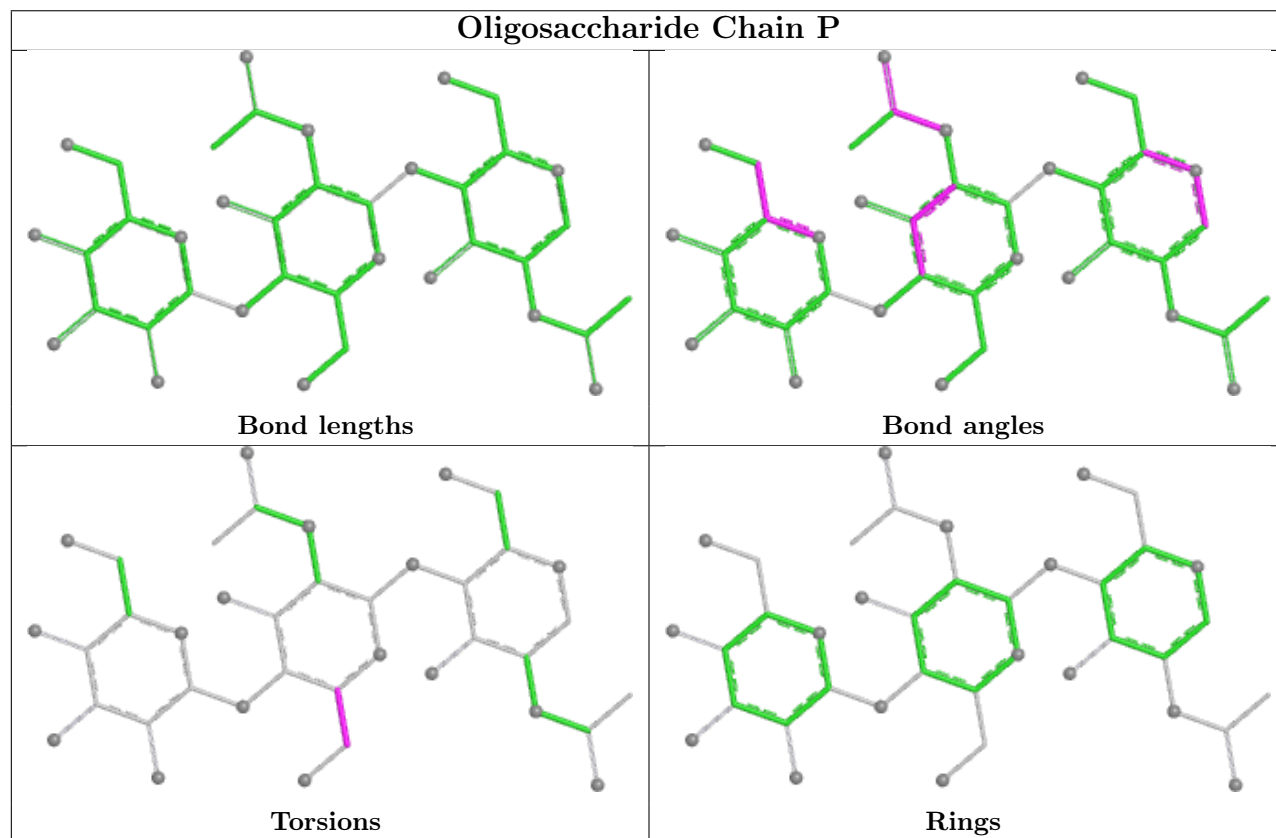
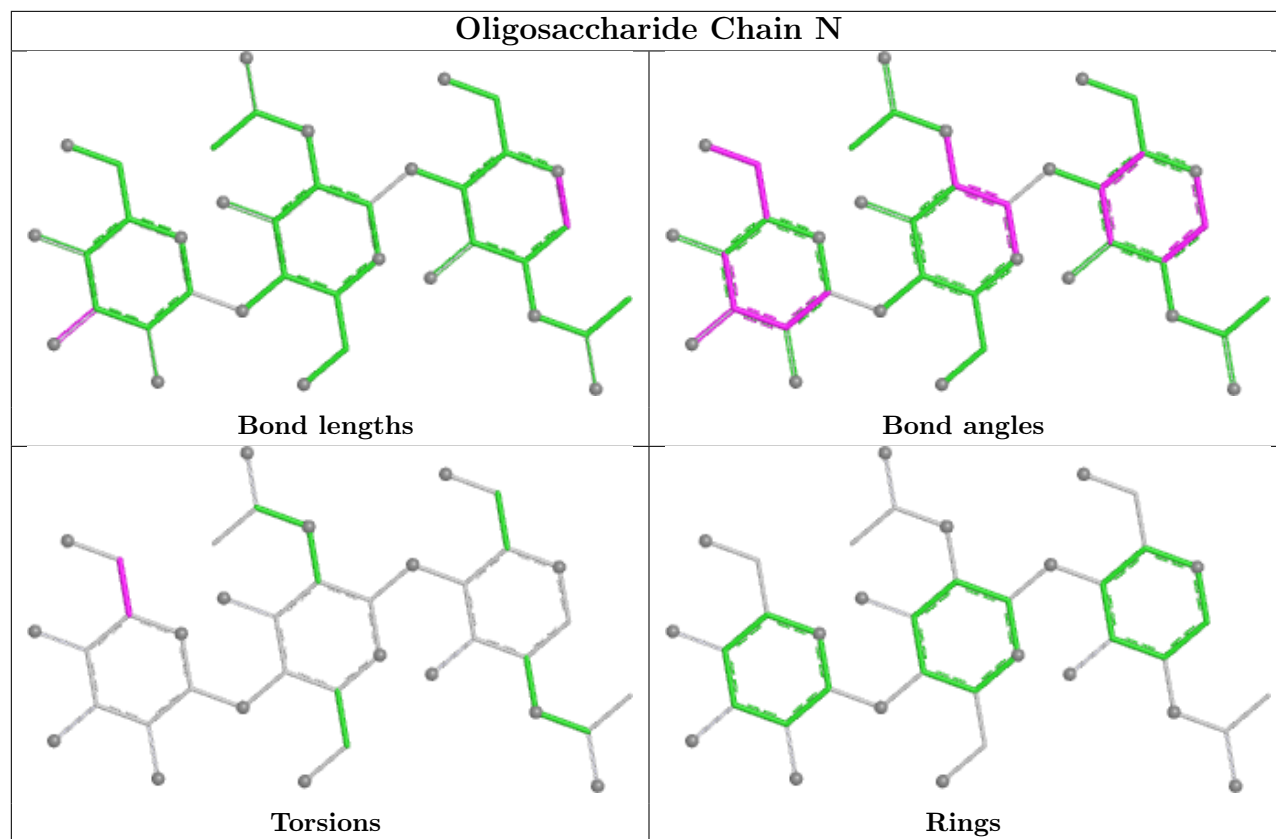


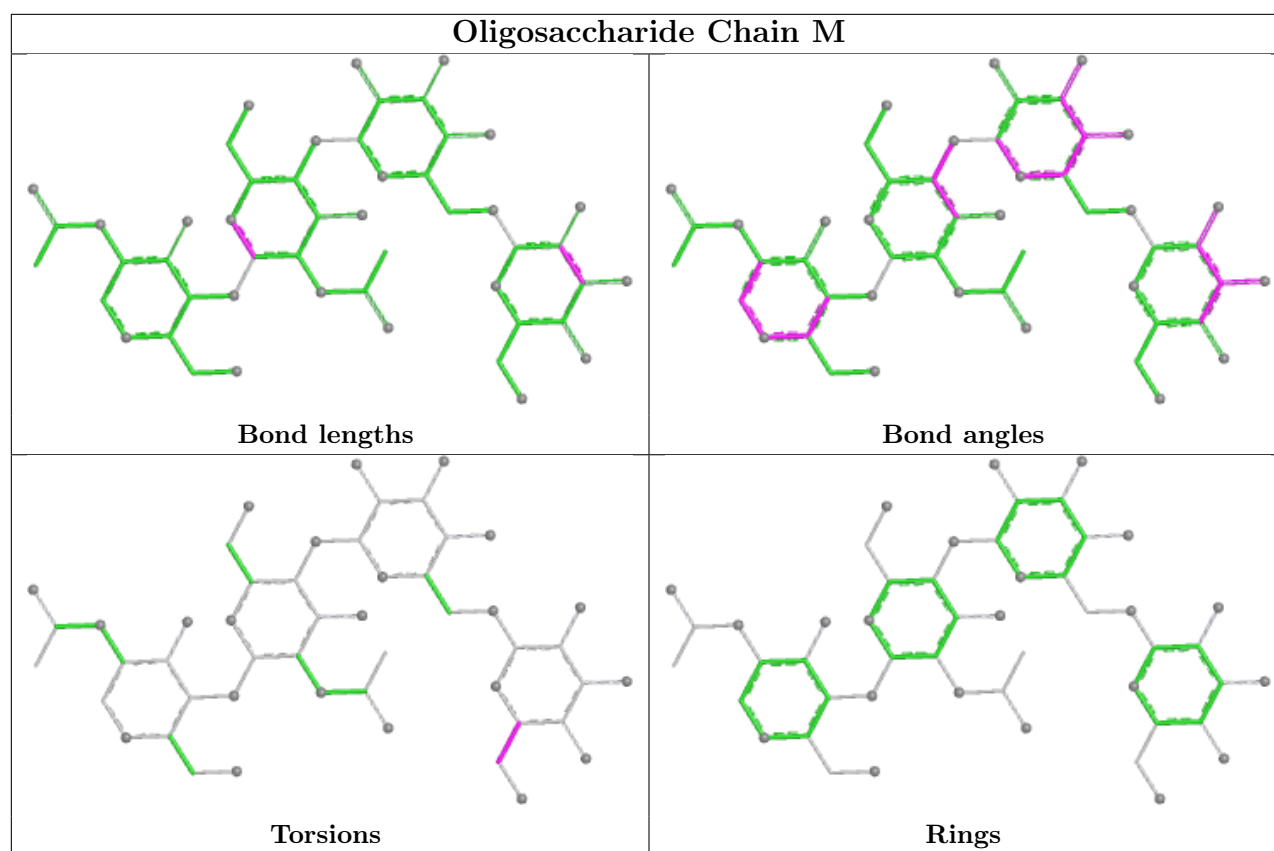












5.6 Ligand geometry [i](#)

18 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	NAG	B	1013	1	14,14,15	0.73	0	17,19,21	1.78	5 (29%)
7	NAG	B	1011	1	14,14,15	0.68	0	17,19,21	1.02	0
7	NAG	C	912	1	14,14,15	0.69	0	17,19,21	1.71	2 (11%)
6	MBL	C	901	-	18,18,18	0.87	1 (5%)	20,23,23	1.51	4 (20%)
7	NAG	B	1010	1	14,14,15	0.76	1 (7%)	17,19,21	1.78	4 (23%)
7	NAG	D	1006	1	14,14,15	0.53	0	17,19,21	1.60	3 (17%)
7	NAG	D	1011	1	14,14,15	0.65	0	17,19,21	1.91	5 (29%)
7	NAG	A	912	1	14,14,15	0.58	0	17,19,21	2.45	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MBL	A	901	-	18,18,18	1.00	0	20,23,23	1.37	4 (20%)
6	MBL	A	915	-	18,18,18	0.70	1 (5%)	20,23,23	1.74	4 (20%)
7	NAG	D	1010	1	14,14,15	0.74	0	17,19,21	1.20	3 (17%)
7	NAG	C	914	1	14,14,15	0.89	1 (7%)	17,19,21	0.94	1 (5%)
7	NAG	A	914	1	14,14,15	0.72	0	17,19,21	2.21	6 (35%)
7	NAG	A	913	1	14,14,15	0.76	0	17,19,21	1.47	2 (11%)
7	NAG	C	913	1	14,14,15	0.94	1 (7%)	17,19,21	1.30	3 (17%)
7	NAG	C	907	1	14,14,15	0.86	0	17,19,21	1.52	3 (17%)
6	MBL	C	915	-	18,18,18	1.04	2 (11%)	20,23,23	1.52	4 (20%)
7	NAG	B	1012	1	14,14,15	0.89	1 (7%)	17,19,21	1.42	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	1013	1	-	4/6/23/26	0/1/1/1
7	NAG	B	1011	1	-	0/6/23/26	0/1/1/1
7	NAG	C	912	1	-	0/6/23/26	0/1/1/1
6	MBL	C	901	-	-	0/9/9/9	0/2/2/2
7	NAG	B	1010	1	-	0/6/23/26	0/1/1/1
7	NAG	D	1006	1	-	4/6/23/26	0/1/1/1
7	NAG	D	1011	1	-	2/6/23/26	0/1/1/1
7	NAG	A	912	1	-	0/6/23/26	0/1/1/1
6	MBL	A	901	-	-	0/9/9/9	0/2/2/2
6	MBL	A	915	-	-	0/9/9/9	0/2/2/2
7	NAG	D	1010	1	-	0/6/23/26	0/1/1/1
7	NAG	C	914	1	-	2/6/23/26	0/1/1/1
7	NAG	A	914	1	-	2/6/23/26	0/1/1/1
7	NAG	A	913	1	-	2/6/23/26	0/1/1/1
7	NAG	C	913	1	-	3/6/23/26	0/1/1/1
7	NAG	C	907	1	-	4/6/23/26	0/1/1/1
6	MBL	C	915	-	-	0/9/9/9	0/2/2/2
7	NAG	B	1012	1	-	0/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1012	NAG	O5-C1	-2.46	1.39	1.43
6	C	915	MBL	C6-N1	-2.34	1.35	1.39
6	C	901	MBL	C6-N1	-2.31	1.35	1.39
6	A	915	MBL	C7-C6	2.30	1.41	1.37
7	C	914	NAG	C1-C2	2.30	1.55	1.52
6	C	915	MBL	C7-N	-2.12	1.31	1.36
7	C	913	NAG	O5-C1	-2.02	1.40	1.43
7	B	1010	NAG	O5-C1	-2.02	1.40	1.43

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	912	NAG	O5-C1-C2	5.86	120.35	111.29
7	C	912	NAG	C1-O5-C5	5.60	119.70	112.19
7	A	914	NAG	O5-C1-C2	-5.49	102.80	111.29
6	A	915	MBL	C6-N1-C8	-5.32	102.57	105.46
7	A	912	NAG	C1-O5-C5	5.14	119.07	112.19
7	B	1010	NAG	C1-O5-C5	4.84	118.68	112.19
7	A	914	NAG	C8-C7-N2	4.54	123.65	116.12
7	A	912	NAG	C4-C3-C2	-4.23	104.81	111.02
7	D	1011	NAG	C8-C7-N2	4.09	122.90	116.12
7	A	912	NAG	C1-C2-N2	-3.78	104.47	110.43
7	D	1006	NAG	C8-C7-N2	3.77	122.37	116.12
7	B	1013	NAG	C2-N2-C7	3.59	127.71	122.90
6	C	901	MBL	C6-N1-C8	-3.57	103.52	105.46
7	C	907	NAG	C1-C2-N2	-3.36	105.15	110.43
7	D	1011	NAG	C4-C3-C2	-3.20	106.33	111.02
7	A	913	NAG	O5-C1-C2	-3.14	106.43	111.29
6	C	915	MBL	C3-C6-N1	3.14	124.76	119.95
7	B	1013	NAG	O5-C5-C6	2.99	113.47	107.66
7	A	913	NAG	O4-C4-C3	-2.97	103.36	110.38
7	D	1011	NAG	O5-C1-C2	-2.93	106.76	111.29
7	A	914	NAG	C4-C3-C2	-2.90	106.76	111.02
6	A	915	MBL	C3-C6-C7	-2.87	125.27	129.65
7	B	1013	NAG	C1-O5-C5	2.83	115.98	112.19
7	D	1011	NAG	C2-N2-C7	2.81	126.66	122.90
7	C	913	NAG	C1-O5-C5	2.79	115.92	112.19
7	A	914	NAG	O7-C7-N2	-2.77	117.08	121.98
6	A	915	MBL	N2-C8-N1	-2.74	118.66	124.94
6	A	901	MBL	C7-C6-N1	-2.71	108.16	110.75
6	C	915	MBL	C6-N1-C8	-2.69	104.00	105.46
7	D	1006	NAG	O7-C7-C8	-2.65	117.34	122.05
6	A	901	MBL	C3-C6-N1	2.59	123.92	119.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	915	MBL	C3-C6-C7	-2.54	125.78	129.65
7	C	912	NAG	O5-C1-C2	-2.53	107.38	111.29
6	C	901	MBL	C3-C6-N1	2.52	123.81	119.95
6	A	901	MBL	C6-C7-N	2.51	108.09	106.60
7	D	1011	NAG	O7-C7-N2	-2.48	117.59	121.98
7	B	1012	NAG	C1-O5-C5	2.45	115.47	112.19
7	B	1010	NAG	O7-C7-N2	-2.44	117.68	121.98
6	A	915	MBL	C3-C6-N1	2.39	123.61	119.95
7	D	1006	NAG	O5-C1-C2	-2.37	107.62	111.29
6	C	915	MBL	N2-C8-N1	-2.30	119.66	124.94
6	A	901	MBL	C6-N1-C8	-2.27	104.22	105.46
6	C	901	MBL	C-C1-C3	-2.19	118.21	120.36
7	C	913	NAG	O7-C7-C8	-2.17	118.19	122.05
6	C	901	MBL	C3-C6-C7	-2.15	126.36	129.65
7	D	1010	NAG	O5-C1-C2	-2.15	107.96	111.29
7	C	907	NAG	O4-C4-C3	-2.15	105.32	110.38
7	A	914	NAG	C1-O5-C5	2.12	115.03	112.19
7	B	1010	NAG	C2-N2-C7	-2.11	120.07	122.90
7	D	1010	NAG	O5-C5-C4	-2.11	105.70	110.83
7	C	914	NAG	C1-O5-C5	2.09	114.99	112.19
7	B	1010	NAG	O3-C3-C4	-2.09	105.46	110.38
7	B	1013	NAG	C1-C2-N2	2.08	113.72	110.43
7	D	1010	NAG	O3-C3-C4	2.08	115.28	110.38
7	C	913	NAG	O5-C5-C6	-2.08	103.62	107.66
7	B	1012	NAG	O6-C6-C5	-2.06	104.33	111.33
7	C	907	NAG	C8-C7-N2	2.01	119.46	116.12
7	B	1013	NAG	C4-C3-C2	2.01	113.97	111.02
7	A	914	NAG	C1-C2-N2	2.01	113.60	110.43

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1013	NAG	O5-C5-C6-O6
7	C	907	NAG	O5-C5-C6-O6
7	B	1013	NAG	C4-C5-C6-O6
7	C	907	NAG	C4-C5-C6-O6
7	D	1006	NAG	O5-C5-C6-O6
7	A	914	NAG	C8-C7-N2-C2
7	A	914	NAG	O7-C7-N2-C2
7	B	1013	NAG	C8-C7-N2-C2
7	B	1013	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	C	907	NAG	C8-C7-N2-C2
7	C	907	NAG	O7-C7-N2-C2
7	D	1006	NAG	C8-C7-N2-C2
7	D	1006	NAG	O7-C7-N2-C2
7	D	1011	NAG	C8-C7-N2-C2
7	D	1011	NAG	O7-C7-N2-C2
7	D	1006	NAG	C4-C5-C6-O6
7	C	913	NAG	O5-C5-C6-O6
7	C	914	NAG	C4-C5-C6-O6
7	C	913	NAG	C4-C5-C6-O6
7	C	914	NAG	O5-C5-C6-O6
7	C	913	NAG	C3-C2-N2-C7
7	A	913	NAG	C1-C2-N2-C7
7	A	913	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1011	NAG	1	0
7	D	1010	NAG	1	0
7	A	914	NAG	1	0
7	A	913	NAG	2	0

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	748/811 (92%)	-0.24	8 (1%) 78 74	34, 50, 80, 110	0
1	B	749/811 (92%)	-0.12	13 (1%) 69 65	33, 55, 99, 145	0
1	C	748/811 (92%)	0.17	30 (4%) 42 38	34, 64, 105, 168	0
1	D	746/811 (91%)	0.12	27 (3%) 46 42	36, 63, 121, 169	0
All	All	2991/3244 (92%)	-0.02	78 (2%) 57 53	33, 57, 104, 169	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	817	LEU	6.8
1	D	100	VAL	6.8
1	A	100	VAL	6.3
1	D	732	LEU	5.8
1	B	100	VAL	5.7
1	C	100	VAL	5.6
1	B	457	THR	5.0
1	B	761	THR	4.4
1	B	817	LEU	4.2
1	C	815	VAL	3.9
1	C	761	THR	3.9
1	C	122	LEU	3.7
1	D	814	ILE	3.6
1	B	42	ASN	3.6
1	D	457	THR	3.5
1	D	755	ALA	3.5
1	C	84	GLN	3.5
1	C	64	TYR	3.5
1	C	756	LEU	3.4
1	D	678	PHE	3.4
1	C	678	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	732	LEU	3.2
1	D	64	TYR	3.2
1	C	85	GLY	3.1
1	C	242	PHE	3.0
1	D	813	SER	2.9
1	D	735	VAL	2.9
1	C	123	ASN	2.9
1	A	432	PRO	2.8
1	C	307	PHE	2.8
1	C	762	THR	2.8
1	C	86	LEU	2.8
1	D	751	ILE	2.7
1	B	758	THR	2.7
1	B	760	THR	2.7
1	C	112	ASN	2.6
1	B	759	LYS	2.6
1	D	774	PHE	2.6
1	D	815	VAL	2.6
1	C	113	GLY	2.5
1	D	113	GLY	2.5
1	C	121	PHE	2.5
1	C	778	CYS	2.5
1	D	758	THR	2.5
1	D	767	LEU	2.5
1	C	65	VAL	2.5
1	C	798	LEU	2.4
1	B	495	PHE	2.4
1	D	731	PHE	2.4
1	A	817	LEU	2.4
1	C	59	GLN	2.4
1	C	44	SER	2.3
1	C	777	THR	2.3
1	D	816	SER	2.3
1	C	495	PHE	2.3
1	D	783	PHE	2.3
1	B	64	TYR	2.3
1	D	776	CYS	2.3
1	D	761	THR	2.2
1	B	780	ILE	2.2
1	D	756	LEU	2.2
1	A	458	ASP	2.2
1	C	816	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	470	PHE	2.2
1	D	659	PHE	2.2
1	A	41	GLN	2.2
1	C	758	THR	2.2
1	A	736	SER	2.2
1	A	678	PHE	2.1
1	D	681	TRP	2.1
1	D	86	LEU	2.1
1	D	750	THR	2.1
1	D	34	TYR	2.1
1	C	806	PRO	2.1
1	A	752	ASN	2.1
1	C	96	HIS	2.1
1	D	40	LYS	2.0
1	B	762	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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	MAN	G	4	11/12	0.71	0.13	78,91,95,96	0
7	NAG	A	914	14/15	0.74	0.12	61,68,72,78	0
5	MAN	M	4	11/12	0.76	0.14	76,93,101,102	0
7	NAG	D	1011	14/15	0.79	0.10	79,87,95,106	0
3	NAG	O	2	14/15	0.80	0.12	65,75,87,88	0
7	NAG	D	1006	14/15	0.82	0.12	73,83,92,96	0
2	MAN	H	4	11/12	0.83	0.12	57,75,79,81	0
3	NAG	L	2	14/15	0.84	0.14	70,82,92,93	0
7	NAG	B	1013	14/15	0.85	0.10	66,73,78,78	0
2	MAN	E	4	11/12	0.85	0.11	55,63,68,69	0
7	NAG	A	912	14/15	0.85	0.12	76,83,94,96	0
7	NAG	B	1011	14/15	0.86	0.10	74,88,92,95	0
7	NAG	C	907	14/15	0.86	0.11	66,77,87,95	0
3	NAG	F	2	14/15	0.88	0.12	48,66,70,70	0
7	NAG	C	914	14/15	0.90	0.09	59,64,67,70	0
3	NAG	I	2	14/15	0.90	0.10	54,64,70,71	0
7	NAG	B	1012	14/15	0.90	0.09	56,65,75,78	0
7	NAG	B	1010	14/15	0.90	0.08	50,57,64,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	C	912	14/15	0.91	0.10	56,66,74,82	0
4	NAG	K	2	14/15	0.92	0.08	53,57,64,66	0
2	NAG	G	2	14/15	0.93	0.12	33,45,49,58	0
4	NAG	P	1	14/15	0.93	0.08	42,49,54,54	0
7	NAG	C	913	14/15	0.93	0.10	61,76,82,85	0
2	NAG	H	1	14/15	0.94	0.09	35,42,48,50	0
4	NAG	N	2	14/15	0.95	0.06	42,50,58,58	0
2	NAG	H	2	14/15	0.95	0.06	45,49,58,63	0
4	NAG	J	2	14/15	0.95	0.07	36,44,51,52	0
2	NAG	G	1	14/15	0.95	0.07	38,41,46,49	0
7	NAG	D	1010	14/15	0.95	0.08	51,54,64,65	0
5	NAG	M	2	14/15	0.95	0.06	38,42,51,55	0
5	NAG	M	1	14/15	0.96	0.06	35,38,41,46	0
3	NAG	L	1	14/15	0.96	0.06	40,46,50,54	0
4	NAG	P	2	14/15	0.96	0.07	47,55,63,63	0
4	NAG	K	1	14/15	0.96	0.06	44,47,56,57	0
7	NAG	A	913	14/15	0.96	0.06	56,60,64,64	0
3	NAG	I	1	14/15	0.97	0.06	34,41,45,49	0
2	NAG	E	2	14/15	0.97	0.05	35,40,48,52	0
4	NAG	J	1	14/15	0.97	0.05	29,38,41,43	0
4	NAG	N	1	14/15	0.97	0.06	39,43,45,47	0
2	NAG	E	1	14/15	0.97	0.05	29,35,37,38	0
3	NAG	O	1	14/15	0.97	0.06	45,50,54,61	0
3	NAG	F	1	14/15	0.98	0.05	36,40,47,48	0

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($\text{\AA}^2$)	Q<0.9
2	MAN	G	4	11/12	0.71	0.13	78,91,95,96	0
4	BMA	P	3	11/12	0.71	0.12	69,73,80,81	0
4	BMA	K	3	11/12	0.76	0.13	64,70,79,83	0
5	MAN	M	4	11/12	0.76	0.14	76,93,101,102	0
4	BMA	J	3	11/12	0.78	0.12	53,66,72,72	0
4	BMA	N	3	11/12	0.78	0.12	50,63,71,72	0
3	NAG	O	2	14/15	0.80	0.12	65,75,87,88	0
2	BMA	E	3	11/12	0.82	0.09	50,59,62,62	0
2	BMA	G	3	11/12	0.83	0.10	55,68,79,85	0

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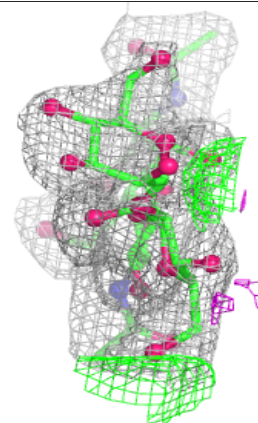
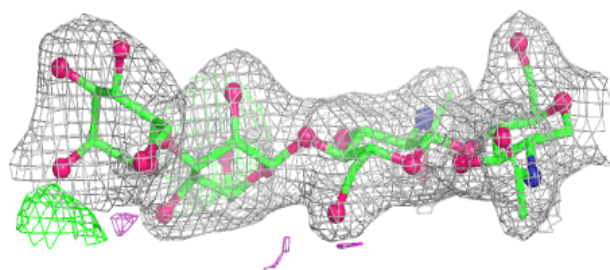
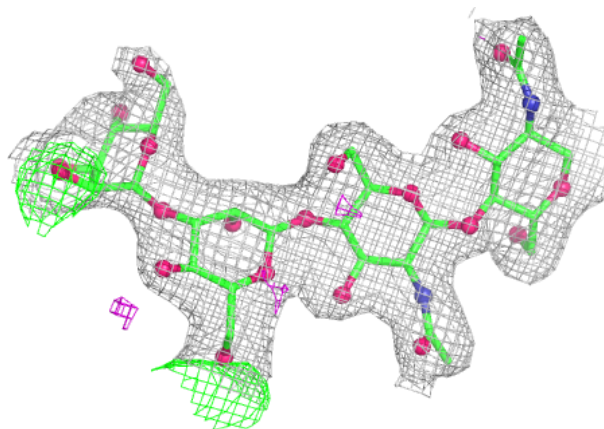
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	H	4	11/12	0.83	0.12	57,75,79,81	0
3	NAG	L	2	14/15	0.84	0.14	70,82,92,93	0
2	MAN	E	4	11/12	0.85	0.11	55,63,68,69	0
2	BMA	H	3	11/12	0.85	0.10	55,66,72,82	0
5	BMA	M	3	11/12	0.87	0.09	57,65,69,84	0
3	NAG	F	2	14/15	0.88	0.12	48,66,70,70	0
3	NAG	I	2	14/15	0.90	0.10	54,64,70,71	0
4	NAG	K	2	14/15	0.92	0.08	53,57,64,66	0
4	NAG	P	1	14/15	0.93	0.08	42,49,54,54	0
2	NAG	G	2	14/15	0.93	0.12	33,45,49,58	0
2	NAG	H	1	14/15	0.94	0.09	35,42,48,50	0
2	NAG	H	2	14/15	0.95	0.06	45,49,58,63	0
4	NAG	J	2	14/15	0.95	0.07	36,44,51,52	0
5	NAG	M	2	14/15	0.95	0.06	38,42,51,55	0
4	NAG	N	2	14/15	0.95	0.06	42,50,58,58	0
2	NAG	G	1	14/15	0.95	0.07	38,41,46,49	0
5	NAG	M	1	14/15	0.96	0.06	35,38,41,46	0
3	NAG	L	1	14/15	0.96	0.06	40,46,50,54	0
4	NAG	P	2	14/15	0.96	0.07	47,55,63,63	0
4	NAG	K	1	14/15	0.96	0.06	44,47,56,57	0
2	NAG	E	2	14/15	0.97	0.05	35,40,48,52	0
4	NAG	J	1	14/15	0.97	0.05	29,38,41,43	0
4	NAG	N	1	14/15	0.97	0.06	39,43,45,47	0
2	NAG	E	1	14/15	0.97	0.05	29,35,37,38	0
3	NAG	I	1	14/15	0.97	0.06	34,41,45,49	0
3	NAG	O	1	14/15	0.97	0.06	45,50,54,61	0
3	NAG	F	1	14/15	0.98	0.05	36,40,47,48	0

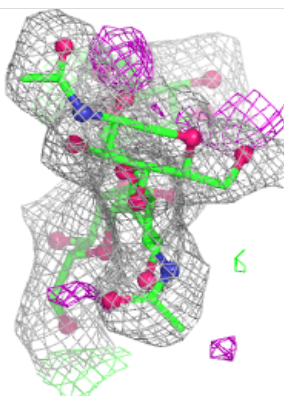
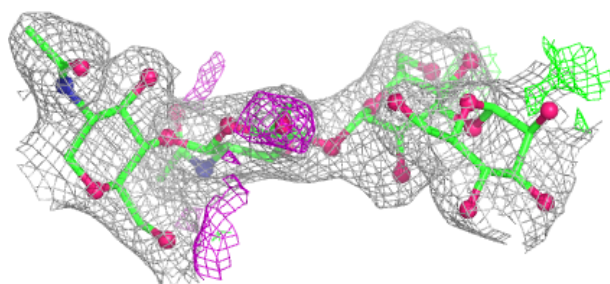
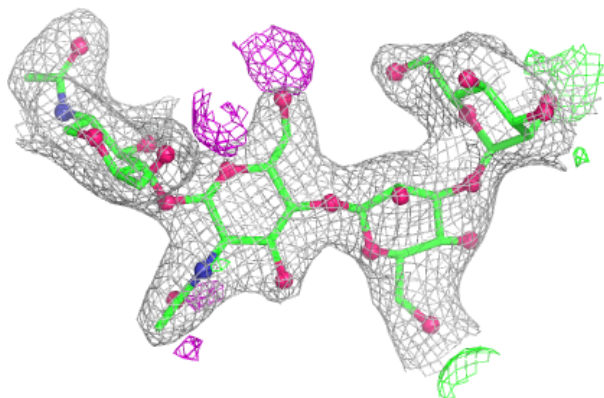
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

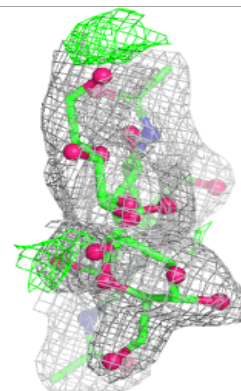
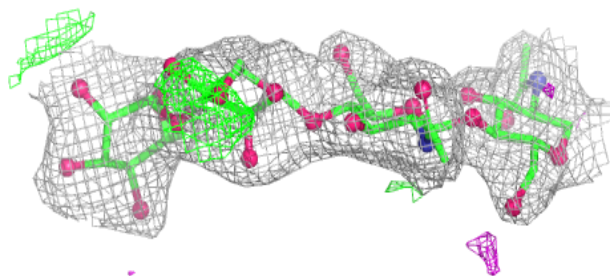
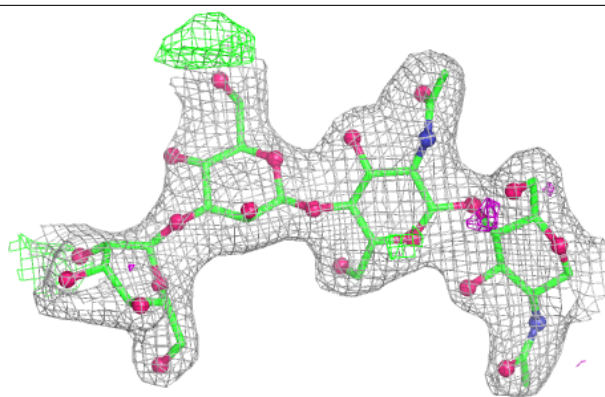
**Electron density around Chain G:**

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

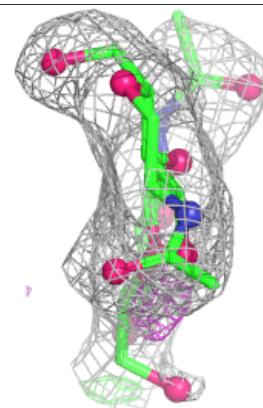
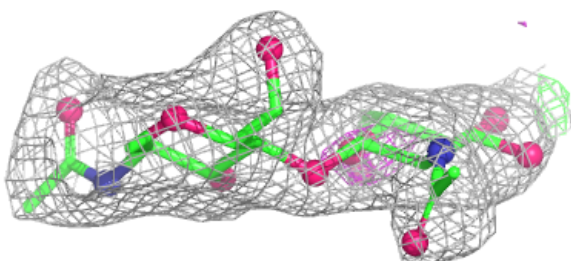
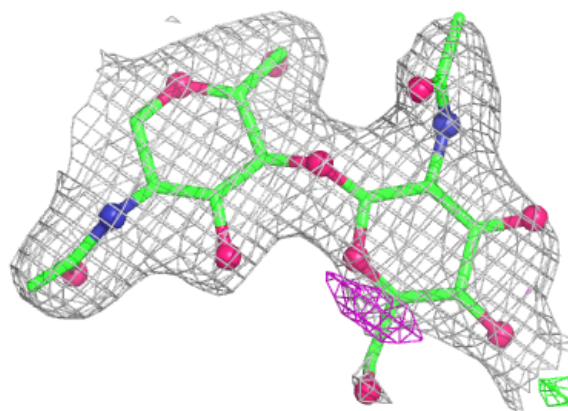


Electron density around Chain H:

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

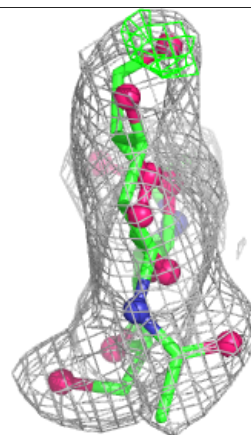
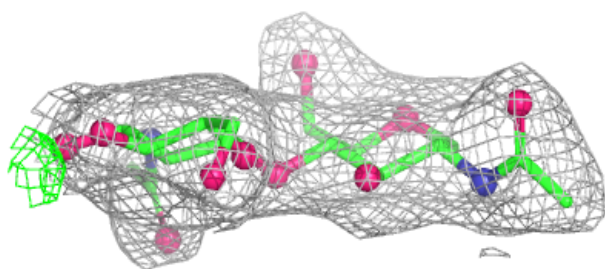
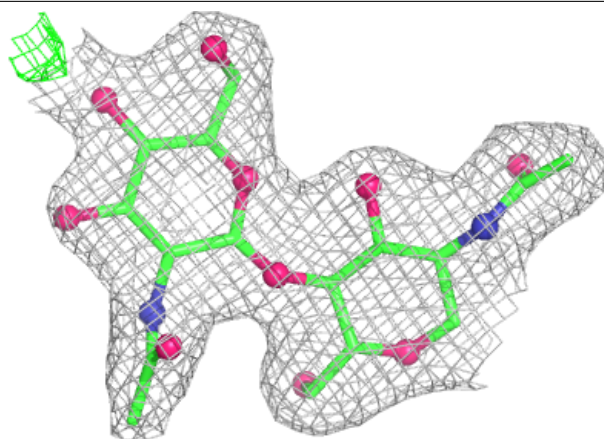
**Electron density around Chain F:**

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



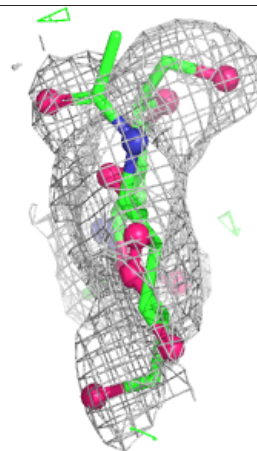
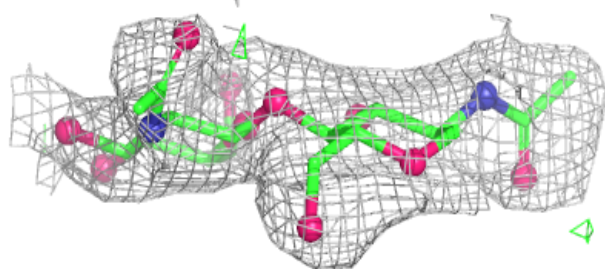
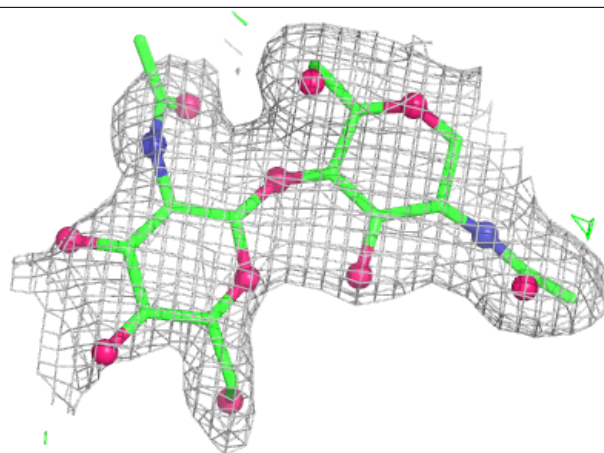
Electron density around Chain I:

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



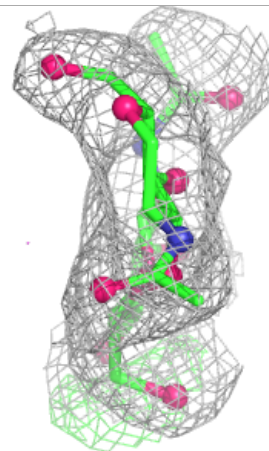
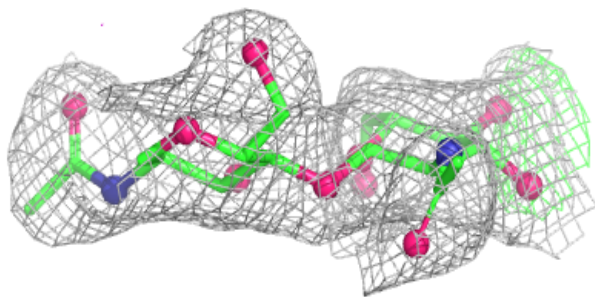
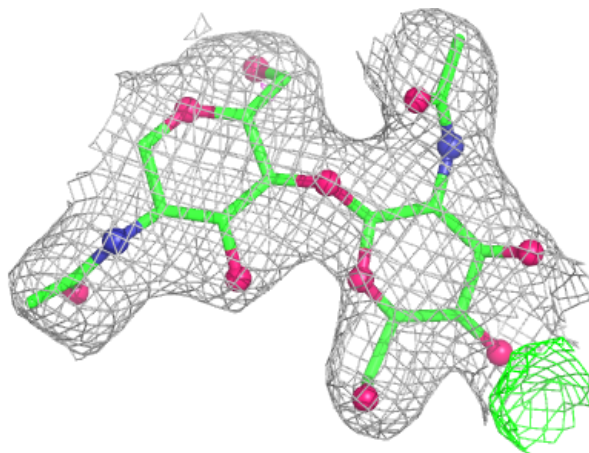
Electron density around Chain L:

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



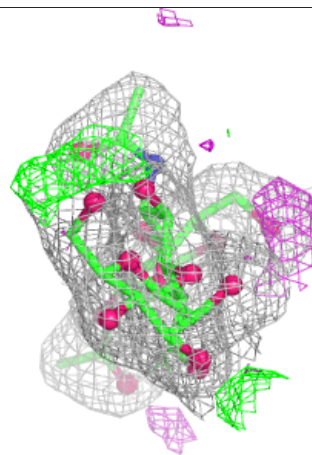
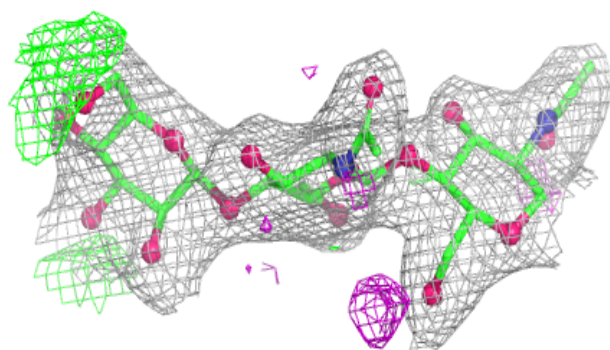
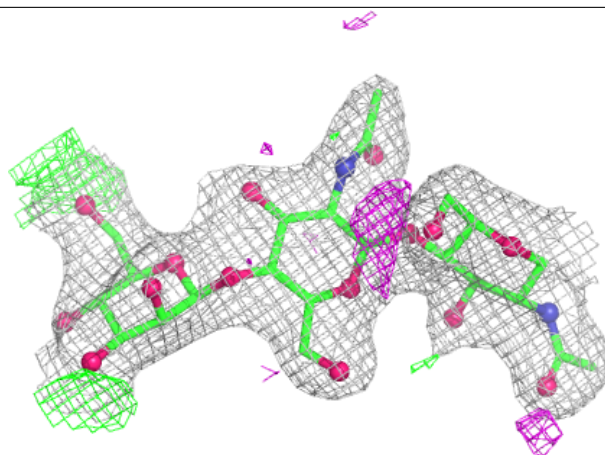
Electron density around Chain O:

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



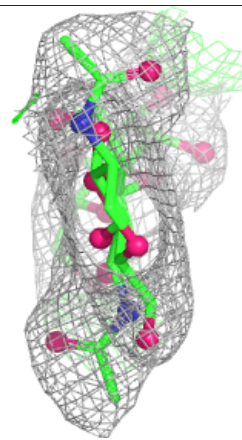
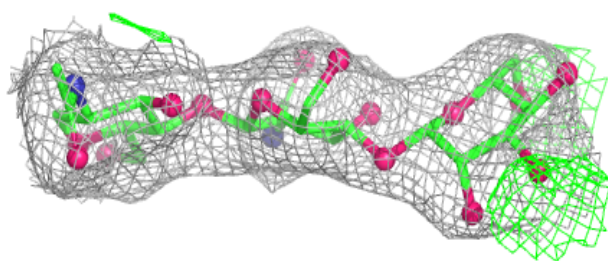
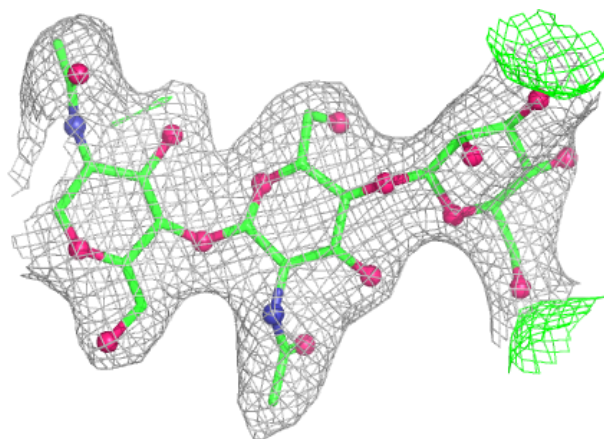
Electron density around Chain J:

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and green (positive)

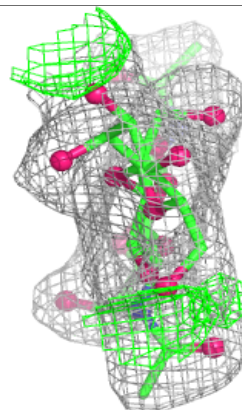
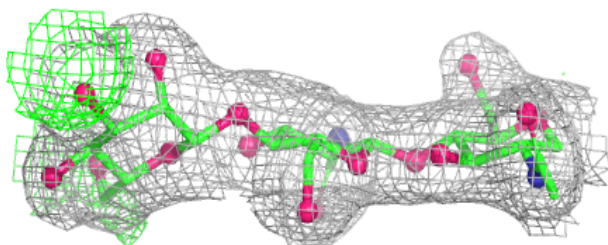
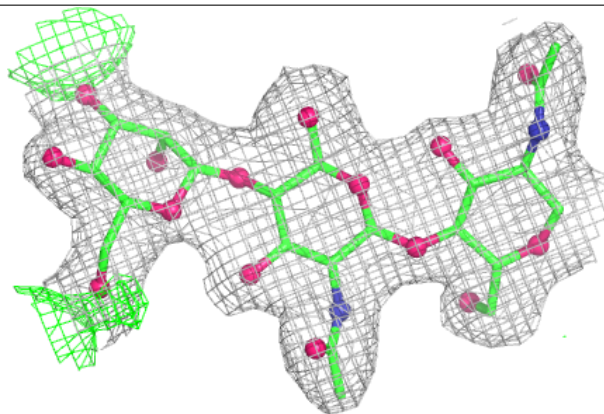


Electron density around Chain K:

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

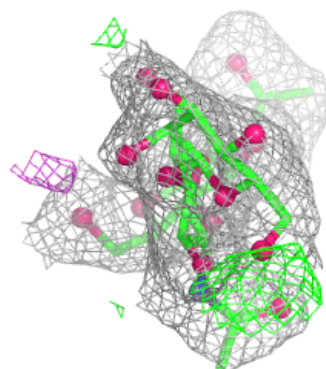
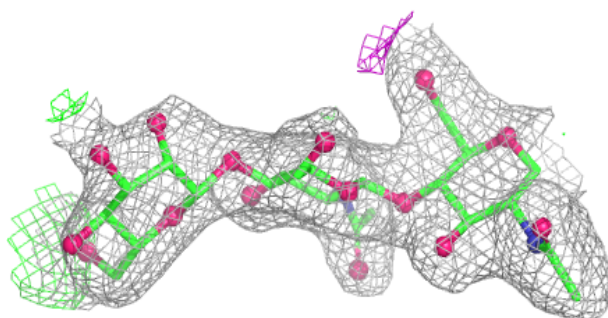
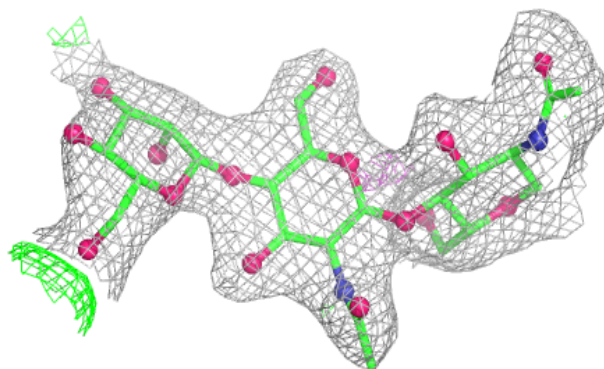
**Electron density around Chain N:**

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

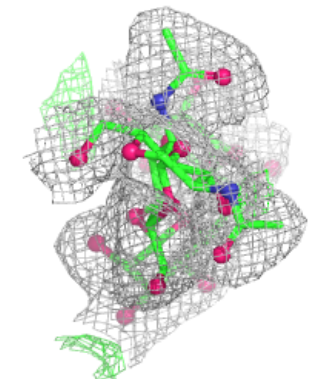
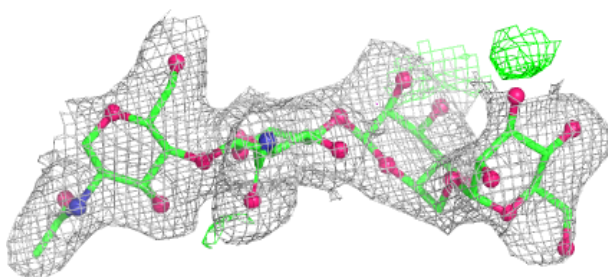
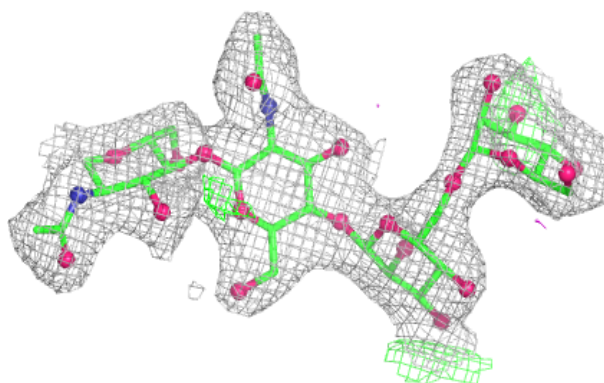


Electron density around Chain P:

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

**Electron density around Chain M:**

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



6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
7	NAG	A	914	14/15	0.74	0.12	61,68,72,78	0
7	NAG	D	1011	14/15	0.79	0.10	79,87,95,106	0
7	NAG	D	1006	14/15	0.82	0.12	73,83,92,96	0
7	NAG	A	912	14/15	0.85	0.12	76,83,94,96	0
7	NAG	B	1013	14/15	0.85	0.10	66,73,78,78	0
7	NAG	B	1011	14/15	0.86	0.10	74,88,92,95	0
7	NAG	C	907	14/15	0.86	0.11	66,77,87,95	0
7	NAG	C	914	14/15	0.90	0.09	59,64,67,70	0
7	NAG	B	1010	14/15	0.90	0.08	50,57,64,72	0
7	NAG	B	1012	14/15	0.90	0.09	56,65,75,78	0
7	NAG	C	912	14/15	0.91	0.10	56,66,74,82	0
7	NAG	C	913	14/15	0.93	0.10	61,76,82,85	0
7	NAG	D	1010	14/15	0.95	0.08	51,54,64,65	0
6	MBL	C	901	17/17	0.95	0.10	50,57,61,63	0
6	MBL	A	901	17/17	0.96	0.08	43,48,54,54	0
6	MBL	A	915	17/17	0.96	0.08	39,44,49,49	0
7	NAG	A	913	14/15	0.96	0.06	56,60,64,64	0
6	MBL	C	915	17/17	0.97	0.07	44,47,55,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.