



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:12 PM UTC

PDB ID : 5L59 / pdb_00005l59
Title : Plexin A1 full extracellular region, domains 1 to 10, to 6 angstrom, spacegroup P2(1)
Authors : Janssen, B.J.C.; Kong, Y.; Malinauskas, T.; Vangoor, V.R.; Coles, C.H.; Kaufmann, R.; Ni, T.; Gilbert, R.J.C.; Padilla-Parra, S.; Pasterkamp, R.J.; Jones, E.Y.
Deposited on : 2016-05-28
Resolution : 6.00 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:

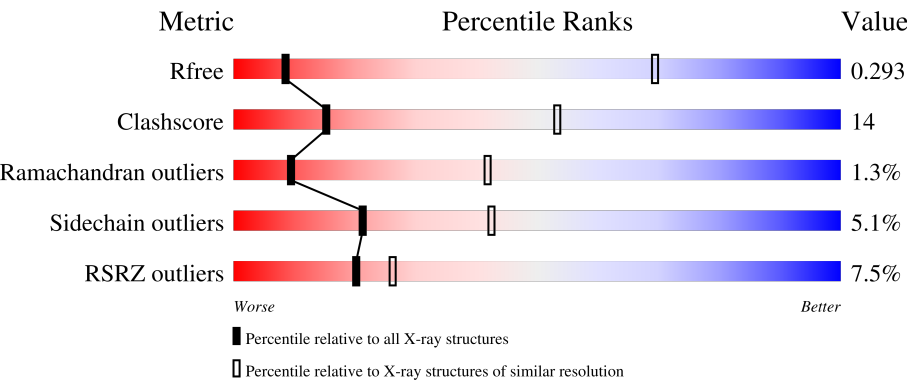
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 6.00 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.



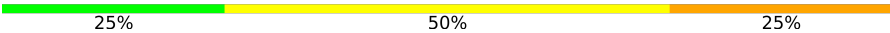
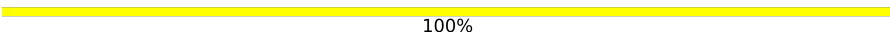
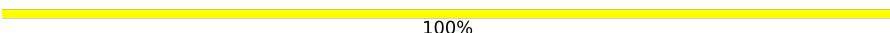
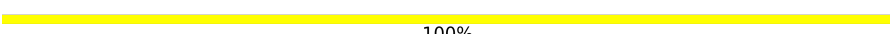
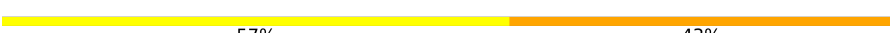
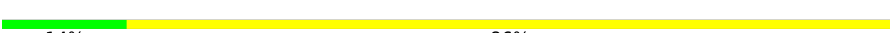
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1143 (8.00-4.00)
Clashscore	190562	1210 (8.00-4.00)
Ramachandran outliers	187476	1034 (8.00-4.00)
Sidechain outliers	187428	1000 (8.00-4.00)
RSRZ outliers	180081	1136 (8.00-4.00)

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	1212	8% 69% 25% • •
1	B	1212	7% 68% 25% • •
2	C	4	25% 50% 25%
2	E	4	100%

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Mol	Chain	Length	Quality of chain
2	K	4	 25% 50% 25%
2	M	4	 100%
2	O	4	 100%
3	D	5	 20% 80%
3	I	5	 100%
4	F	7	 57% 43%
4	J	7	 14% 86%
4	N	7	 14% 43% 43%
4	R	7	 14% 86%
5	G	3	 100%
5	H	3	 100%
5	P	3	 100%
6	L	6	 17% 83%
6	Q	6	 17% 83%

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
4	NAG	J	1	X	-	-	-
4	NAG	R	1	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19191 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.

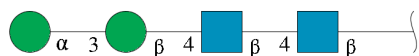
- Molecule 1 is a protein called Plexin-A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1171	Total	C	N	O	S	0	0	0
			9085	5719	1593	1715	58			
1	B	1171	Total	C	N	O	S	0	0	0
			9085	5719	1593	1715	58			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLU	-	expression tag	UNP P70206
A	35	THR	-	expression tag	UNP P70206
A	36	GLY	-	expression tag	UNP P70206
A	1237	ARG	-	expression tag	UNP P70206
A	1238	THR	-	expression tag	UNP P70206
A	1239	LYS	-	expression tag	UNP P70206
A	1240	HIS	-	expression tag	UNP P70206
A	1241	HIS	-	expression tag	UNP P70206
A	1242	HIS	-	expression tag	UNP P70206
A	1243	HIS	-	expression tag	UNP P70206
A	1244	HIS	-	expression tag	UNP P70206
A	1245	HIS	-	expression tag	UNP P70206
B	34	GLU	-	expression tag	UNP P70206
B	35	THR	-	expression tag	UNP P70206
B	36	GLY	-	expression tag	UNP P70206
B	1237	ARG	-	expression tag	UNP P70206
B	1238	THR	-	expression tag	UNP P70206
B	1239	LYS	-	expression tag	UNP P70206
B	1240	HIS	-	expression tag	UNP P70206
B	1241	HIS	-	expression tag	UNP P70206
B	1242	HIS	-	expression tag	UNP P70206
B	1243	HIS	-	expression tag	UNP P70206
B	1244	HIS	-	expression tag	UNP P70206
B	1245	HIS	-	expression tag	UNP P70206

- 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.



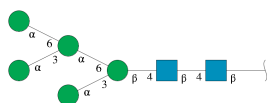
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	E	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	K	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	M	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	O	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 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.



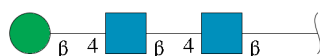
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	I	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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.



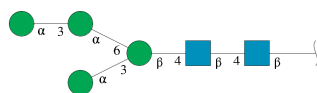
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	J	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	N	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	R	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 5 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.



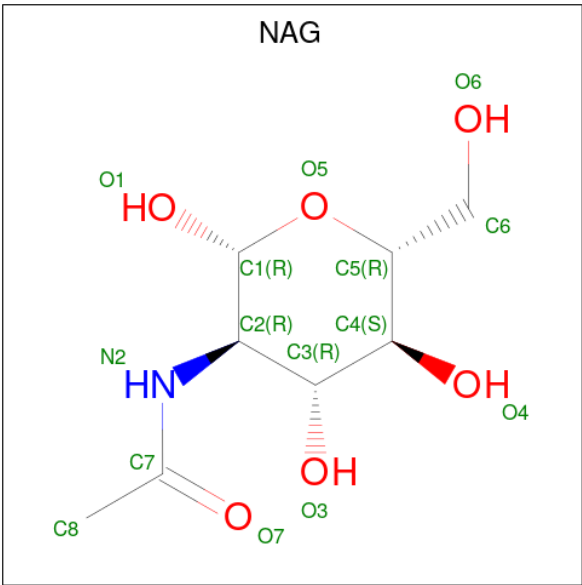
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	P	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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
6	L	6	Total	C	N	O	0	0	0
			72	40	2	30			
6	Q	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

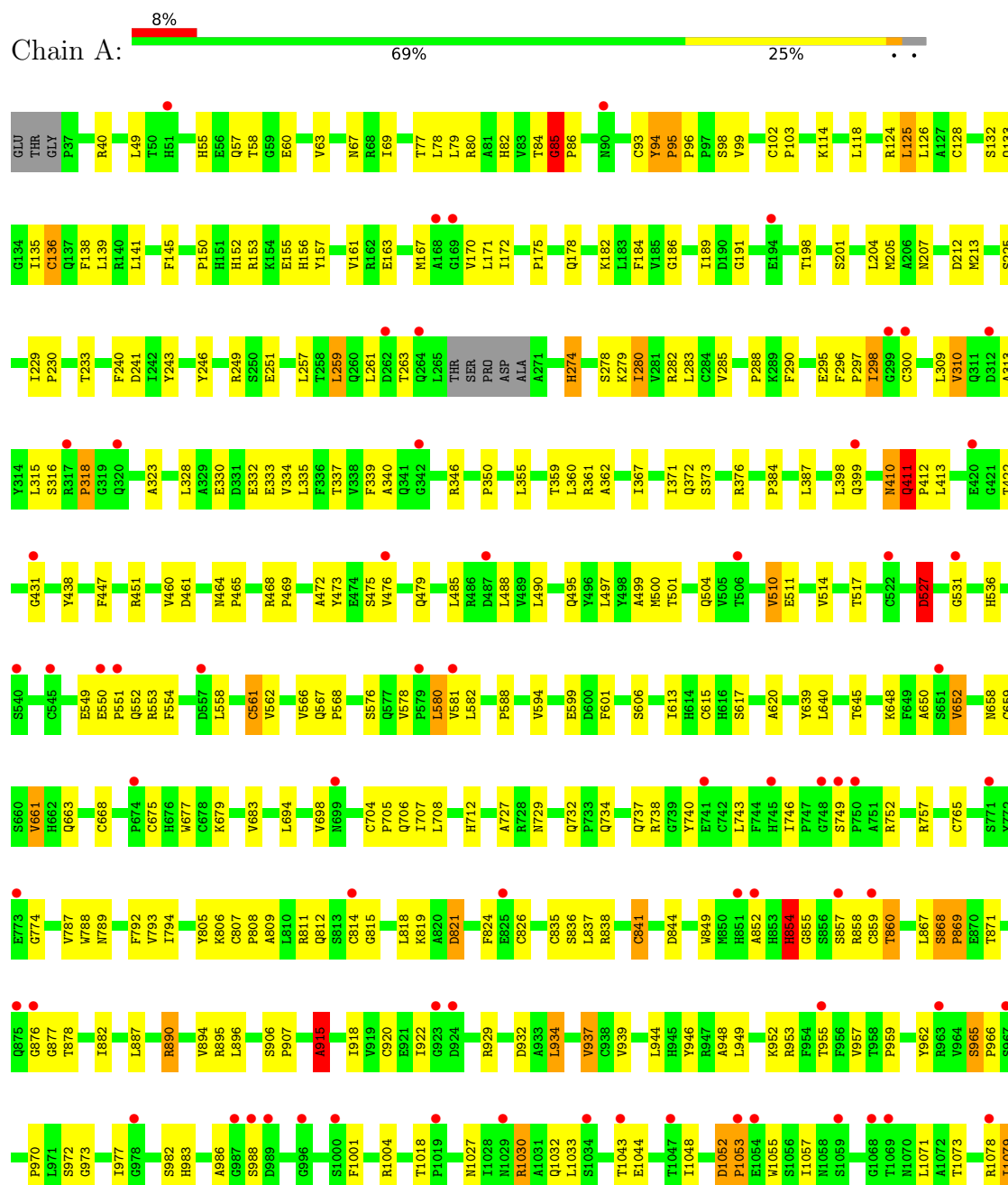


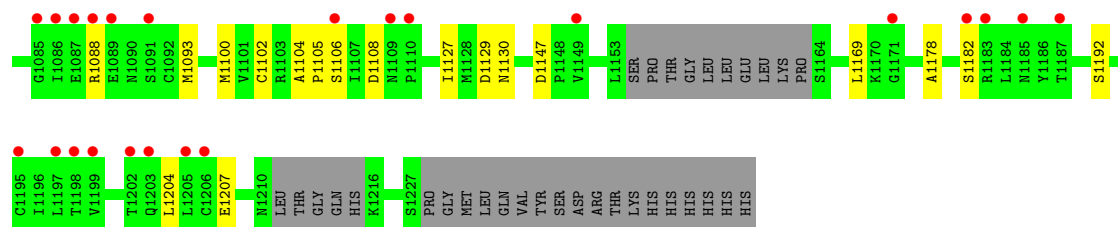
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots

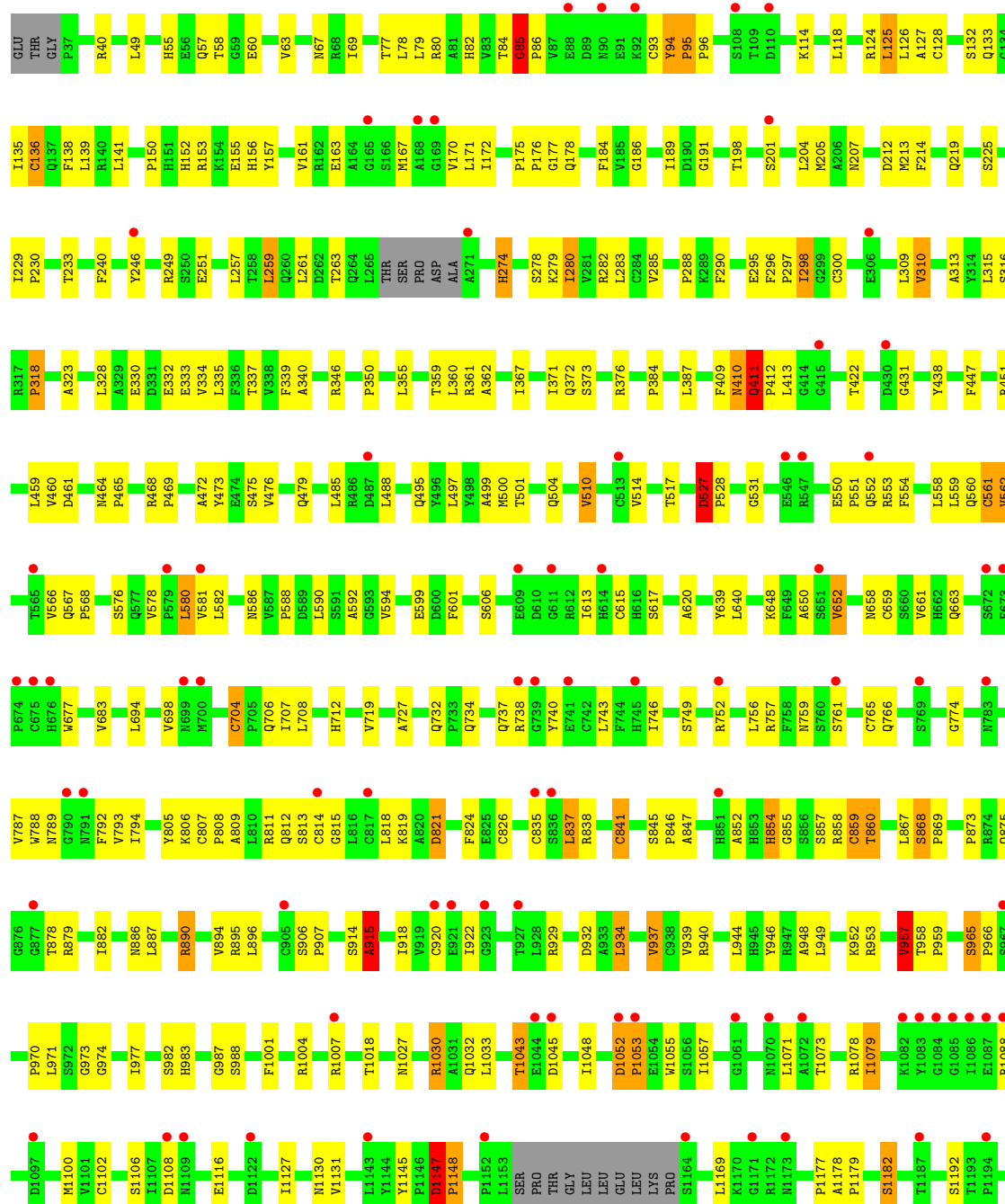
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

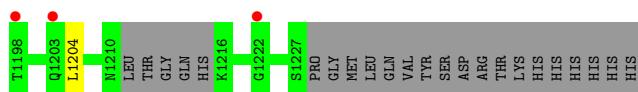
• Molecule 1: Plexin-A1





● Molecule 1: Plexin-A1





- 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



- 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



- 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



- 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



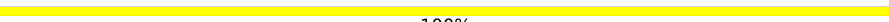
- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 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

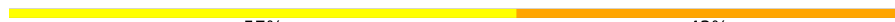


- Molecule 3: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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 F:  57% 43%

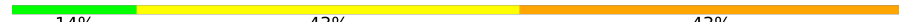
MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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 J:  14% 86%

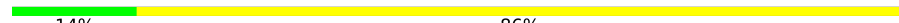
MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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 N:  14% 43% 43%

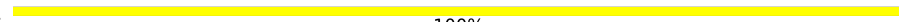
MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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 R:  14% 86%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

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

Chain G:  100%

MAG1
MAG2
BMA3

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

Chain H:  100%

MAG1
MAG2
BMA3

- Molecule 5: 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 6: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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 L:  17% 83%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 6: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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 Q:  17% 83%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	139.99Å 196.45Å 144.94Å 90.00° 94.57° 90.00°	Depositor
Resolution (Å)	58.22 – 6.00 58.22 – 6.00	Depositor EDS
% Data completeness (in resolution range)	94.3 (58.22-6.00) 76.2 (58.22-6.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 6.17Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.274 , 0.299 0.270 , 0.293	Depositor DCC
R_{free} test set	1004 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	291.6	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.62 , 995.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.077 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19191	wwPDB-VP
Average B, all atoms (Å ²)	272.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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

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	0.69	5/9293 (0.1%)	0.90	22/12628 (0.2%)
1	B	0.93	8/9296 (0.1%)	1.11	32/12639 (0.3%)
All	All	0.82	13/18589 (0.1%)	1.01	54/25267 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	10
All	All	0	18

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	561	CYS	C-N	59.77	2.00	1.33
1	A	859	CYS	C-N	-33.99	0.89	1.33
1	A	510	VAL	C-N	31.13	1.75	1.33
1	B	859	CYS	C-N	30.67	1.76	1.33
1	B	1147	ASP	C-N	26.55	1.96	1.33
1	B	1043	THR	C-N	23.07	1.64	1.33
1	B	957	VAL	C-N	13.71	1.61	1.33
1	A	561	CYS	C-N	-11.81	1.20	1.33
1	A	957	VAL	C-N	-11.03	1.25	1.33
1	B	510	VAL	C-N	-10.14	1.19	1.33
1	A	806	LYS	C-N	9.44	1.54	1.33
1	B	704	CYS	C-N	7.42	1.51	1.33
1	B	806	LYS	C-N	5.65	1.41	1.33

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1043	THR	O-C-N	39.48	172.91	123.16
1	B	1043	THR	CA-C-N	-33.54	73.09	120.71
1	B	1043	THR	C-N-CA	-33.54	73.09	120.71
1	B	1147	ASP	O-C-N	-24.68	92.94	121.32
1	B	859	CYS	O-C-N	-16.26	101.10	122.72
1	B	704	CYS	CA-C-N	15.09	138.70	119.84
1	B	704	CYS	C-N-CA	15.09	138.70	119.84
1	B	704	CYS	O-C-N	-14.48	104.67	121.32
1	B	806	LYS	O-C-N	12.95	138.55	123.27
1	A	561	CYS	O-C-N	-10.55	109.83	122.81
1	A	561	CYS	CA-C-N	9.29	135.11	121.18
1	A	561	CYS	C-N-CA	9.29	135.11	121.18
1	B	1147	ASP	C-N-CD	-8.22	91.30	125.00
1	B	527	ASP	CA-C-N	8.20	127.86	119.82
1	B	527	ASP	C-N-CA	8.20	127.86	119.82
1	A	527	ASP	CA-C-N	8.13	127.78	119.82
1	A	527	ASP	C-N-CA	8.13	127.78	119.82
1	A	1052	ASP	N-CA-C	7.67	123.68	110.02
1	B	1052	ASP	N-CA-C	7.62	123.58	110.02
1	A	868	SER	CA-C-N	7.44	129.14	119.84
1	A	868	SER	C-N-CA	7.44	129.14	119.84
1	B	868	SER	CA-C-N	7.36	129.04	119.84
1	B	868	SER	C-N-CA	7.36	129.04	119.84
1	B	957	VAL	CA-C-N	-7.29	104.01	121.80
1	B	957	VAL	C-N-CA	-7.29	104.01	121.80
1	A	809	ALA	N-CA-C	-6.02	105.59	113.17
1	B	809	ALA	N-CA-C	-5.91	105.73	113.17
1	B	841	CYS	CA-C-N	5.82	125.76	119.76
1	B	841	CYS	C-N-CA	5.82	125.76	119.76
1	B	510	VAL	O-C-N	-5.82	116.00	121.87
1	B	712	HIS	N-CA-C	5.78	118.44	110.35
1	A	85	GLY	CA-C-N	5.77	127.05	119.84
1	A	85	GLY	C-N-CA	5.77	127.05	119.84
1	B	85	GLY	CA-C-N	5.76	127.04	119.84
1	B	85	GLY	C-N-CA	5.76	127.04	119.84
1	A	841	CYS	CA-C-N	5.76	125.69	119.76
1	A	841	CYS	C-N-CA	5.76	125.69	119.76
1	B	965	SER	CA-C-N	-5.74	112.66	119.84
1	B	965	SER	C-N-CA	-5.74	112.66	119.84
1	A	965	SER	CA-C-N	-5.71	112.71	119.84
1	A	965	SER	C-N-CA	-5.71	112.71	119.84
1	A	712	HIS	N-CA-C	5.70	118.33	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	854	HIS	N-CA-C	-5.67	105.76	114.16
1	A	854	HIS	N-CA-C	-5.65	105.80	114.16
1	B	965	SER	N-CA-C	5.50	121.96	109.81
1	A	965	SER	N-CA-C	5.46	121.87	109.81
1	A	316	SER	N-CA-C	5.12	114.90	108.45
1	B	1053	PRO	N-CA-C	-5.11	101.95	112.47
1	A	1053	PRO	N-CA-C	-5.10	101.97	112.47
1	B	295	GLU	N-CA-C	5.09	115.85	107.20
1	B	316	SER	N-CA-C	5.08	114.85	108.45
1	A	295	GLU	N-CA-C	5.07	115.81	107.20
1	A	915	ALA	N-CA-C	5.03	121.52	110.80
1	B	915	ALA	N-CA-C	5.01	121.46	110.80

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1052	ASP	Peptide
1	A	410	ASN	Peptide
1	A	527	ASP	Peptide
1	A	807	CYS	Peptide
1	A	85	GLY	Peptide
1	A	868	SER	Peptide
1	A	94	TYR	Peptide
1	A	965	SER	Peptide
1	B	1052	ASP	Peptide
1	B	410	ASN	Peptide
1	B	527	ASP	Peptide
1	B	704	CYS	Mainchain
1	B	807	CYS	Peptide
1	B	85	GLY	Peptide
1	B	868	SER	Peptide
1	B	94	TYR	Peptide
1	B	957	VAL	Mainchain
1	B	965	SER	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	9085	0	8876	245	25
1	B	9085	0	8878	287	41
2	C	50	0	43	1	0
2	E	50	0	43	0	0
2	K	50	0	43	1	0
2	M	50	0	43	0	0
2	O	50	0	43	0	0
3	D	61	0	51	0	0
3	I	61	0	52	0	0
4	F	83	0	70	4	0
4	J	83	0	70	0	0
4	N	83	0	70	2	0
4	R	83	0	70	0	0
5	G	39	0	34	0	0
5	H	39	0	34	0	0
5	P	39	0	34	0	0
6	L	72	0	60	0	0
6	Q	72	0	61	0	0
7	A	28	0	26	0	0
7	B	28	0	26	0	0
All	All	19191	0	18627	515	43

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 14.

All (515) 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:A:855:GLY:HA3	1:A:890:ARG:NH2	1.22	1.48
1:A:510:VAL:C	1:A:511:GLU:N	1.75	1.44
1:B:859:CYS:C	1:B:860:THR:N	1.76	1.44
1:B:1116:GLU:O	1:B:1177:PRO:CD	1.68	1.42
1:B:813:SER:HB2	1:B:886:ASN:CG	1.48	1.38
1:B:813:SER:HB2	1:B:886:ASN:OD1	1.22	1.36
1:A:855:GLY:CA	1:A:890:ARG:NH2	1.88	1.35
1:B:858:ARG:HB3	1:B:940:ARG:NH2	1.43	1.30
1:B:813:SER:CB	1:B:886:ASN:OD1	1.80	1.29
1:B:1147:ASP:C	1:B:1148:PRO:N	1.96	1.24
1:A:98:SER:C	1:B:756:LEU:HD21	1.58	1.24
1:B:561:CYS:C	1:B:562:VAL:N	1.99	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:ASN:C	1:A:659:CYS:N	2.04	1.15
1:A:704:CYS:C	1:A:705:PRO:N	2.07	1.13
1:B:855:GLY:C	1:B:890:ARG:HH22	1.56	1.13
1:A:855:GLY:CA	1:A:890:ARG:HH22	1.52	1.12
1:A:877:GLY:HA3	1:A:1030:ARG:HG3	1.16	1.12
1:A:99:VAL:O	1:B:766:GLN:NE2	1.83	1.10
1:B:813:SER:HB2	1:B:886:ASN:ND2	1.64	1.10
1:A:99:VAL:HA	1:B:756:LEU:HD11	1.17	1.10
1:B:411:GLN:HG2	1:B:412:PRO:HD2	1.35	1.09
1:B:1116:GLU:O	1:B:1177:PRO:HD2	0.92	1.08
1:B:658:ASN:C	1:B:659:CYS:N	2.12	1.07
1:A:411:GLN:HG2	1:A:412:PRO:HD2	1.35	1.05
1:B:860:THR:HA	1:B:946:TYR:CE1	1.93	1.04
1:A:860:THR:HA	1:A:946:TYR:CE1	1.93	1.02
1:A:855:GLY:C	1:A:890:ARG:NH2	2.19	1.01
1:B:855:GLY:C	1:B:890:ARG:NH2	2.19	0.99
1:B:860:THR:HA	1:B:946:TYR:HE1	1.28	0.98
1:A:1043:THR:C	1:A:1044:GLU:N	2.21	0.97
1:B:855:GLY:CA	1:B:890:ARG:HH22	1.75	0.97
1:B:855:GLY:HA3	1:B:890:ARG:NH2	1.79	0.96
1:B:859:CYS:O	1:B:946:TYR:CE1	2.20	0.95
1:B:858:ARG:HB3	1:B:940:ARG:HH22	1.19	0.94
1:A:860:THR:HA	1:A:946:TYR:HE1	1.29	0.94
1:A:468:ARG:HG2	1:A:469:PRO:HD2	1.51	0.92
1:A:189:ILE:HD12	1:A:198:THR:HG23	1.52	0.91
1:B:189:ILE:HD12	1:B:198:THR:HG23	1.52	0.91
1:A:98:SER:O	1:B:756:LEU:HD21	1.70	0.91
1:B:855:GLY:CA	1:B:890:ARG:NH2	2.33	0.91
1:B:468:ARG:HG2	1:B:469:PRO:HD2	1.51	0.89
1:B:813:SER:OG	1:B:886:ASN:OD1	1.91	0.89
1:B:94:TYR:CD2	1:B:95:PRO:HD3	2.08	0.89
1:A:973:GLY:O	1:A:1129:ASP:HB3	1.72	0.89
1:A:94:TYR:CD2	1:A:95:PRO:HD3	2.08	0.88
1:B:855:GLY:O	1:B:890:ARG:NH2	2.07	0.88
1:B:459:LEU:HD21	1:B:528:PRO:HG3	1.56	0.88
1:B:859:CYS:C	1:B:946:TYR:CE1	2.51	0.88
1:B:819:LYS:NZ	1:B:914:SER:O	2.07	0.87
1:A:98:SER:CA	1:B:756:LEU:HD21	2.05	0.87
1:B:859:CYS:C	1:B:946:TYR:HE1	1.83	0.87
1:B:1147:ASP:C	1:B:1148:PRO:CD	2.48	0.86
1:A:808:PRO:HD2	1:A:835:CYS:O	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:VAL:HA	1:B:756:LEU:CD1	2.06	0.85
1:B:1116:GLU:O	1:B:1177:PRO:CG	2.25	0.84
1:B:808:PRO:HD2	1:B:835:CYS:O	1.76	0.84
1:B:567:GLN:HB3	1:B:568:PRO:HD3	1.61	0.81
1:A:98:SER:CB	1:B:756:LEU:CD2	2.59	0.81
1:B:818:LEU:HB3	1:B:852:ALA:HB2	1.62	0.81
1:B:813:SER:HB2	1:B:886:ASN:HD21	1.46	0.81
1:A:98:SER:CB	1:B:756:LEU:HD21	2.11	0.81
1:B:553:ARG:HD2	1:B:588:PRO:HG3	1.63	0.81
1:A:818:LEU:HB3	1:A:852:ALA:HB2	1.63	0.80
1:A:567:GLN:HB3	1:A:568:PRO:HD3	1.62	0.80
1:A:855:GLY:CA	1:A:890:ARG:HH21	1.75	0.80
1:A:280:ILE:HB	1:A:298:ILE:HD12	1.64	0.79
1:A:876:GLY:O	1:A:1030:ARG:HB2	1.82	0.79
1:B:789:ASN:HD22	1:B:792:PHE:HE2	1.31	0.79
1:A:789:ASN:HD22	1:A:792:PHE:HE2	1.31	0.79
1:B:153:ARG:H	1:B:156:HIS:HD2	1.30	0.78
1:A:411:GLN:CG	1:A:412:PRO:HD2	2.14	0.78
1:A:153:ARG:H	1:A:156:HIS:HD2	1.30	0.78
1:A:855:GLY:HA3	1:A:890:ARG:HH21	0.97	0.78
1:B:259:LEU:HD23	1:B:346:ARG:HG3	1.66	0.77
1:B:858:ARG:HB3	1:B:940:ARG:HH21	1.47	0.77
1:B:411:GLN:CG	1:B:412:PRO:HD2	2.14	0.77
1:A:877:GLY:HA3	1:A:1030:ARG:CG	2.06	0.76
1:A:895:ARG:O	1:A:896:LEU:HB2	1.85	0.76
1:B:280:ILE:HB	1:B:298:ILE:HD12	1.64	0.76
1:A:98:SER:HB2	1:B:756:LEU:CD2	2.14	0.76
1:A:259:LEU:HD23	1:A:346:ARG:HG3	1.66	0.75
1:B:230:PRO:O	1:B:233:THR:HG22	1.86	0.75
1:B:895:ARG:O	1:B:896:LEU:HB2	1.85	0.75
1:A:230:PRO:O	1:A:233:THR:HG22	1.86	0.74
1:A:743:LEU:HD22	1:A:752:ARG:HG2	1.70	0.73
1:A:877:GLY:CA	1:A:1030:ARG:HG3	2.09	0.73
1:B:813:SER:CB	1:B:886:ASN:CG	2.42	0.72
1:A:171:LEU:HD22	1:A:204:LEU:HD11	1.72	0.72
1:B:82:HIS:HD2	1:B:84:THR:HG22	1.55	0.72
1:B:743:LEU:HD22	1:B:752:ARG:HG2	1.70	0.72
1:B:1145:TYR:OH	1:B:1179:PRO:HD2	1.90	0.72
1:A:82:HIS:HD2	1:A:84:THR:HG22	1.55	0.71
1:B:553:ARG:HD2	1:B:588:PRO:CG	2.20	0.71
1:B:171:LEU:HD22	1:B:204:LEU:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:TYR:CG	1:A:824:PHE:CD1	2.79	0.71
1:B:472:ALA:HB3	1:B:527:ASP:OD1	1.91	0.71
1:B:852:ALA:HA	1:B:857:SER:OG	1.90	0.70
1:B:663:GLN:NE2	4:N:6:MAN:O6	2.24	0.70
1:B:1079:ILE:HD11	1:B:1102:CYS:HB3	1.73	0.70
1:B:1116:GLU:HG2	1:B:1177:PRO:HD3	1.74	0.70
1:A:852:ALA:HA	1:A:857:SER:OG	1.91	0.70
1:B:974:GLY:HA3	1:B:1130:ASN:HB2	1.73	0.70
1:A:606:SER:HB3	1:A:615:CYS:HB3	1.74	0.70
1:A:860:THR:CA	1:A:946:TYR:HE1	2.03	0.70
1:B:860:THR:CA	1:B:946:TYR:HE1	2.03	0.69
1:A:138:PHE:CZ	1:A:213:MET:HE2	2.28	0.69
1:A:55:HIS:HE2	1:A:141:LEU:HD21	1.57	0.69
1:B:310:VAL:HG22	1:B:339:PHE:CE1	2.28	0.69
1:B:606:SER:HB3	1:B:615:CYS:HB3	1.74	0.69
1:B:55:HIS:HE2	1:B:141:LEU:HD21	1.57	0.69
1:A:310:VAL:HG22	1:A:339:PHE:CE1	2.28	0.69
1:A:114:LYS:HE2	1:A:167:MET:HE3	1.75	0.68
1:A:1079:ILE:HD11	1:A:1102:CYS:HB3	1.73	0.68
1:B:114:LYS:HE2	1:B:167:MET:HE3	1.75	0.68
1:B:138:PHE:CZ	1:B:213:MET:HE2	2.28	0.68
1:A:468:ARG:CG	1:A:469:PRO:HD2	2.24	0.68
1:A:566:VAL:HG22	1:A:582:LEU:HD23	1.76	0.67
1:B:813:SER:CB	1:B:886:ASN:ND2	2.51	0.67
1:A:175:PRO:HG2	1:A:178:GLN:HG3	1.77	0.67
1:A:746:ILE:HB	1:A:749:SER:O	1.95	0.67
1:B:895:ARG:HA	1:B:907:PRO:HG2	1.76	0.67
1:B:468:ARG:CG	1:B:469:PRO:HD2	2.24	0.67
1:B:746:ILE:HB	1:B:749:SER:O	1.95	0.67
1:B:973:GLY:O	1:B:1130:ASN:HB3	1.95	0.67
1:A:98:SER:O	1:B:756:LEU:CD2	2.40	0.66
1:A:895:ARG:HA	1:A:907:PRO:HG2	1.76	0.66
1:B:813:SER:CB	1:B:886:ASN:HD21	2.09	0.66
1:B:566:VAL:HG22	1:B:582:LEU:HD23	1.76	0.66
1:A:472:ALA:HB3	1:A:527:ASP:OD1	1.95	0.66
1:A:855:GLY:C	1:A:890:ARG:HH22	1.94	0.66
1:B:315:LEU:HD11	1:B:333:GLU:HB3	1.78	0.66
1:B:973:GLY:O	1:B:1130:ASN:CB	2.44	0.65
1:A:69:ILE:HD12	1:A:84:THR:HG21	1.79	0.65
1:B:175:PRO:HG2	1:B:178:GLN:HG3	1.77	0.65
1:A:99:VAL:CA	1:B:756:LEU:HD11	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:ILE:HD12	1:A:1147:ASP:OD1	1.96	0.65
1:B:1057:ILE:HD12	1:B:1147:ASP:OD1	1.97	0.65
1:A:855:GLY:N	1:A:890:ARG:HH22	1.93	0.65
1:B:1147:ASP:C	1:B:1148:PRO:HD3	2.21	0.65
1:B:858:ARG:CB	1:B:940:ARG:HH22	2.04	0.64
1:B:1116:GLU:C	1:B:1177:PRO:CD	2.66	0.64
1:A:315:LEU:HD11	1:A:333:GLU:HB3	1.78	0.64
1:B:69:ILE:HD12	1:B:84:THR:HG21	1.79	0.64
1:B:553:ARG:HD2	1:B:588:PRO:CB	2.28	0.64
1:B:472:ALA:CB	1:B:527:ASP:OD1	2.46	0.64
1:B:957:VAL:C	1:B:958:THR:OG1	2.41	0.64
1:A:550:GLU:HB3	1:A:551:PRO:HD2	1.80	0.63
1:B:550:GLU:HB3	1:B:551:PRO:HD2	1.80	0.63
1:B:887:LEU:HB2	1:B:915:ALA:HA	1.80	0.63
1:A:536:HIS:HA	1:A:645:THR:HG21	1.80	0.63
1:A:98:SER:C	1:B:756:LEU:CD2	2.54	0.63
1:A:58:THR:OG1	1:A:60:GLU:HG2	1.99	0.62
1:A:887:LEU:HB2	1:A:915:ALA:HA	1.80	0.62
1:B:560:GLN:O	1:B:586:ASN:HB3	2.00	0.62
1:A:939:VAL:HG22	1:A:946:TYR:HB3	1.82	0.62
1:A:871:THR:OG1	1:A:986:ALA:HA	1.99	0.62
1:B:58:THR:OG1	1:B:60:GLU:HG2	1.99	0.62
1:B:939:VAL:HG22	1:B:946:TYR:HB3	1.82	0.61
1:A:732:GLN:HG2	1:A:757:ARG:HH22	1.66	0.61
1:B:858:ARG:CB	1:B:940:ARG:NH2	2.39	0.61
1:A:259:LEU:HD23	1:A:346:ARG:CG	2.31	0.61
1:A:639:TYR:CD2	1:A:648:LYS:HD2	2.36	0.61
1:A:740:TYR:CD1	1:A:788:TRP:HB3	2.36	0.61
1:B:578:VAL:H	1:B:617:SER:HB3	1.66	0.61
1:B:740:TYR:CD1	1:B:788:TRP:HB3	2.36	0.61
1:B:1145:TYR:OH	1:B:1179:PRO:CD	2.49	0.61
1:B:732:GLN:HG2	1:B:757:ARG:HH22	1.66	0.61
1:B:560:GLN:C	1:B:586:ASN:HD22	2.09	0.60
1:A:663:GLN:NE2	4:F:6:MAN:O6	2.34	0.60
1:A:661:VAL:HG13	4:F:1:NAG:O6	2.01	0.60
1:B:259:LEU:HD23	1:B:346:ARG:CG	2.31	0.60
1:A:578:VAL:H	1:A:617:SER:HB3	1.66	0.60
1:B:639:TYR:CD2	1:B:648:LYS:HD2	2.36	0.60
1:B:878:THR:HG23	1:B:987:GLY:HA2	1.84	0.60
1:A:55:HIS:NE2	1:A:141:LEU:HD21	2.17	0.60
1:B:879:ARG:HB2	1:B:988:SER:OG	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:878:THR:HB	1:A:922:ILE:HD12	1.84	0.59
1:B:55:HIS:NE2	1:B:141:LEU:HD21	2.17	0.59
1:B:859:CYS:SG	1:B:860:THR:N	2.75	0.59
1:B:878:THR:HB	1:B:922:ILE:HD12	1.84	0.59
1:B:153:ARG:N	1:B:156:HIS:HD2	1.99	0.59
1:A:153:ARG:N	1:A:156:HIS:HD2	1.99	0.59
1:B:1116:GLU:C	1:B:1177:PRO:HG2	2.27	0.59
1:A:485:LEU:HD12	1:A:500:MET:HG2	1.86	0.58
1:B:153:ARG:H	1:B:156:HIS:CD2	2.18	0.58
1:A:246:TYR:CD2	1:A:313:ALA:HB3	2.39	0.58
1:B:485:LEU:HD12	1:B:500:MET:HG2	1.86	0.58
1:A:447:PHE:HZ	1:A:510:VAL:HG23	1.69	0.57
1:B:719:VAL:HG21	1:B:837:LEU:CD1	2.33	0.57
1:B:1116:GLU:O	1:B:1177:PRO:HG2	2.05	0.57
1:A:732:GLN:HG2	1:A:757:ARG:NH2	2.20	0.57
1:B:132:SER:HB2	1:B:135:ILE:HG12	1.87	0.57
1:B:337:THR:O	1:B:355:LEU:HD12	2.05	0.57
1:B:973:GLY:C	1:B:1130:ASN:HB3	2.30	0.57
1:B:447:PHE:HZ	1:B:510:VAL:HG23	1.69	0.57
1:B:246:TYR:CD2	1:B:313:ALA:HB3	2.39	0.57
1:B:531:GLY:HA3	1:B:554:PHE:CZ	2.40	0.57
1:B:970:PRO:CB	1:B:1131:VAL:CG2	2.83	0.57
1:A:808:PRO:HG3	1:A:835:CYS:HB3	1.87	0.57
1:B:859:CYS:O	1:B:860:THR:N	2.33	0.57
1:A:132:SER:HB2	1:A:135:ILE:HG12	1.87	0.56
1:B:172:ILE:HG22	1:B:249:ARG:HD2	1.87	0.56
1:A:531:GLY:HA3	1:A:554:PHE:CZ	2.40	0.56
1:A:661:VAL:HG22	4:F:1:NAG:O5	2.05	0.56
1:B:732:GLN:HG2	1:B:757:ARG:NH2	2.20	0.56
1:B:1147:ASP:O	1:B:1148:PRO:N	2.37	0.56
1:A:789:ASN:HB3	1:A:792:PHE:CD2	2.41	0.56
1:A:1055:TRP:CE2	1:A:1178:ALA:HB1	2.40	0.56
1:B:296:PHE:CE1	1:B:367:ILE:HG12	2.41	0.56
1:A:337:THR:O	1:A:355:LEU:HD12	2.05	0.56
1:B:789:ASN:HB3	1:B:792:PHE:CD2	2.41	0.56
1:B:808:PRO:HG3	1:B:835:CYS:HB3	1.87	0.56
1:A:172:ILE:HG22	1:A:249:ARG:HD2	1.87	0.56
1:A:567:GLN:HB2	1:A:581:VAL:HG22	1.87	0.56
1:B:567:GLN:HB2	1:B:581:VAL:HG22	1.87	0.55
1:A:98:SER:O	1:B:756:LEU:CG	2.54	0.55
1:A:566:VAL:HG22	1:A:582:LEU:CD2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:738:ARG:HB2	1:B:789:ASN:HA	1.89	0.55
1:B:1116:GLU:HG2	1:B:1177:PRO:CD	2.36	0.55
1:A:296:PHE:CE1	1:A:367:ILE:HG12	2.41	0.55
1:B:566:VAL:HG22	1:B:582:LEU:CD2	2.37	0.55
1:B:737:GLN:HG2	1:B:789:ASN:ND2	2.22	0.55
1:A:98:SER:HB2	1:B:756:LEU:HD23	1.89	0.55
1:B:318:PRO:HG2	1:B:323:ALA:HB2	1.89	0.55
1:A:93:CYS:O	1:A:133:GLN:NE2	2.40	0.55
1:A:318:PRO:HG2	1:A:323:ALA:HB2	1.89	0.55
1:B:93:CYS:O	1:B:133:GLN:NE2	2.40	0.55
1:B:282:ARG:HG3	1:B:283:LEU:N	2.22	0.55
1:B:552:GLN:O	1:B:588:PRO:HD3	2.06	0.55
1:B:279:LYS:HG2	1:B:297:PRO:HA	1.87	0.55
1:A:464:ASN:CG	1:A:465:PRO:HD2	2.32	0.54
1:A:279:LYS:HG2	1:A:297:PRO:HA	1.87	0.54
1:B:464:ASN:CG	1:B:465:PRO:HD2	2.32	0.54
1:A:738:ARG:HB2	1:A:789:ASN:HA	1.89	0.54
1:A:488:LEU:HD12	1:A:499:ALA:HA	1.89	0.54
1:A:679:LYS:HE2	1:A:729:ASN:HB3	1.89	0.54
1:B:1055:TRP:CZ2	1:B:1182:SER:HB2	2.43	0.54
1:A:282:ARG:HG3	1:A:283:LEU:N	2.22	0.54
1:A:970:PRO:CG	1:A:1129:ASP:OD2	2.56	0.54
1:B:1116:GLU:HG2	1:B:1177:PRO:CG	2.38	0.54
1:A:737:GLN:HG2	1:A:789:ASN:ND2	2.22	0.54
1:B:205:MET:HG3	1:B:212:ASP:HB3	1.90	0.53
1:B:789:ASN:HB3	1:B:792:PHE:HD2	1.73	0.53
1:A:789:ASN:HB3	1:A:792:PHE:HD2	1.73	0.53
1:A:332:GLU:OE2	1:A:361:ARG:NH2	2.41	0.53
1:A:805:TYR:CD1	1:A:824:PHE:HD1	2.26	0.53
1:B:488:LEU:HD12	1:B:499:ALA:HA	1.89	0.53
1:A:124:ARG:HD2	1:A:138:PHE:HD2	1.74	0.53
1:A:640:LEU:HD12	1:A:650:ALA:HB3	1.91	0.53
1:A:126:LEU:HD11	1:A:136:CYS:SG	2.49	0.53
1:A:170:VAL:HG11	1:A:249:ARG:HB2	1.91	0.53
1:A:205:MET:HG3	1:A:212:ASP:HB3	1.90	0.53
1:A:278:SER:HB3	1:A:310:VAL:HG23	1.91	0.53
1:A:310:VAL:HG22	1:A:339:PHE:HE1	1.72	0.53
1:B:278:SER:HB3	1:B:310:VAL:HG23	1.91	0.53
1:A:58:THR:CB	1:A:60:GLU:HG2	2.39	0.52
1:B:126:LEU:HD11	1:B:136:CYS:SG	2.49	0.52
1:B:332:GLU:OE2	1:B:361:ARG:NH2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:859:CYS:C	1:B:860:THR:CA	2.76	0.52
1:B:58:THR:CB	1:B:60:GLU:HG2	2.40	0.52
1:A:153:ARG:H	1:A:156:HIS:CD2	2.18	0.52
1:B:677:TRP:HB3	1:B:698:VAL:HB	1.92	0.52
1:A:447:PHE:CZ	1:A:510:VAL:HG23	2.45	0.52
1:A:869:PRO:HG3	1:A:988:SER:OG	2.10	0.52
1:B:821:ASP:HB2	1:B:824:PHE:CD2	2.45	0.52
1:A:461:ASP:HA	1:A:464:ASN:HB3	1.92	0.52
1:B:124:ARG:HD2	1:B:138:PHE:HD2	1.74	0.52
1:B:640:LEU:HD12	1:B:650:ALA:HB3	1.91	0.51
1:A:438:TYR:CE1	1:A:510:VAL:HG21	2.46	0.51
1:A:821:ASP:HB2	1:A:824:PHE:CD2	2.44	0.51
1:A:854:HIS:C	1:A:890:ARG:HH22	2.18	0.51
1:B:447:PHE:CZ	1:B:510:VAL:HG23	2.45	0.51
1:B:438:TYR:CE1	1:B:510:VAL:HG21	2.46	0.51
1:B:170:VAL:HG11	1:B:249:ARG:HB2	1.91	0.51
1:B:461:ASP:HA	1:B:464:ASN:HB3	1.92	0.51
1:A:153:ARG:NH2	1:A:212:ASP:HA	2.26	0.51
1:B:153:ARG:NH2	1:B:212:ASP:HA	2.26	0.51
1:A:229:ILE:HD12	1:A:240:PHE:HE2	1.76	0.51
1:A:431:GLY:HA3	1:A:451:ARG:HD2	1.93	0.51
1:B:229:ILE:HD12	1:B:240:PHE:HE2	1.76	0.51
1:B:55:HIS:CE1	1:B:57:GLN:HB2	2.46	0.51
1:B:971:LEU:N	1:B:1045:ASP:OD1	2.41	0.51
1:B:859:CYS:O	1:B:946:TYR:CD1	2.64	0.50
1:B:970:PRO:HB2	1:B:1131:VAL:CG2	2.42	0.50
1:A:472:ALA:CB	1:A:527:ASP:OD1	2.59	0.50
1:A:677:TRP:HB3	1:A:698:VAL:HB	1.92	0.50
1:A:55:HIS:CE1	1:A:57:GLN:HB2	2.46	0.50
1:A:805:TYR:OH	1:A:824:PHE:O	2.27	0.50
1:A:805:TYR:HB3	1:A:824:PHE:CE1	2.47	0.50
4:F:1:NAG:H61	4:F:2:NAG:HN2	1.76	0.50
1:A:186:GLY:HA2	1:A:198:THR:O	2.12	0.50
1:A:510:VAL:C	1:A:511:GLU:CA	2.77	0.50
1:B:310:VAL:HG22	1:B:339:PHE:HE1	1.72	0.50
1:B:553:ARG:HG2	1:B:588:PRO:HB3	1.92	0.50
1:B:186:GLY:HA2	1:B:198:THR:O	2.12	0.50
1:B:875:GLN:O	1:B:1030:ARG:NH1	2.45	0.50
4:N:1:NAG:H61	4:N:2:NAG:HN2	1.77	0.50
1:A:323:ALA:HA	1:A:328:LEU:HD12	1.94	0.50
1:A:708:LEU:H	1:A:727:ALA:HA	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:ALA:HA	1:B:328:LEU:HD12	1.93	0.50
1:A:145:PHE:HD1	1:B:734:GLN:OE1	1.96	0.49
1:B:172:ILE:HD11	1:B:184:PHE:HE2	1.77	0.49
1:B:431:GLY:HA3	1:B:451:ARG:HD2	1.94	0.49
1:A:172:ILE:HD11	1:A:184:PHE:HE2	1.77	0.49
1:B:708:LEU:H	1:B:727:ALA:HA	1.77	0.49
1:B:1116:GLU:CG	1:B:1177:PRO:HD3	2.42	0.49
1:A:495:GLN:O	1:A:510:VAL:HG12	2.13	0.49
1:B:153:ARG:HB2	1:B:156:HIS:CD2	2.48	0.49
1:A:1027:ASN:HB3	1:A:1032:GLN:HG3	1.95	0.48
1:B:495:GLN:O	1:B:510:VAL:HG12	2.13	0.48
1:B:1147:ASP:HB3	1:B:1148:PRO:CD	2.43	0.48
1:A:460:VAL:HA	1:A:469:PRO:HB3	1.95	0.48
1:B:40:ARG:NH2	2:K:1:NAG:O3	2.47	0.48
1:B:501:THR:OG1	1:B:504:GLN:N	2.44	0.48
1:A:145:PHE:HE1	1:B:734:GLN:NE2	2.12	0.48
1:B:96:PRO:HD2	1:B:157:TYR:CZ	2.48	0.48
1:B:859:CYS:O	1:B:946:TYR:HE1	1.75	0.48
1:A:40:ARG:NH2	2:C:1:NAG:O3	2.47	0.48
1:B:719:VAL:HG21	1:B:837:LEU:HD13	1.95	0.48
1:B:970:PRO:HB2	1:B:1131:VAL:HG22	1.94	0.48
1:A:63:VAL:HG13	1:A:500:MET:HE1	1.96	0.48
1:A:96:PRO:HD2	1:A:157:TYR:CZ	2.48	0.48
1:A:98:SER:O	1:B:756:LEU:HD11	2.14	0.48
1:A:939:VAL:CG2	1:A:946:TYR:HB3	2.42	0.48
1:B:1027:ASN:HB3	1:B:1032:GLN:HG3	1.95	0.47
1:A:153:ARG:HB2	1:A:156:HIS:CD2	2.48	0.47
1:B:63:VAL:HG13	1:B:500:MET:HE1	1.96	0.47
1:B:460:VAL:HA	1:B:469:PRO:HB3	1.96	0.47
1:B:907:PRO:HA	1:B:920:CYS:HA	1.96	0.47
1:B:567:GLN:CB	1:B:581:VAL:HG22	2.44	0.47
1:B:821:ASP:HB2	1:B:824:PHE:CE2	2.50	0.47
1:A:821:ASP:HB2	1:A:824:PHE:CE2	2.49	0.47
1:B:973:GLY:C	1:B:1130:ASN:CB	2.88	0.47
1:A:372:GLN:O	1:A:376:ARG:HD3	2.15	0.47
1:A:447:PHE:CD2	1:A:497:LEU:HD22	2.50	0.47
1:B:172:ILE:HD13	1:B:285:VAL:HG13	1.97	0.47
1:B:939:VAL:CG2	1:B:946:TYR:HB3	2.42	0.47
1:A:907:PRO:HA	1:A:920:CYS:HA	1.96	0.47
1:A:934:LEU:HD23	1:A:953:ARG:HB3	1.97	0.47
1:B:372:GLN:O	1:B:376:ARG:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:934:LEU:HD23	1:B:953:ARG:HB3	1.97	0.47
1:A:567:GLN:CB	1:A:581:VAL:HG22	2.44	0.47
1:A:461:ASP:CA	1:A:464:ASN:HB3	2.45	0.47
1:A:805:TYR:CE2	1:A:824:PHE:HB3	2.50	0.47
1:A:818:LEU:HD22	1:A:852:ALA:H	1.80	0.46
1:B:566:VAL:CG2	1:B:652:VAL:HG21	2.45	0.46
1:B:952:LYS:HD2	1:B:952:LYS:HA	1.70	0.46
1:A:145:PHE:CE1	1:B:734:GLN:NE2	2.84	0.46
1:B:818:LEU:HD22	1:B:852:ALA:H	1.80	0.46
1:A:566:VAL:CG2	1:A:652:VAL:HG21	2.45	0.46
1:A:805:TYR:CZ	1:A:824:PHE:O	2.68	0.46
1:A:860:THR:HG22	1:A:946:TYR:OH	2.16	0.46
1:B:447:PHE:CD2	1:B:497:LEU:HD22	2.50	0.46
1:B:805:TYR:CE2	1:B:824:PHE:HB3	2.51	0.46
1:A:553:ARG:HD2	1:A:588:PRO:HG3	1.98	0.46
1:A:877:GLY:HA2	1:A:1030:ARG:NE	2.31	0.46
1:B:461:ASP:CA	1:B:464:ASN:HB3	2.45	0.46
1:A:805:TYR:CE2	1:A:824:PHE:O	2.69	0.46
1:B:1055:TRP:HZ2	1:B:1182:SER:HB2	1.81	0.46
1:B:558:LEU:HD12	1:B:561:CYS:SG	2.56	0.45
1:A:79:LEU:O	1:A:80:ARG:HG3	2.16	0.45
1:B:201:SER:HB2	1:B:290:PHE:HE1	1.81	0.45
1:B:937:VAL:HG23	1:B:948:ALA:HB3	1.98	0.45
1:B:1043:THR:HG21	1:B:1073:THR:HG21	1.98	0.45
1:A:501:THR:OG1	1:A:504:GLN:N	2.44	0.45
1:A:558:LEU:HD12	1:A:561:CYS:SG	2.56	0.45
1:A:566:VAL:HG23	1:A:652:VAL:HG21	1.98	0.45
1:B:125:LEU:HD23	1:B:139:LEU:HB2	1.99	0.45
1:B:887:LEU:HD23	1:B:918:ILE:HD11	1.98	0.45
1:A:887:LEU:HD23	1:A:918:ILE:HD11	1.98	0.45
1:B:860:THR:HG22	1:B:946:TYR:OH	2.16	0.45
1:B:79:LEU:O	1:B:80:ARG:HG3	2.17	0.45
1:B:815:GLY:O	1:B:819:LYS:HB2	2.17	0.45
1:A:172:ILE:HD13	1:A:285:VAL:HG13	1.97	0.45
1:A:858:ARG:HE	1:A:946:TYR:HE2	1.64	0.45
1:A:98:SER:OG	1:B:756:LEU:CD2	2.64	0.45
1:A:132:SER:CB	1:A:135:ILE:HG12	2.47	0.45
1:A:937:VAL:HG23	1:A:948:ALA:HB3	1.98	0.45
1:A:102:CYS:HA	1:A:103:PRO:HD3	1.87	0.44
1:B:1088:ARG:HD2	1:B:1106:SER:O	2.18	0.44
1:B:1145:TYR:OH	1:B:1178:ALA:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:SER:HB2	1:A:290:PHE:HE1	1.81	0.44
1:A:932:ASP:OD1	1:A:932:ASP:N	2.50	0.44
1:B:132:SER:CB	1:B:135:ILE:HG12	2.47	0.44
1:B:932:ASP:OD1	1:B:932:ASP:N	2.50	0.44
1:A:125:LEU:HD23	1:A:139:LEU:HB2	1.99	0.44
1:A:1078:ARG:HG3	1:A:1127:ILE:HB	1.99	0.44
1:A:1088:ARG:HD2	1:A:1106:SER:O	2.18	0.44
1:B:566:VAL:HG23	1:B:652:VAL:HG21	1.98	0.44
1:A:952:LYS:HD2	1:A:952:LYS:HA	1.70	0.44
1:B:894:VAL:HG11	1:B:918:ILE:HD13	1.99	0.44
1:A:550:GLU:HB2	1:A:553:ARG:HG3	2.00	0.44
1:A:972:SER:C	1:A:1130:ASN:HB3	2.42	0.44
1:B:67:ASN:CB	1:B:85:GLY:HA3	2.48	0.44
1:B:359:THR:HG23	1:B:362:ALA:CB	2.48	0.44
1:B:789:ASN:ND2	1:B:792:PHE:HE2	2.09	0.44
1:A:815:GLY:O	1:A:819:LYS:HB2	2.17	0.44
1:B:808:PRO:HB2	1:B:811:ARG:H	1.82	0.44
1:A:860:THR:CA	1:A:946:TYR:CE1	2.81	0.44
1:A:805:TYR:CG	1:A:824:PHE:HD1	2.29	0.43
1:A:805:TYR:CD1	1:A:824:PHE:CD1	3.06	0.43
1:A:740:TYR:HE1	1:A:794:ILE:HD11	1.83	0.43
1:A:808:PRO:HB2	1:A:811:ARG:H	1.82	0.43
1:B:155:GLU:OE1	1:B:155:GLU:N	2.51	0.43
1:B:818:LEU:HB3	1:B:852:ALA:CB	2.41	0.43
1:B:161:VAL:HG12	1:B:163:GLU:H	1.84	0.43
1:A:67:ASN:CB	1:A:85:GLY:HA3	2.48	0.43
1:B:740:TYR:HE1	1:B:794:ILE:HD11	1.83	0.43
1:B:973:GLY:O	1:B:1130:ASN:N	2.51	0.43
1:A:359:THR:HG23	1:A:362:ALA:CB	2.48	0.43
1:A:576:SER:OG	1:A:620:ALA:N	2.51	0.43
1:A:838:ARG:NH1	1:A:841:CYS:O	2.51	0.43
1:B:261:LEU:HD11	1:B:274:HIS:CB	2.48	0.43
1:B:559:LEU:O	1:B:586:ASN:ND2	2.50	0.43
1:B:706:GLN:O	1:B:727:ALA:HB1	2.19	0.43
1:B:838:ARG:NH1	1:B:841:CYS:O	2.51	0.43
1:A:161:VAL:HG12	1:A:163:GLU:H	1.83	0.43
1:A:639:TYR:HD2	1:A:648:LYS:HD2	1.84	0.43
1:A:818:LEU:HB3	1:A:852:ALA:CB	2.41	0.43
1:B:150:PRO:HB2	1:B:156:HIS:ND1	2.34	0.43
1:A:155:GLU:N	1:A:155:GLU:OE1	2.51	0.43
1:A:261:LEU:HD11	1:A:274:HIS:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:VAL:HG11	1:A:918:ILE:HD13	1.99	0.43
1:B:476:VAL:HB	1:B:479:GLN:HG2	2.01	0.43
1:B:553:ARG:CD	1:B:588:PRO:CB	2.96	0.43
1:A:58:THR:HB	1:A:60:GLU:HG2	2.01	0.43
1:B:58:THR:HB	1:B:60:GLU:HG2	2.01	0.43
1:B:1078:ARG:HG3	1:B:1127:ILE:HB	1.99	0.43
1:A:150:PRO:HB2	1:A:156:HIS:ND1	2.34	0.43
1:A:789:ASN:ND2	1:A:792:PHE:HE2	2.09	0.43
1:B:550:GLU:HB2	1:B:553:ARG:HG3	2.00	0.43
1:A:468:ARG:HG2	1:A:469:PRO:CD	2.36	0.43
1:B:606:SER:CB	1:B:615:CYS:HB3	2.47	0.43
1:A:410:ASN:O	1:A:411:GLN:O	2.37	0.42
1:A:787:VAL:HG22	1:A:793:VAL:HG22	2.01	0.42
1:A:818:LEU:HD22	1:A:852:ALA:N	2.34	0.42
1:B:576:SER:OG	1:B:620:ALA:N	2.51	0.42
1:B:410:ASN:O	1:B:411:GLN:O	2.37	0.42
1:B:818:LEU:HD22	1:B:852:ALA:N	2.34	0.42
1:B:959:PRO:HA	1:B:983:HIS:HB2	2.01	0.42
1:A:69:ILE:CD1	1:A:84:THR:HG21	2.48	0.42
1:A:309:LEU:O	1:A:339:PHE:HA	2.19	0.42
1:A:706:GLN:O	1:A:727:ALA:HB1	2.19	0.42
1:A:824:PHE:C	1:A:826:CYS:H	2.27	0.42
1:A:476:VAL:HB	1:A:479:GLN:HG2	2.01	0.42
1:A:972:SER:HB3	1:A:1130:ASN:HB3	2.02	0.42
1:B:309:LEU:O	1:B:339:PHE:HA	2.19	0.42
1:B:263:THR:HB	1:B:384:PRO:HB2	2.02	0.42
1:B:787:VAL:HG22	1:B:793:VAL:HG22	2.01	0.42
1:A:263:THR:HB	1:A:384:PRO:HB2	2.01	0.42
1:A:340:ALA:HB1	1:A:350:PRO:HG2	2.02	0.42
1:A:599:GLU:C	1:A:601:PHE:H	2.28	0.42
1:A:371:ILE:C	1:A:373:SER:H	2.28	0.42
1:A:959:PRO:HA	1:A:983:HIS:HB2	2.01	0.42
1:A:1169:LEU:HB2	1:A:1204:LEU:HB2	2.02	0.42
1:B:340:ALA:HB1	1:B:350:PRO:HG2	2.02	0.42
1:B:1071:LEU:HD13	1:B:1100:MET:HE3	2.01	0.42
1:B:568:PRO:HG2	1:B:580:LEU:HD23	2.01	0.42
1:B:824:PHE:C	1:B:826:CYS:H	2.27	0.42
1:B:970:PRO:HB3	1:B:1131:VAL:CG2	2.48	0.42
1:B:1001:PHE:HZ	1:B:1004:ARG:HB2	1.85	0.42
1:B:1116:GLU:C	1:B:1177:PRO:CG	2.86	0.42
1:B:468:ARG:HG2	1:B:469:PRO:CD	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:GLU:C	1:B:601:PHE:H	2.28	0.41
1:B:1116:GLU:HG2	1:B:1177:PRO:HG3	2.02	0.41
1:A:552:GLN:O	1:A:588:PRO:HD3	2.20	0.41
1:A:1001:PHE:HZ	1:A:1004:ARG:HB2	1.85	0.41
1:B:371:ILE:C	1:B:373:SER:H	2.28	0.41
1:A:582:LEU:HB2	1:A:613:ILE:HB	2.02	0.41
1:A:1071:LEU:HD13	1:A:1100:MET:HE3	2.01	0.41
1:B:150:PRO:O	1:B:156:HIS:HB3	2.21	0.41
1:B:906:SER:HA	1:B:907:PRO:HD3	1.77	0.41
1:A:568:PRO:HG2	1:A:580:LEU:HD23	2.01	0.41
1:B:189:ILE:HG22	1:B:191:GLY:H	1.85	0.41
1:A:871:THR:HG22	1:A:955:THR:HB	2.02	0.41
1:B:49:LEU:HD13	1:B:500:MET:HE2	2.02	0.41
1:B:488:LEU:HG	1:B:497:LEU:HD11	2.02	0.41
1:A:49:LEU:HD13	1:A:500:MET:HE2	2.02	0.41
1:B:461:ASP:CB	1:B:464:ASN:HB3	2.50	0.41
1:A:313:ALA:HB1	1:A:335:LEU:HD11	2.03	0.41
1:B:69:ILE:CD1	1:B:84:THR:HG21	2.48	0.41
1:B:136:CYS:HB3	1:B:214:PHE:CZ	2.56	0.41
1:B:459:LEU:HD23	1:B:459:LEU:HA	1.95	0.41
1:B:582:LEU:HB2	1:B:613:ILE:HB	2.02	0.41
1:A:261:LEU:HD11	1:A:274:HIS:HB3	2.03	0.41
1:A:461:ASP:CB	1:A:464:ASN:HB3	2.50	0.41
1:A:488:LEU:HG	1:A:497:LEU:HD11	2.02	0.41
1:A:944:LEU:HD12	1:A:944:LEU:H	1.85	0.41
1:A:1104:ALA:HA	1:A:1105:PRO:HD3	1.89	0.41
1:B:313:ALA:HB1	1:B:335:LEU:HD11	2.03	0.41
1:B:473:TYR:CE2	1:B:475:SER:HB2	2.56	0.41
1:B:944:LEU:H	1:B:944:LEU:HD12	1.85	0.41
1:B:1147:ASP:CA	1:B:1148:PRO:HD3	2.51	0.41
1:A:150:PRO:O	1:A:156:HIS:HB3	2.21	0.41
1:A:189:ILE:HG22	1:A:191:GLY:H	1.86	0.41
1:A:241:ASP:HB3	1:A:243:TYR:CZ	2.56	0.41
1:A:473:TYR:CE2	1:A:475:SER:HB2	2.56	0.41
1:A:734:GLN:O	1:A:737:GLN:HB2	2.21	0.41
1:B:409:PHE:C	1:B:411:GLN:H	2.29	0.41
1:A:225:SER:HB3	1:A:288:PRO:O	2.20	0.40
1:B:590:LEU:C	1:B:592:ALA:N	2.79	0.40
1:B:855:GLY:HA3	1:B:890:ARG:HH22	1.43	0.40
1:B:1169:LEU:HB2	1:B:1204:LEU:HB2	2.02	0.40
1:B:873:PRO:HD2	1:B:878:THR:OG1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:CYS:O	1:A:675:CYS:HB2	2.22	0.40
1:B:205:MET:N	1:B:213:MET:SD	2.93	0.40
1:A:490:LEU:HD23	1:A:497:LEU:HB2	2.03	0.40
1:A:836:SER:O	1:A:849:TRP:NE1	2.54	0.40
1:A:906:SER:HA	1:A:907:PRO:HD3	1.77	0.40
1:B:189:ILE:CD1	1:B:198:THR:HG23	2.37	0.40
1:B:225:SER:HB3	1:B:288:PRO:O	2.21	0.40
1:B:860:THR:CA	1:B:946:TYR:CE1	2.81	0.40
1:A:1043:THR:OG1	1:A:1073:THR:HB	2.21	0.40
1:B:69:ILE:HD13	1:B:127:ALA:HB1	2.04	0.40
1:B:759:ASN:C	1:B:761:SER:H	2.29	0.40

All (43) 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:A:399:GLN:N	1:B:1007:ARG:NH2[2_445]	0.67	1.53
1:A:398:LEU:C	1:B:1007:ARG:NH2[2_445]	0.78	1.42
1:A:962:TYR:OH	1:B:361:ARG:NH1[1_656]	1.02	1.18
1:B:176:PRO:CG	1:B:846:PRO:CD[1_554]	1.10	1.10
1:A:399:GLN:N	1:B:1007:ARG:CZ[2_445]	1.25	0.95
1:A:398:LEU:C	1:B:1007:ARG:CZ[2_445]	1.28	0.92
1:B:219:GLN:CG	1:B:944:LEU:CD2[1_554]	1.29	0.91
1:A:399:GLN:NE2	1:B:1007:ARG:CG[2_445]	1.36	0.84
1:B:219:GLN:O	1:B:944:LEU:CD1[1_554]	1.43	0.77
1:B:177:GLY:CA	1:B:847:ALA:CB[1_554]	1.56	0.64
1:A:398:LEU:O	1:B:1007:ARG:NH1[2_445]	1.61	0.59
1:B:176:PRO:CB	1:B:846:PRO:CD[1_554]	1.62	0.58
1:A:962:TYR:CZ	1:B:361:ARG:NH1[1_656]	1.69	0.51
1:A:398:LEU:O	1:B:1007:ARG:NH2[2_445]	1.73	0.47
1:B:219:GLN:C	1:B:944:LEU:CD1[1_554]	1.76	0.44
1:A:399:GLN:NE2	1:B:1007:ARG:CB[2_445]	1.80	0.40
1:A:399:GLN:CA	1:B:1007:ARG:NH2[2_445]	1.80	0.40
1:A:398:LEU:C	1:B:1007:ARG:NH1[2_445]	1.82	0.38
1:A:399:GLN:CD	1:B:1007:ARG:CG[2_445]	1.82	0.38
1:B:177:GLY:C	1:B:847:ALA:CB[1_554]	1.82	0.38
1:A:399:GLN:N	1:B:1007:ARG:NE[2_445]	1.84	0.36
1:B:219:GLN:CB	1:B:944:LEU:CD2[1_554]	1.84	0.36
1:A:398:LEU:O	1:B:1007:ARG:CZ[2_445]	1.86	0.34
1:B:219:GLN:CA	1:B:944:LEU:CD1[1_554]	1.87	0.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:PRO:O	1:B:847:ALA:N[1_554]	1.89	0.31
1:A:962:TYR:OH	1:B:361:ARG:CZ[1_656]	1.97	0.23
1:B:176:PRO:CG	1:B:846:PRO:CG[1_554]	1.99	0.21
1:A:399:GLN:CG	1:B:1007:ARG:CG[2_445]	2.00	0.20
1:A:398:LEU:CA	1:B:1007:ARG:NH2[2_445]	2.01	0.19
1:B:176:PRO:CA	1:B:845:SER:OG[1_554]	2.01	0.19
1:B:176:PRO:CB	1:B:845:SER:OG[1_554]	2.03	0.17
1:A:962:TYR:CE2	1:B:361:ARG:NH1[1_656]	2.04	0.16
1:B:177:GLY:CA	1:B:847:ALA:CA[1_554]	2.04	0.16
1:B:219:GLN:O	1:B:944:LEU:CG[1_554]	2.04	0.16
1:B:176:PRO:O	1:B:846:PRO:CG[1_554]	2.07	0.13
1:B:219:GLN:N	1:B:944:LEU:CD1[1_554]	2.07	0.13
1:B:176:PRO:CD	1:B:846:PRO:CG[1_554]	2.11	0.09
1:A:399:GLN:CA	1:B:1007:ARG:CZ[2_445]	2.12	0.08
1:A:399:GLN:CG	1:B:1007:ARG:NE[2_445]	2.13	0.07
1:A:182:LYS:CE	1:A:844:ASP:OD1[1_455]	2.15	0.05
1:A:1093:MET:CE	1:B:376:ARG:O[1_656]	2.17	0.03
1:A:399:GLN:NE2	1:B:1007:ARG:CA[2_445]	2.19	0.01
1:A:549:GLU:O	1:A:1207:GLU:OE2[2_545]	2.19	0.01

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	1155/1212 (95%)	1049 (91%)	92 (8%)	14 (1%)	10	44
1	B	1161/1212 (96%)	1048 (90%)	96 (8%)	17 (2%)	8	39
All	All	2316/2424 (96%)	2097 (90%)	188 (8%)	31 (1%)	9	42

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	PRO

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Mol	Chain	Res	Type
1	A	95	PRO
1	A	411	GLN
1	A	869	PRO
1	A	915	ALA
1	A	1192	SER
1	B	86	PRO
1	B	95	PRO
1	B	411	GLN
1	B	869	PRO
1	B	915	ALA
1	B	1147	ASP
1	B	1148	PRO
1	B	1192	SER
1	A	251	GLU
1	A	1053	PRO
1	A	1182	SER
1	B	251	GLU
1	B	1053	PRO
1	B	1182	SER
1	A	694	LEU
1	B	694	LEU
1	A	966	PRO
1	B	966	PRO
1	A	318	PRO
1	A	1108	ASP
1	B	318	PRO
1	B	1108	ASP
1	B	957	VAL
1	A	774	GLY
1	B	774	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1015/1051 (97%)	963 (95%)	52 (5%)	21	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1015/1051 (97%)	963 (95%)	52 (5%)	21	42
All	All	2030/2102 (97%)	1926 (95%)	104 (5%)	21	42

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	THR
1	A	78	LEU
1	A	118	LEU
1	A	125	LEU
1	A	128	CYS
1	A	136	CYS
1	A	152	HIS
1	A	207	ASN
1	A	257	LEU
1	A	259	LEU
1	A	274	HIS
1	A	280	ILE
1	A	298	ILE
1	A	300	CYS
1	A	310	VAL
1	A	330	GLU
1	A	334	VAL
1	A	360	LEU
1	A	387	LEU
1	A	411	GLN
1	A	413	LEU
1	A	422	THR
1	A	514	VAL
1	A	517	THR
1	A	562	VAL
1	A	580	LEU
1	A	594	VAL
1	A	652	VAL
1	A	661	VAL
1	A	683	VAL
1	A	707	ILE
1	A	765	CYS
1	A	812	GLN
1	A	814	CYS
1	A	821	ASP
1	A	837	LEU

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Mol	Chain	Res	Type
1	A	854	HIS
1	A	860	THR
1	A	867	LEU
1	A	882	ILE
1	A	890	ARG
1	A	929	ARG
1	A	934	LEU
1	A	937	VAL
1	A	949	LEU
1	A	977	ILE
1	A	982	SER
1	A	1018	THR
1	A	1030	ARG
1	A	1033	LEU
1	A	1048	ILE
1	A	1079	ILE
1	B	77	THR
1	B	78	LEU
1	B	118	LEU
1	B	125	LEU
1	B	128	CYS
1	B	136	CYS
1	B	152	HIS
1	B	207	ASN
1	B	257	LEU
1	B	259	LEU
1	B	274	HIS
1	B	280	ILE
1	B	298	ILE
1	B	300	CYS
1	B	310	VAL
1	B	330	GLU
1	B	334	VAL
1	B	360	LEU
1	B	387	LEU
1	B	411	GLN
1	B	413	LEU
1	B	422	THR
1	B	514	VAL
1	B	517	THR
1	B	562	VAL
1	B	580	LEU

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Mol	Chain	Res	Type
1	B	594	VAL
1	B	652	VAL
1	B	661	VAL
1	B	683	VAL
1	B	707	ILE
1	B	765	CYS
1	B	812	GLN
1	B	814	CYS
1	B	821	ASP
1	B	837	LEU
1	B	854	HIS
1	B	860	THR
1	B	867	LEU
1	B	882	ILE
1	B	890	ARG
1	B	929	ARG
1	B	934	LEU
1	B	937	VAL
1	B	949	LEU
1	B	977	ILE
1	B	982	SER
1	B	1018	THR
1	B	1030	ARG
1	B	1033	LEU
1	B	1048	ILE
1	B	1079	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	156	HIS
1	A	260	GLN
1	A	441	GLN
1	A	536	HIS
1	A	542	GLN
1	A	563	GLN
1	A	616	HIS
1	A	663	GLN
1	A	706	GLN
1	A	729	ASN
1	A	764	GLN

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Mol	Chain	Res	Type
1	A	766	GLN
1	A	899	HIS
1	A	931	HIS
1	A	983	HIS
1	A	1035	ASN
1	B	57	GLN
1	B	156	HIS
1	B	260	GLN
1	B	441	GLN
1	B	536	HIS
1	B	542	GLN
1	B	563	GLN
1	B	586	ASN
1	B	616	HIS
1	B	663	GLN
1	B	686	ASN
1	B	706	GLN
1	B	729	ASN
1	B	764	GLN
1	B	766	GLN
1	B	791	ASN
1	B	899	HIS
1	B	931	HIS
1	B	1027	ASN
1	B	1035	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

79 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	C	1	2,1	14,14,15	0.80	0	17,19,21	1.74	3 (17%)
2	NAG	C	2	2	14,14,15	0.57	0	17,19,21	1.54	2 (11%)
2	BMA	C	3	2	11,11,12	0.64	0	15,15,17	0.72	0
2	MAN	C	4	2	11,11,12	0.62	0	15,15,17	0.93	1 (6%)
3	NAG	D	1	1,3	14,14,15	0.65	0	17,19,21	1.20	1 (5%)
3	NAG	D	2	3	14,14,15	0.49	0	17,19,21	1.25	1 (5%)
3	BMA	D	3	3	11,11,12	0.53	0	15,15,17	0.56	0
3	MAN	D	4	3	11,11,12	0.66	0	15,15,17	0.88	1 (6%)
3	MAN	D	5	3	11,11,12	0.56	0	15,15,17	1.17	2 (13%)
2	NAG	E	1	2,1	14,14,15	0.65	0	17,19,21	1.27	1 (5%)
2	NAG	E	2	2	14,14,15	0.58	0	17,19,21	1.21	2 (11%)
2	BMA	E	3	2	11,11,12	0.80	1 (9%)	15,15,17	1.92	3 (20%)
2	MAN	E	4	2	11,11,12	0.57	0	15,15,17	1.01	1 (6%)
4	NAG	F	1	4,1	14,14,15	0.67	0	17,19,21	1.18	1 (5%)
4	NAG	F	2	4	14,14,15	0.53	0	17,19,21	1.16	2 (11%)
4	BMA	F	3	4	11,11,12	0.58	0	15,15,17	1.54	3 (20%)
4	MAN	F	4	4	11,11,12	0.60	0	15,15,17	0.87	1 (6%)
4	MAN	F	5	4	11,11,12	0.52	0	15,15,17	1.22	1 (6%)
4	MAN	F	6	4	11,11,12	0.56	0	15,15,17	1.29	2 (13%)
4	MAN	F	7	4	11,11,12	0.58	0	15,15,17	0.84	1 (6%)
5	NAG	G	1	5,1	14,14,15	0.64	0	17,19,21	1.05	1 (5%)
5	NAG	G	2	5	14,14,15	0.67	0	17,19,21	1.12	1 (5%)
5	BMA	G	3	5	11,11,12	0.42	0	15,15,17	1.64	2 (13%)
5	NAG	H	1	5,1	14,14,15	0.57	0	17,19,21	1.11	1 (5%)
5	NAG	H	2	5	14,14,15	0.57	0	17,19,21	1.18	2 (11%)
5	BMA	H	3	5	11,11,12	0.47	0	15,15,17	1.12	2 (13%)
3	NAG	I	1	1,3	14,14,15	0.58	0	17,19,21	1.07	1 (5%)
3	NAG	I	2	3	14,14,15	0.58	0	17,19,21	1.12	1 (5%)
3	BMA	I	3	3	11,11,12	0.52	0	15,15,17	1.17	2 (13%)
3	MAN	I	4	3	11,11,12	0.72	0	15,15,17	1.18	1 (6%)
3	MAN	I	5	3	11,11,12	0.59	0	15,15,17	1.00	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	J	1	4,1	14,14,15	0.66	0	17,19,21	1.29	2 (11%)
4	NAG	J	2	4	14,14,15	0.53	0	17,19,21	1.45	3 (17%)
4	BMA	J	3	4	11,11,12	0.37	0	15,15,17	0.75	1 (6%)
4	MAN	J	4	4	11,11,12	0.61	0	15,15,17	0.89	0
4	MAN	J	5	4	11,11,12	0.61	0	15,15,17	1.13	1 (6%)
4	MAN	J	6	4	11,11,12	0.63	0	15,15,17	0.96	1 (6%)
4	MAN	J	7	4	11,11,12	0.60	0	15,15,17	1.04	2 (13%)
2	NAG	K	1	2,1	14,14,15	0.80	0	17,19,21	1.74	3 (17%)
2	NAG	K	2	2	14,14,15	0.58	0	17,19,21	1.53	1 (5%)
2	BMA	K	3	2	11,11,12	0.63	0	15,15,17	0.73	0
2	MAN	K	4	2	11,11,12	0.62	0	15,15,17	0.93	1 (6%)
6	NAG	L	1	6,1	14,14,15	0.65	0	17,19,21	1.20	1 (5%)
6	NAG	L	2	6	14,14,15	0.50	0	17,19,21	1.25	1 (5%)
6	BMA	L	3	6	11,11,12	0.52	0	15,15,17	0.58	0
6	MAN	L	4	6	11,11,12	0.66	0	15,15,17	0.89	1 (6%)
6	MAN	L	5	6	11,11,12	0.56	0	15,15,17	1.17	2 (13%)
6	MAN	L	6	6	11,11,12	0.58	0	15,15,17	1.02	1 (6%)
2	NAG	M	1	2,1	14,14,15	0.65	0	17,19,21	1.26	1 (5%)
2	NAG	M	2	2	14,14,15	0.55	0	17,19,21	1.23	2 (11%)
2	BMA	M	3	2	11,11,12	0.80	1 (9%)	15,15,17	1.92	3 (20%)
2	MAN	M	4	2	11,11,12	0.57	0	15,15,17	1.00	1 (6%)
4	NAG	N	1	4,1	14,14,15	0.66	0	17,19,21	1.19	1 (5%)
4	NAG	N	2	4	14,14,15	0.54	0	17,19,21	1.15	2 (11%)
4	BMA	N	3	4	11,11,12	0.60	0	15,15,17	1.53	3 (20%)
4	MAN	N	4	4	11,11,12	0.62	0	15,15,17	0.86	0
4	MAN	N	5	4	11,11,12	0.53	0	15,15,17	1.23	1 (6%)
4	MAN	N	6	4	11,11,12	0.57	0	15,15,17	1.28	2 (13%)
4	MAN	N	7	4	11,11,12	0.57	0	15,15,17	0.83	1 (6%)
2	NAG	O	1	2,1	14,14,15	0.63	0	17,19,21	1.06	1 (5%)
2	NAG	O	2	2	14,14,15	0.68	0	17,19,21	1.11	1 (5%)
2	BMA	O	3	2	11,11,12	0.43	0	15,15,17	1.64	2 (13%)
2	MAN	O	4	2	11,11,12	0.54	0	15,15,17	0.87	1 (6%)
5	NAG	P	1	5,1	14,14,15	0.58	0	17,19,21	1.11	1 (5%)
5	NAG	P	2	5	14,14,15	0.56	0	17,19,21	1.19	2 (11%)
5	BMA	P	3	5	11,11,12	0.47	0	15,15,17	1.13	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	Q	1	6,1	14,14,15	0.61	0	17,19,21	1.07	1 (5%)
6	NAG	Q	2	6	14,14,15	0.59	0	17,19,21	1.13	1 (5%)
6	BMA	Q	3	6	11,11,12	0.53	0	15,15,17	1.17	2 (13%)
6	MAN	Q	4	6	11,11,12	0.73	0	15,15,17	1.18	2 (13%)
6	MAN	Q	5	6	11,11,12	0.59	0	15,15,17	1.00	2 (13%)
6	MAN	Q	6	6	11,11,12	0.64	0	15,15,17	0.80	0
4	NAG	R	1	4,1	14,14,15	0.67	0	17,19,21	1.30	2 (11%)
4	NAG	R	2	4	14,14,15	0.53	0	17,19,21	1.46	3 (17%)
4	BMA	R	3	4	11,11,12	0.39	0	15,15,17	0.75	1 (6%)
4	MAN	R	4	4	11,11,12	0.62	0	15,15,17	0.89	0
4	MAN	R	5	4	11,11,12	0.61	0	15,15,17	1.14	1 (6%)
4	MAN	R	6	4	11,11,12	0.62	0	15,15,17	0.96	1 (6%)
4	MAN	R	7	4	11,11,12	0.61	0	15,15,17	1.04	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	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	1/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
3	MAN	D	5	3	-	0/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
4	NAG	F	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
4	MAN	F	4	4	-	1/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	F	6	4	-	0/2/19/22	0/1/1/1
4	MAN	F	7	4	-	2/2/19/22	0/1/1/1
5	NAG	G	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	2/2/19/22	0/1/1/1
5	NAG	H	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	BMA	H	3	5	-	2/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	BMA	I	3	3	-	1/2/19/22	0/1/1/1
3	MAN	I	4	3	-	2/2/19/22	0/1/1/1
3	MAN	I	5	3	-	1/2/19/22	0/1/1/1
4	NAG	J	1	4,1	1/1/5/7	2/6/23/26	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	MAN	J	4	4	-	0/2/19/22	0/1/1/1
4	MAN	J	5	4	-	2/2/19/22	0/1/1/1
4	MAN	J	6	4	-	1/2/19/22	0/1/1/1
4	MAN	J	7	4	-	2/2/19/22	0/1/1/1
2	NAG	K	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	BMA	K	3	2	-	2/2/19/22	0/1/1/1
2	MAN	K	4	2	-	1/2/19/22	0/1/1/1
6	NAG	L	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	L	2	6	-	1/6/23/26	0/1/1/1
6	BMA	L	3	6	-	0/2/19/22	0/1/1/1
6	MAN	L	4	6	-	2/2/19/22	0/1/1/1
6	MAN	L	5	6	-	0/2/19/22	0/1/1/1
6	MAN	L	6	6	-	0/2/19/22	0/1/1/1
2	NAG	M	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	BMA	M	3	2	-	0/2/19/22	0/1/1/1
2	MAN	M	4	2	-	0/2/19/22	0/1/1/1
4	NAG	N	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	BMA	N	3	4	-	2/2/19/22	0/1/1/1
4	MAN	N	4	4	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	N	5	4	-	0/2/19/22	0/1/1/1
4	MAN	N	6	4	-	0/2/19/22	0/1/1/1
4	MAN	N	7	4	-	2/2/19/22	0/1/1/1
2	NAG	O	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	2/6/23/26	0/1/1/1
2	BMA	O	3	2	-	2/2/19/22	0/1/1/1
2	MAN	O	4	2	-	1/2/19/22	0/1/1/1
5	NAG	P	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1
5	BMA	P	3	5	-	2/2/19/22	0/1/1/1
6	NAG	Q	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	2/6/23/26	0/1/1/1
6	BMA	Q	3	6	-	1/2/19/22	0/1/1/1
6	MAN	Q	4	6	-	2/2/19/22	0/1/1/1
6	MAN	Q	5	6	-	1/2/19/22	0/1/1/1
6	MAN	Q	6	6	-	1/2/19/22	0/1/1/1
4	NAG	R	1	4,1	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
4	BMA	R	3	4	-	1/2/19/22	0/1/1/1
4	MAN	R	4	4	-	0/2/19/22	0/1/1/1
4	MAN	R	5	4	-	2/2/19/22	0/1/1/1
4	MAN	R	6	4	-	1/2/19/22	0/1/1/1
4	MAN	R	7	4	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	3	BMA	C2-C3	2.06	1.55	1.52
2	E	3	BMA	C2-C3	2.06	1.55	1.52

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	3	BMA	C1-C2-C3	6.14	118.58	109.64
2	E	3	BMA	C1-C2-C3	6.11	118.54	109.64
2	C	1	NAG	C4-C3-C2	5.16	118.58	111.02
2	K	1	NAG	C4-C3-C2	5.16	118.58	111.02
2	C	2	NAG	C4-C3-C2	4.90	118.20	111.02
2	K	2	NAG	C4-C3-C2	4.87	118.16	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	3	BMA	C1-O5-C5	4.69	118.47	112.19
5	G	3	BMA	C1-O5-C5	4.66	118.43	112.19
4	N	5	MAN	C1-O5-C5	4.29	117.93	112.19
4	F	5	MAN	C1-O5-C5	4.25	117.88	112.19
2	M	1	NAG	C4-C3-C2	4.07	116.99	111.02
2	E	1	NAG	C4-C3-C2	4.07	116.99	111.02
6	L	2	NAG	C1-O5-C5	4.04	117.59	112.19
3	D	2	NAG	C1-O5-C5	4.02	117.57	112.19
4	N	1	NAG	C4-C3-C2	3.98	116.84	111.02
4	F	1	NAG	C4-C3-C2	3.96	116.82	111.02
4	F	6	MAN	C1-O5-C5	3.71	117.16	112.19
4	F	3	BMA	C3-C4-C5	3.70	116.93	110.23
4	N	6	MAN	C1-O5-C5	3.69	117.14	112.19
4	N	3	BMA	C3-C4-C5	3.66	116.87	110.23
3	I	4	MAN	C1-C2-C3	3.55	114.81	109.64
6	Q	4	MAN	C1-C2-C3	3.54	114.81	109.64
3	D	5	MAN	C1-O5-C5	3.40	116.74	112.19
6	L	5	MAN	C1-O5-C5	3.40	116.74	112.19
3	I	1	NAG	C1-O5-C5	3.32	116.64	112.19
6	Q	1	NAG	C1-O5-C5	3.32	116.64	112.19
5	P	1	NAG	C4-C3-C2	3.31	115.86	111.02
5	H	1	NAG	C4-C3-C2	3.29	115.84	111.02
5	P	3	BMA	C1-O5-C5	3.25	116.54	112.19
5	H	3	BMA	C1-O5-C5	3.18	116.45	112.19
2	O	3	BMA	C1-C2-C3	3.18	114.27	109.64
5	G	3	BMA	C1-C2-C3	3.18	114.27	109.64
5	G	2	NAG	C4-C3-C2	3.06	115.51	111.02
2	O	1	NAG	C4-C3-C2	3.06	115.50	111.02
5	G	1	NAG	C4-C3-C2	3.03	115.46	111.02
4	J	2	NAG	C4-C3-C2	3.03	115.45	111.02
2	C	1	NAG	C3-C4-C5	3.03	115.72	110.23
4	R	2	NAG	C4-C3-C2	3.02	115.44	111.02
2	M	2	NAG	C1-O5-C5	3.01	116.23	112.19
2	O	2	NAG	C4-C3-C2	3.01	115.44	111.02
2	K	1	NAG	C3-C4-C5	3.00	115.68	110.23
5	P	2	NAG	C4-C3-C2	2.99	115.40	111.02
5	H	2	NAG	C4-C3-C2	2.99	115.39	111.02
2	E	2	NAG	C1-O5-C5	2.98	116.18	112.19
3	I	3	BMA	C3-C4-C5	2.96	115.60	110.23
4	N	3	BMA	C2-C3-C4	2.95	116.05	110.86
6	Q	3	BMA	C3-C4-C5	2.94	115.57	110.23
4	J	5	MAN	C1-C2-C3	2.94	113.92	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	5	MAN	C1-C2-C3	2.94	113.92	109.64
4	F	3	BMA	C2-C3-C4	2.92	116.00	110.86
4	R	2	NAG	C3-C4-C5	2.88	115.45	110.23
4	J	2	NAG	C3-C4-C5	2.87	115.43	110.23
6	L	1	NAG	C4-C3-C2	2.86	115.20	111.02
6	L	6	MAN	C1-O5-C5	2.85	116.01	112.19
3	D	1	NAG	C4-C3-C2	2.80	115.12	111.02
4	F	3	BMA	C1-C2-C3	2.71	113.59	109.64
2	E	2	NAG	C4-C3-C2	2.69	114.96	111.02
2	M	2	NAG	C4-C3-C2	2.69	114.96	111.02
4	N	3	BMA	C1-C2-C3	2.67	113.53	109.64
2	O	4	MAN	C1-O5-C5	2.60	115.67	112.19
4	R	2	NAG	O5-C1-C2	-2.57	107.32	111.29
4	J	2	NAG	O5-C1-C2	-2.54	107.36	111.29
3	I	5	MAN	C1-O5-C5	2.49	115.52	112.19
6	Q	5	MAN	C1-O5-C5	2.47	115.50	112.19
4	F	6	MAN	C1-C2-C3	2.47	113.25	109.64
4	J	7	MAN	C1-C2-C3	2.47	113.23	109.64
4	N	6	MAN	C1-C2-C3	2.45	113.22	109.64
3	D	5	MAN	C1-C2-C3	2.45	113.21	109.64
4	R	7	MAN	C1-C2-C3	2.44	113.20	109.64
6	L	5	MAN	C1-C2-C3	2.42	113.17	109.64
2	K	1	NAG	C2-N2-C7	2.41	126.13	122.90
2	C	1	NAG	C2-N2-C7	2.40	126.12	122.90
2	E	3	BMA	C2-C3-C4	2.37	115.04	110.86
4	R	1	NAG	C4-C3-C2	2.37	114.49	111.02
2	E	4	MAN	C1-O5-C5	2.36	115.35	112.19
4	R	6	MAN	C1-C2-C3	2.34	113.05	109.64
2	M	3	BMA	C2-C3-C4	2.34	114.97	110.86
4	R	7	MAN	C1-O5-C5	2.34	115.32	112.19
4	J	1	NAG	C4-C3-C2	2.33	114.44	111.02
4	J	6	MAN	C1-C2-C3	2.32	113.03	109.64
2	M	4	MAN	C1-O5-C5	2.32	115.30	112.19
5	P	2	NAG	O5-C1-C2	-2.29	107.75	111.29
4	J	7	MAN	C1-O5-C5	2.28	115.25	112.19
5	H	2	NAG	O5-C1-C2	-2.27	107.78	111.29
5	P	3	BMA	C1-C2-C3	2.24	112.91	109.64
4	F	7	MAN	C1-O5-C5	2.23	115.18	112.19
5	H	3	BMA	C1-C2-C3	2.23	112.89	109.64
6	Q	5	MAN	C1-C2-C3	2.23	112.89	109.64
4	N	7	MAN	C1-O5-C5	2.20	115.14	112.19
2	M	3	BMA	C1-O5-C5	2.20	115.13	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	BMA	C1-O5-C5	2.20	115.13	112.19
3	I	5	MAN	C1-C2-C3	2.19	112.83	109.64
6	L	4	MAN	C1-C2-C3	2.19	112.83	109.64
4	F	2	NAG	C3-C4-C5	2.18	114.19	110.23
3	D	4	MAN	C1-C2-C3	2.18	112.82	109.64
2	K	4	MAN	C1-C2-C3	2.17	112.81	109.64
2	C	4	MAN	C1-C2-C3	2.16	112.79	109.64
4	N	2	NAG	C3-C4-C5	2.15	114.12	110.23
6	Q	3	BMA	C2-C3-C4	2.14	114.62	110.86
3	I	3	BMA	C2-C3-C4	2.13	114.60	110.86
4	J	3	BMA	C1-O5-C5	2.10	115.00	112.19
4	R	3	BMA	C1-O5-C5	2.09	114.99	112.19
4	F	2	NAG	O5-C1-C2	-2.09	108.06	111.29
4	N	2	NAG	O5-C1-C2	-2.08	108.07	111.29
4	R	1	NAG	C2-N2-C7	2.07	125.68	122.90
6	Q	2	NAG	C2-N2-C7	2.07	125.68	122.90
3	I	2	NAG	C2-N2-C7	2.05	125.64	122.90
4	J	1	NAG	C2-N2-C7	2.02	125.61	122.90
4	F	4	MAN	O5-C5-C6	2.02	111.59	107.66
2	C	2	NAG	C1-C2-N2	-2.01	107.26	110.43
6	Q	4	MAN	O5-C5-C6	2.00	111.56	107.66

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	J	1	NAG	C1
4	R	1	NAG	C1

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	1	NAG	O5-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
5	G	3	BMA	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
2	O	3	BMA	O5-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
5	P	2	NAG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	R	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6
6	L	1	NAG	O5-C5-C6-O6
6	L	4	MAN	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
6	Q	2	NAG	O5-C5-C6-O6
2	O	3	BMA	C4-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
6	L	4	MAN	C4-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
5	G	3	BMA	C4-C5-C6-O6
6	L	1	NAG	C4-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
6	Q	2	NAG	C4-C5-C6-O6
4	N	3	BMA	O5-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
5	H	3	BMA	O5-C5-C6-O6
5	P	3	BMA	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
6	L	2	NAG	O5-C5-C6-O6
4	J	3	BMA	O5-C5-C6-O6
4	R	3	BMA	O5-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
5	P	1	NAG	C4-C5-C6-O6
4	F	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	N	3	BMA	C4-C5-C6-O6
4	J	7	MAN	C4-C5-C6-O6
4	R	7	MAN	C4-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	K	3	BMA	C4-C5-C6-O6
5	H	3	BMA	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
5	P	3	BMA	C4-C5-C6-O6
4	F	7	MAN	C4-C5-C6-O6
4	N	7	MAN	C4-C5-C6-O6
3	I	4	MAN	C4-C5-C6-O6
6	Q	4	MAN	C4-C5-C6-O6
4	J	5	MAN	C4-C5-C6-O6
4	R	5	MAN	C4-C5-C6-O6
4	J	7	MAN	O5-C5-C6-O6
4	R	7	MAN	O5-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
2	K	4	MAN	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
3	I	3	BMA	O5-C5-C6-O6
4	J	5	MAN	O5-C5-C6-O6
4	R	5	MAN	O5-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
5	P	1	NAG	O5-C5-C6-O6
6	Q	3	BMA	O5-C5-C6-O6
3	I	5	MAN	C4-C5-C6-O6
6	Q	5	MAN	C4-C5-C6-O6
4	N	7	MAN	O5-C5-C6-O6
4	F	7	MAN	O5-C5-C6-O6
3	I	4	MAN	O5-C5-C6-O6
6	Q	4	MAN	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	K	3	BMA	O5-C5-C6-O6
6	Q	6	MAN	C4-C5-C6-O6
4	F	4	MAN	O5-C5-C6-O6
4	N	4	MAN	O5-C5-C6-O6
4	J	6	MAN	C4-C5-C6-O6
4	R	6	MAN	C4-C5-C6-O6

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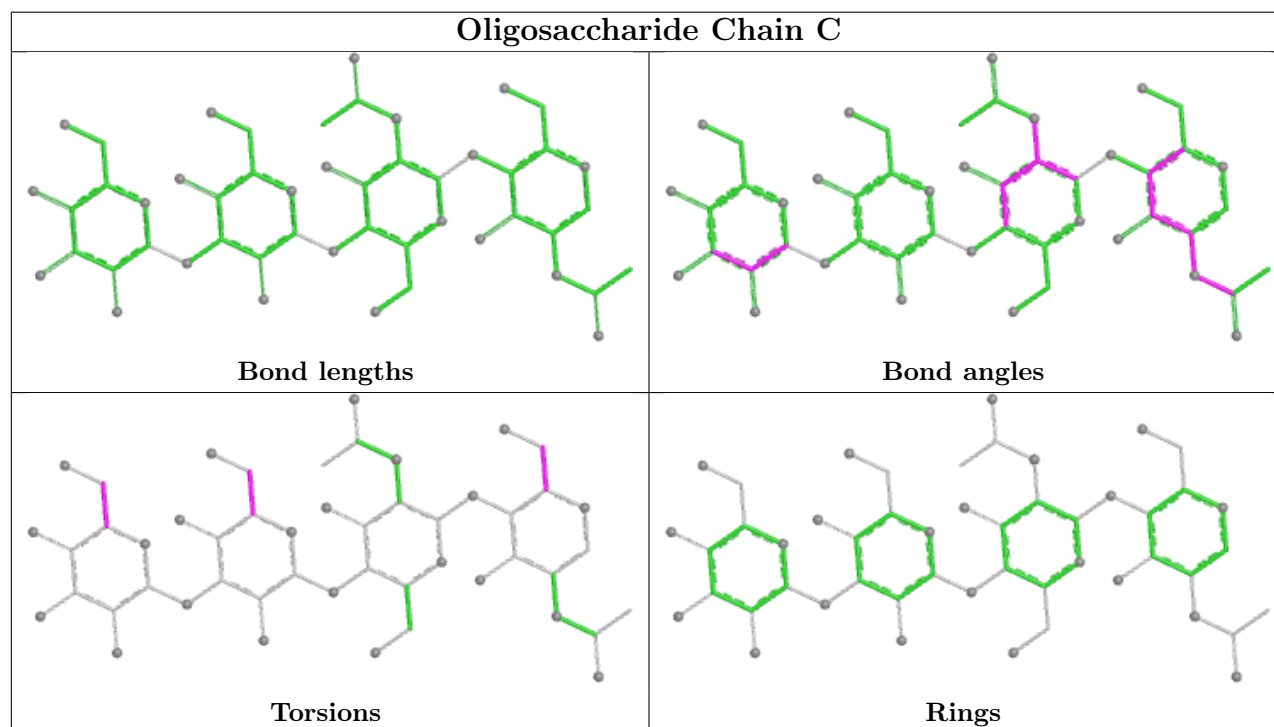
Mol	Chain	Res	Type	Atoms
2	O	4	MAN	C4-C5-C6-O6

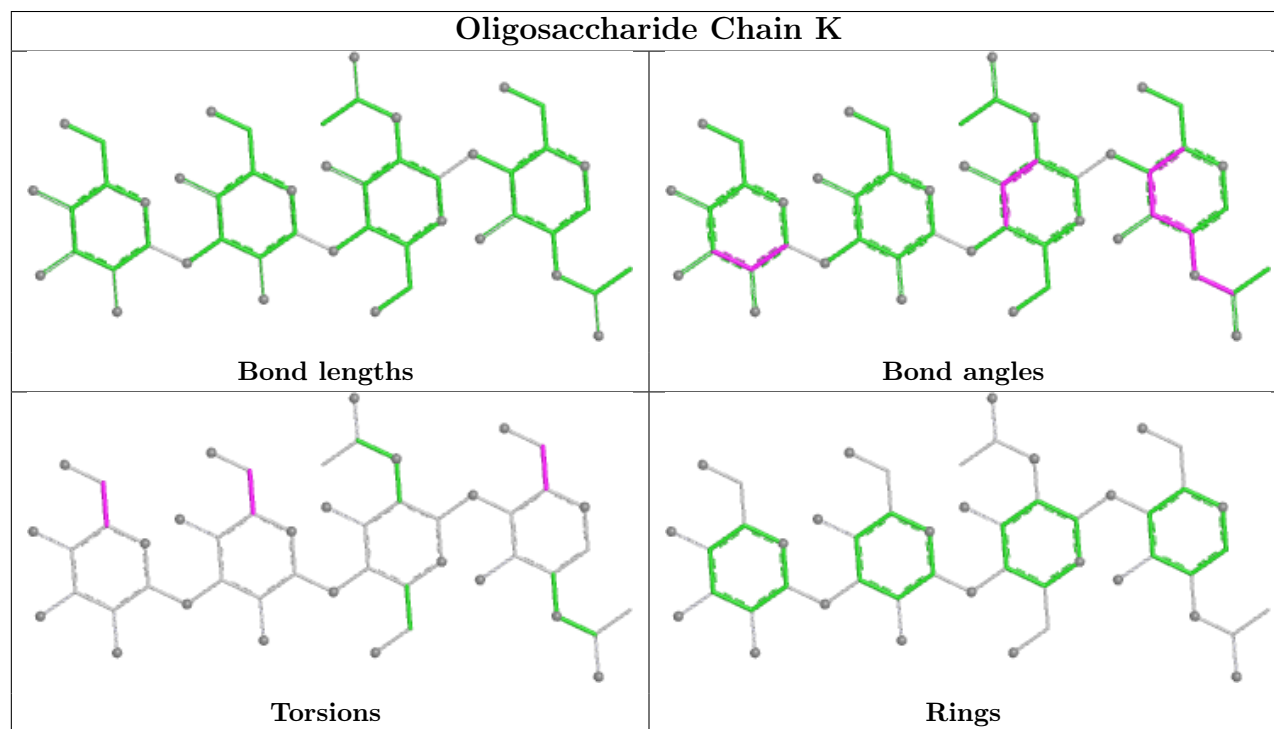
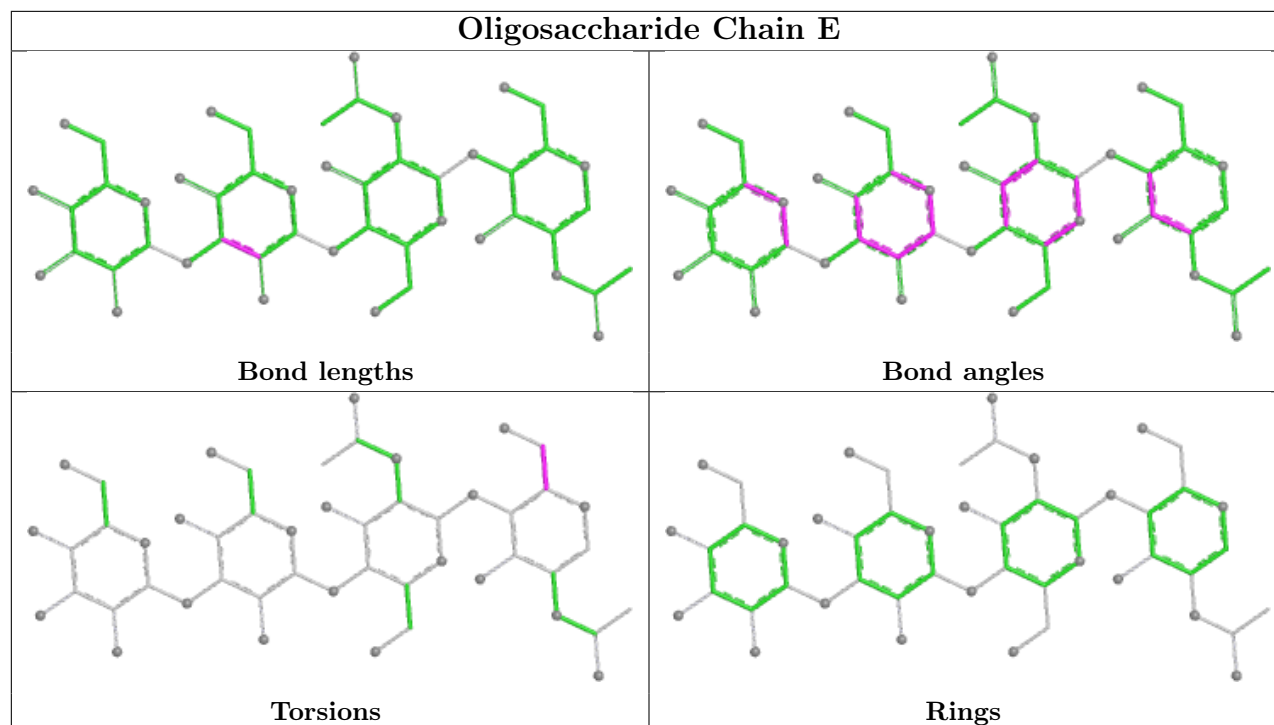
There are no ring outliers.

8 monomers are involved in 8 short contacts:

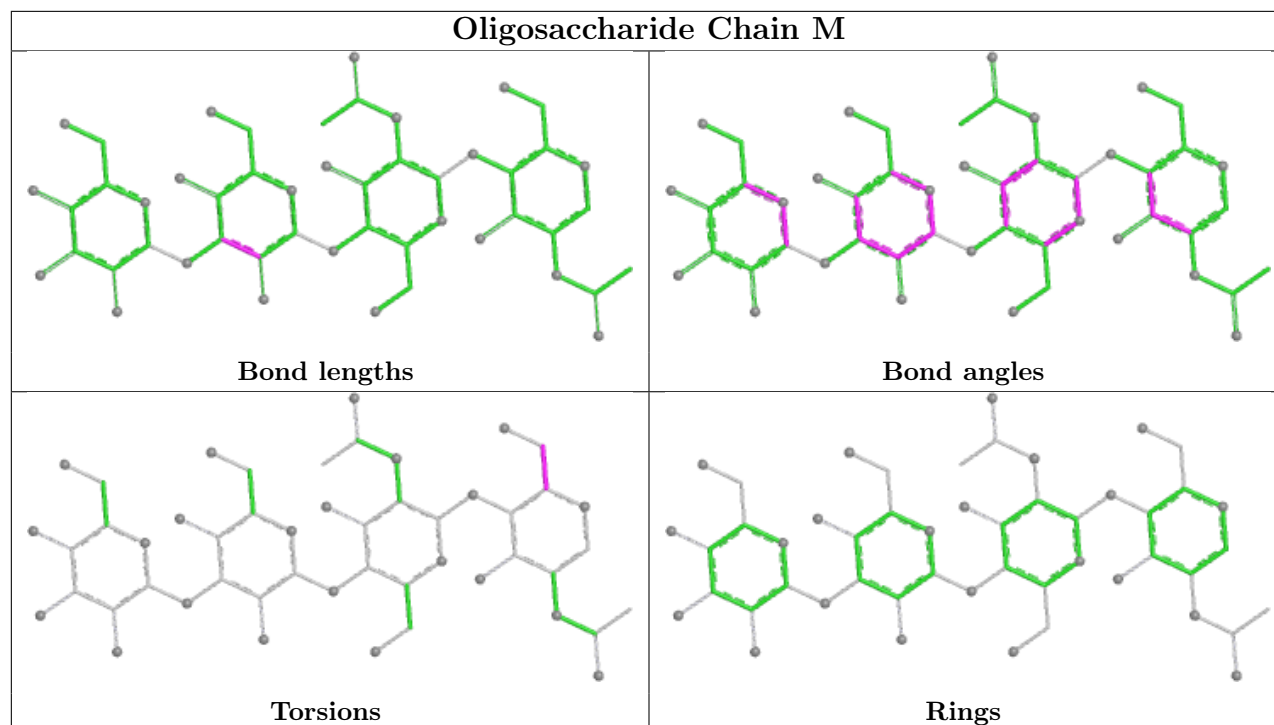
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
4	N	1	NAG	1	0
4	F	1	NAG	3	0
4	N	6	MAN	1	0
4	F	2	NAG	1	0
4	N	2	NAG	1	0
2	K	1	NAG	1	0
4	F	6	MAN	1	0

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

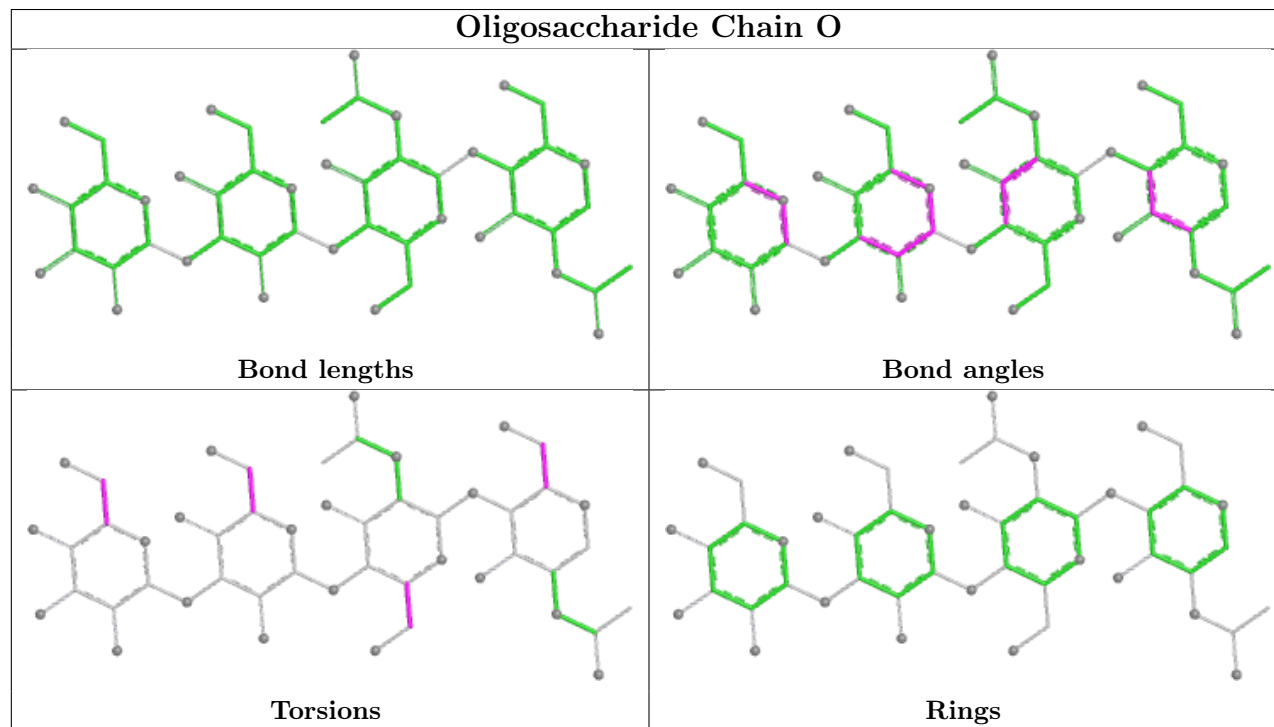


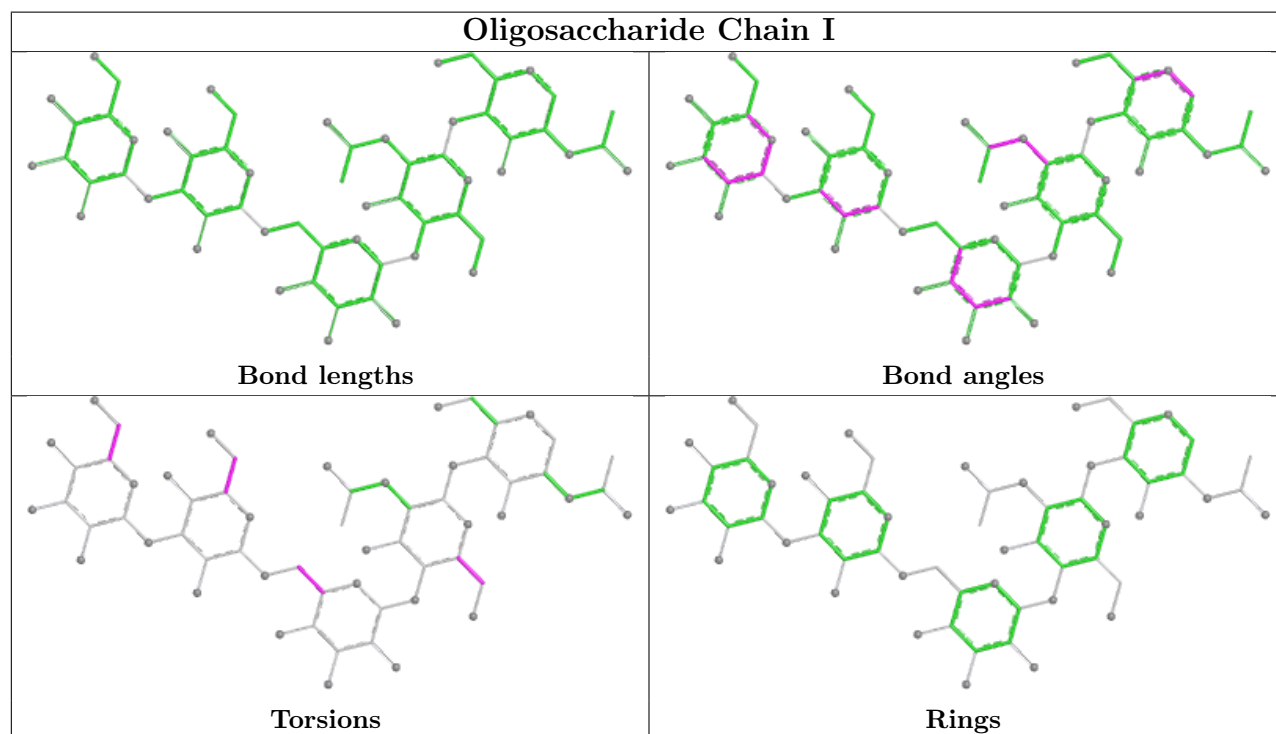
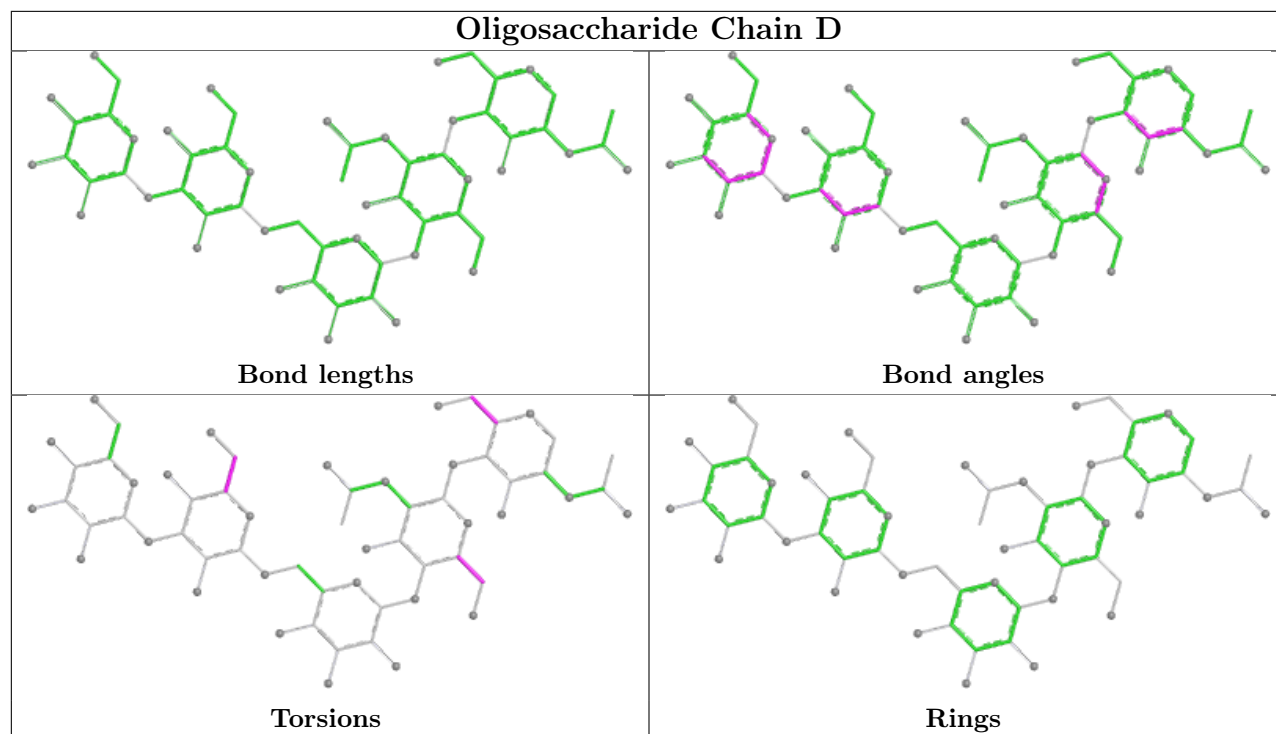


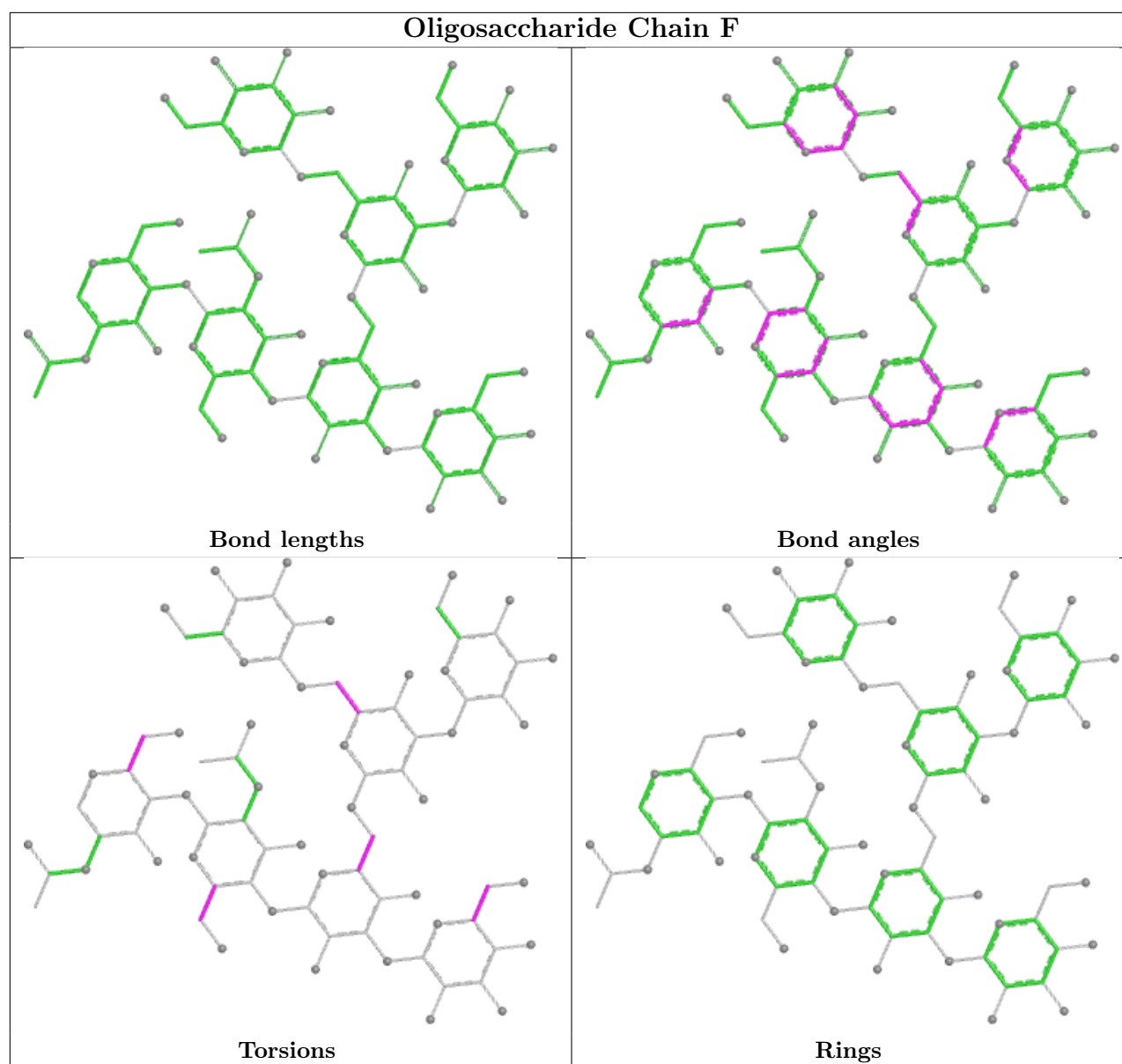
Oligosaccharide Chain M

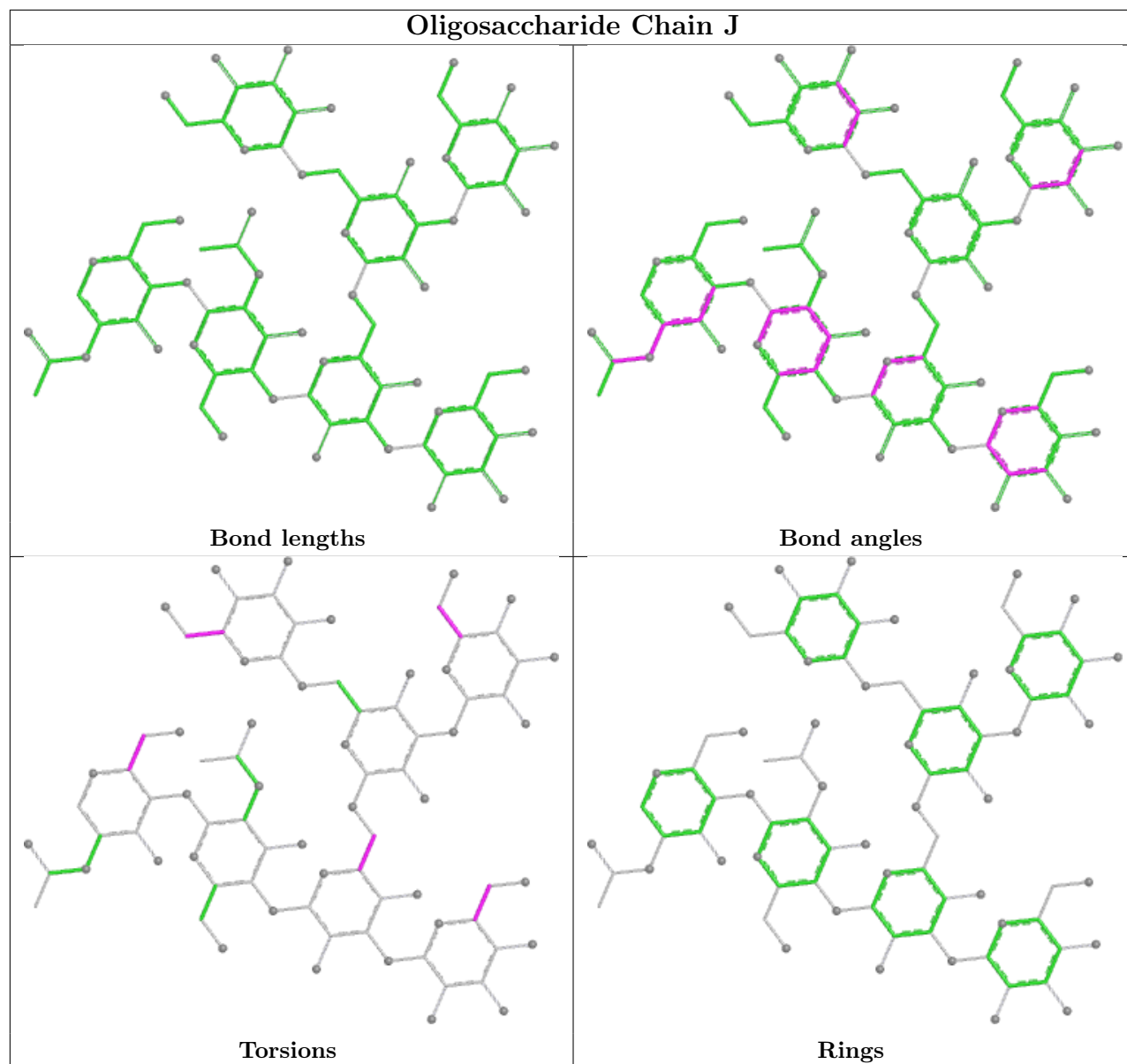


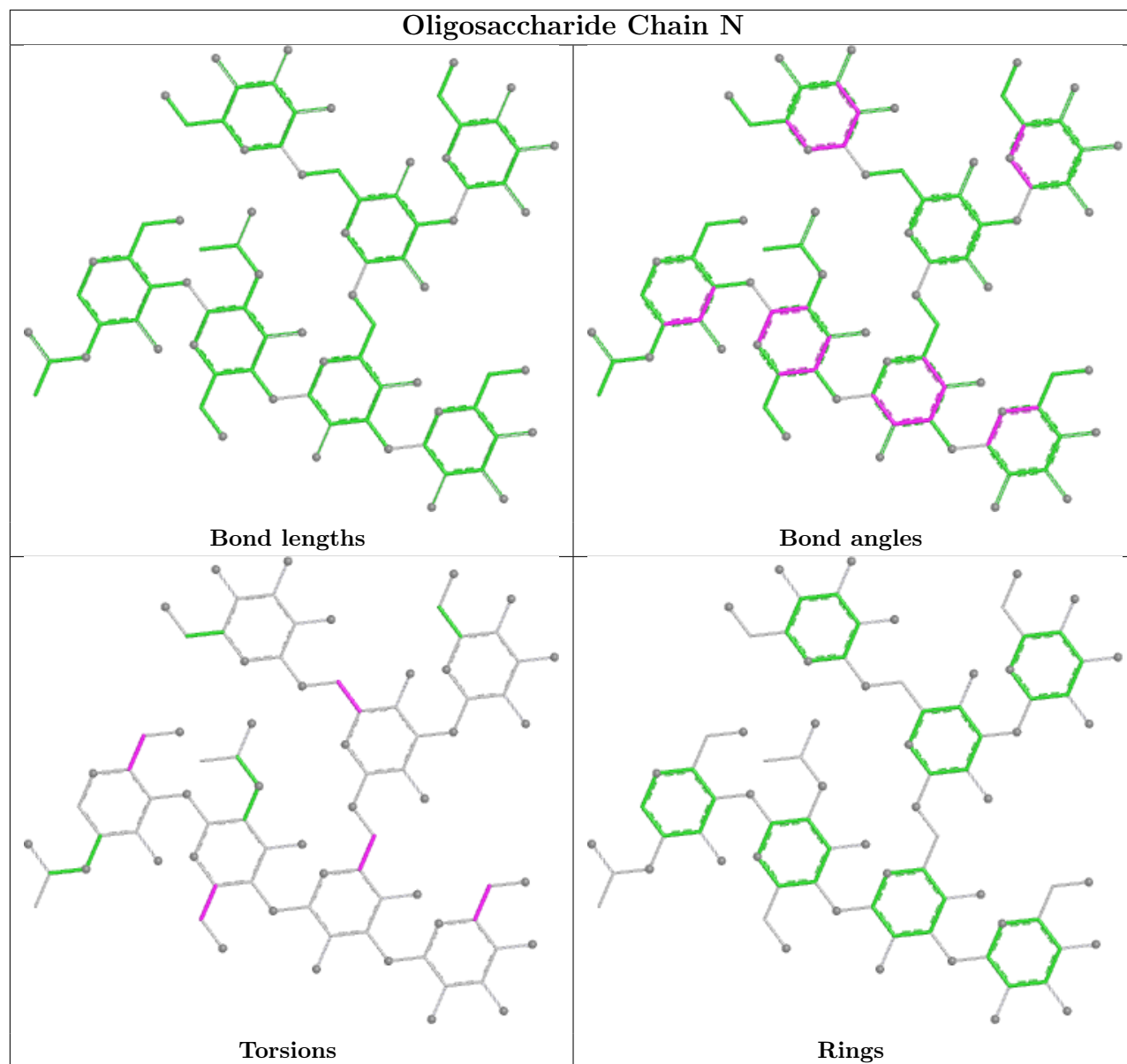
Oligosaccharide Chain O

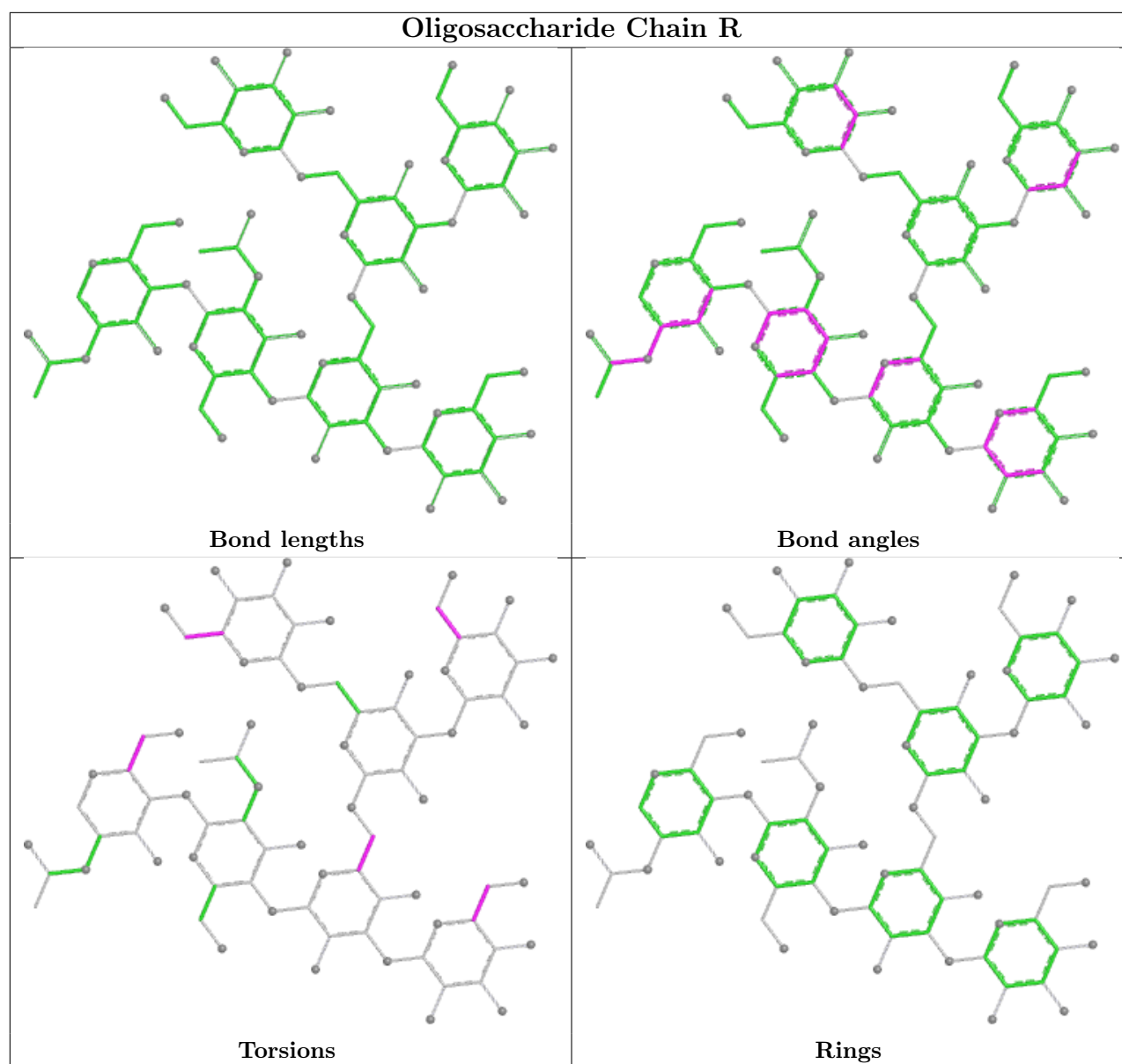


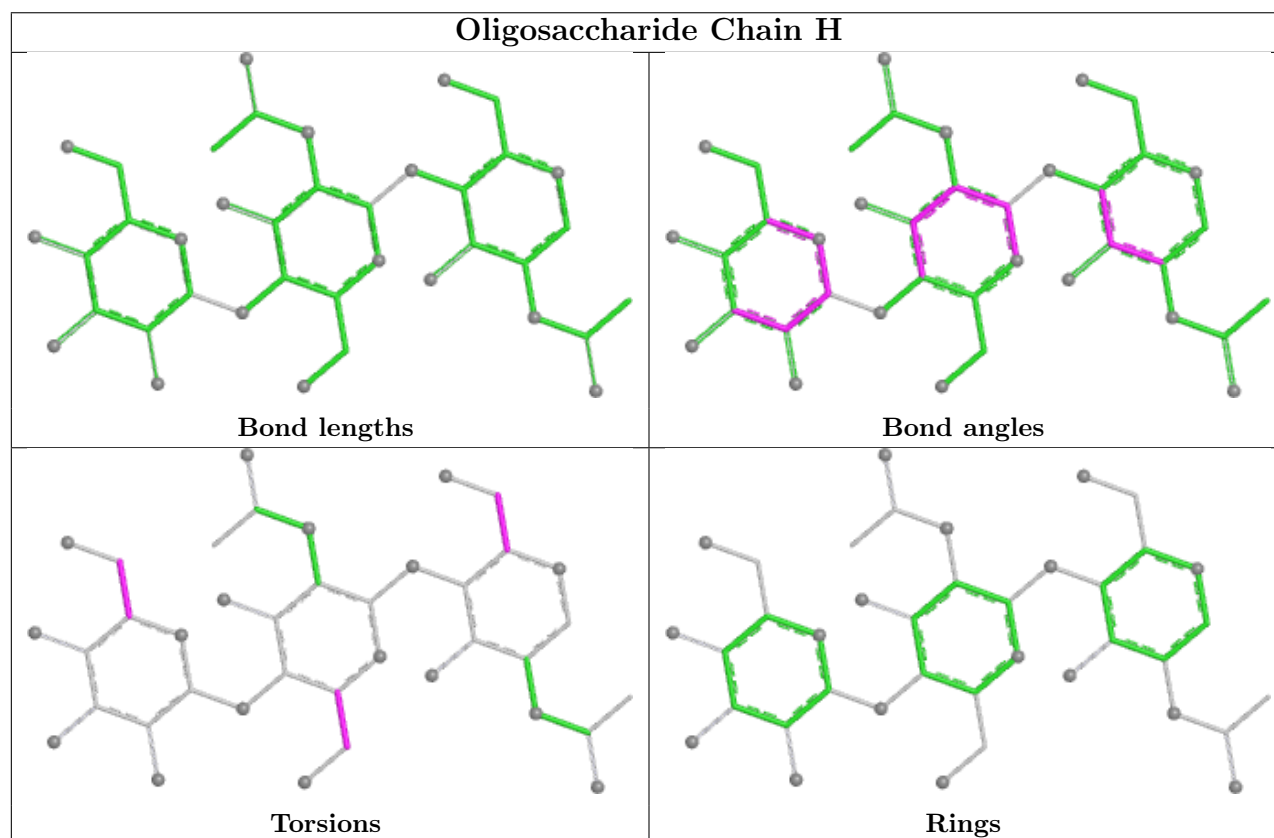
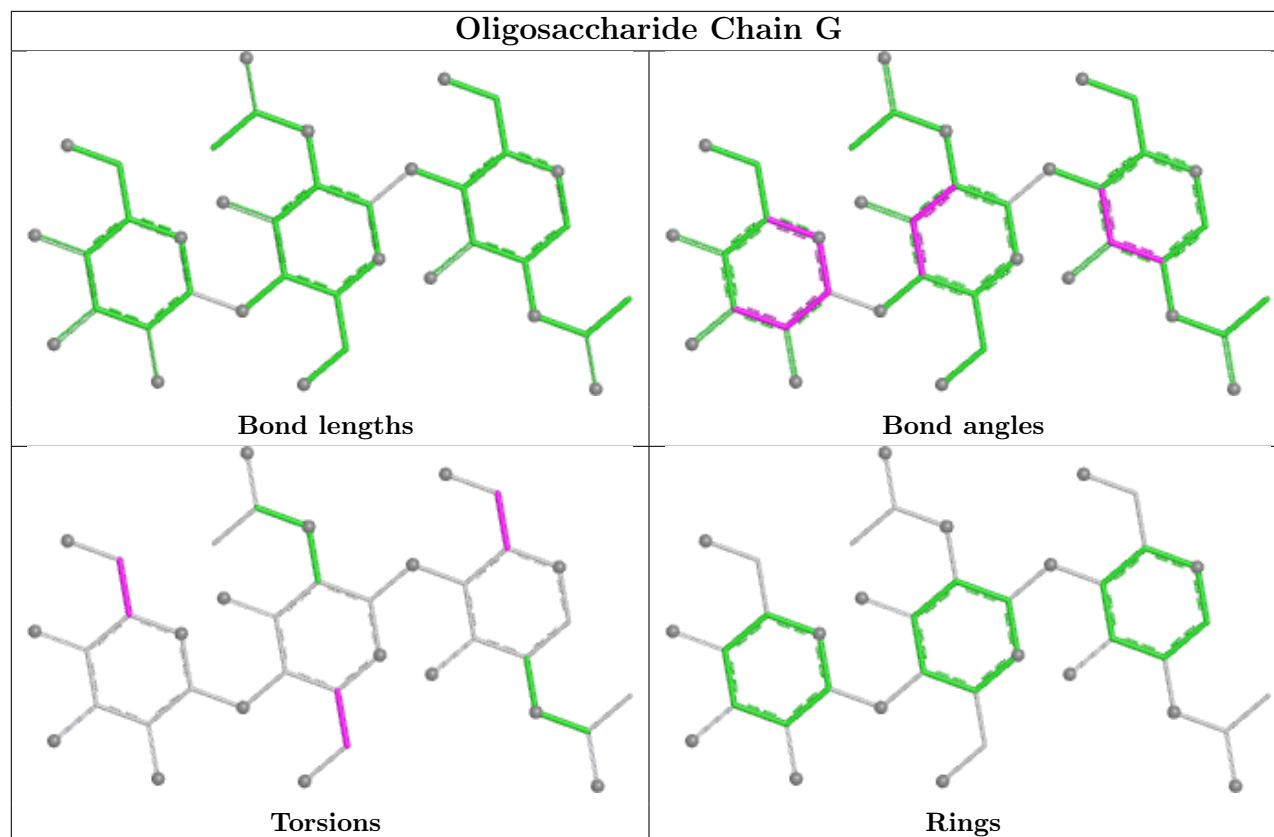


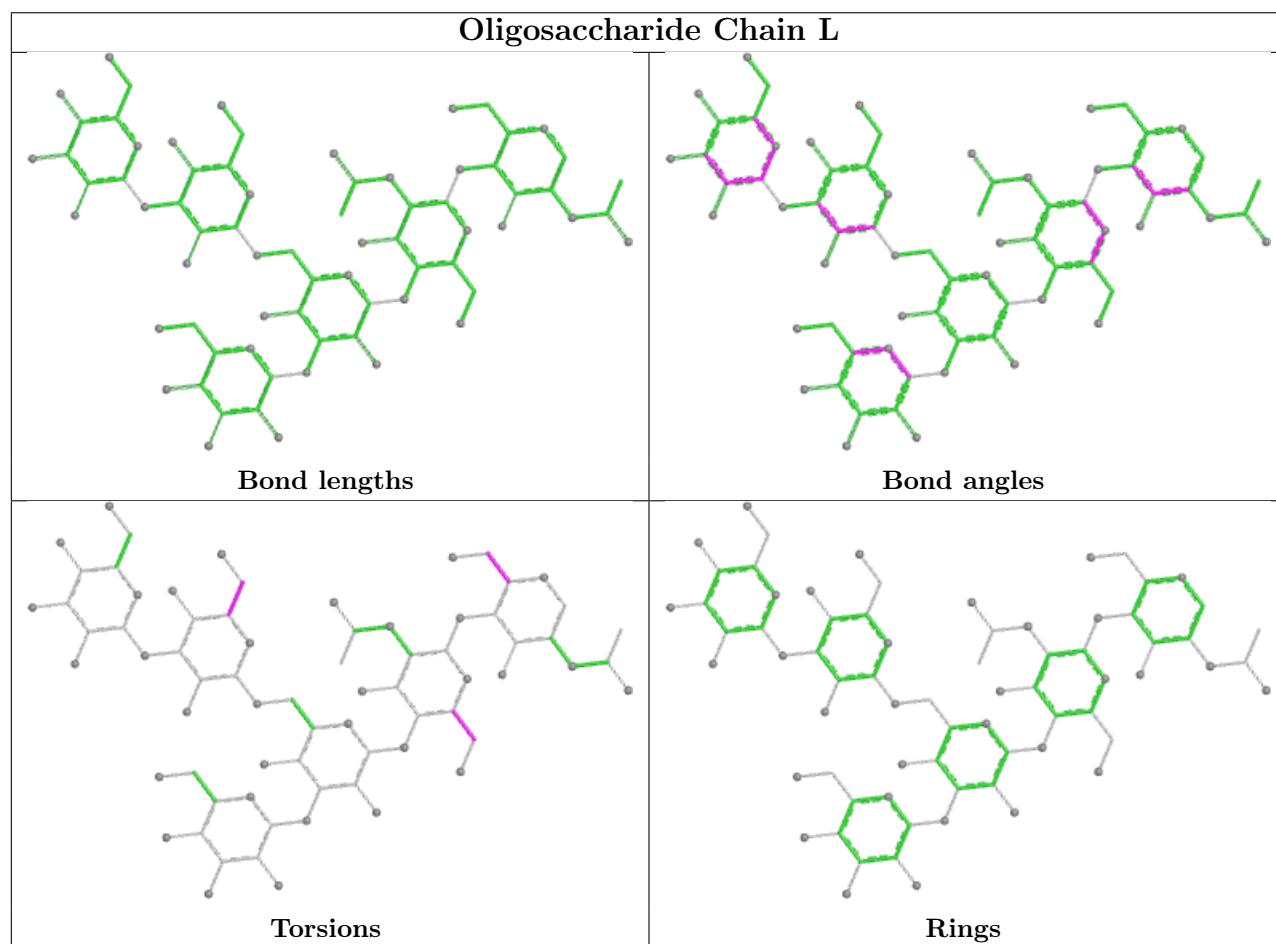
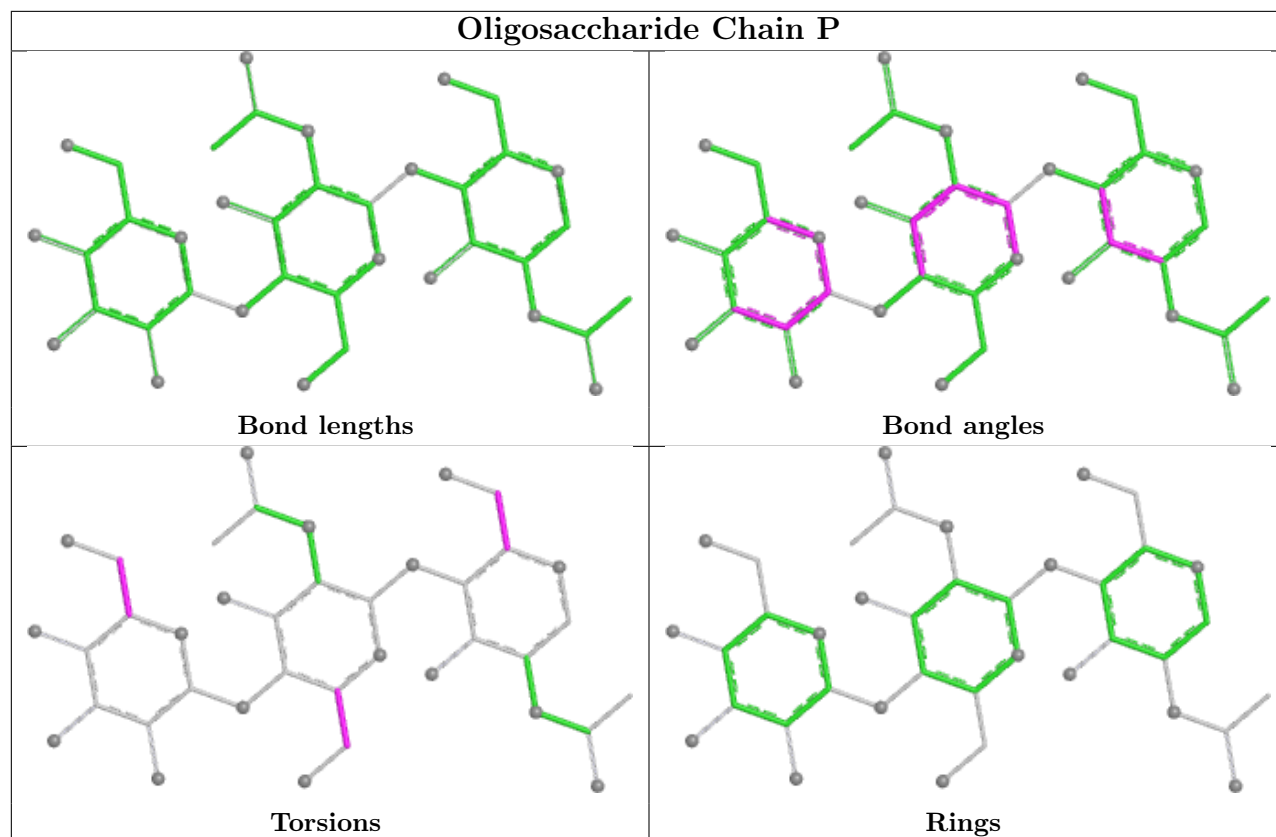


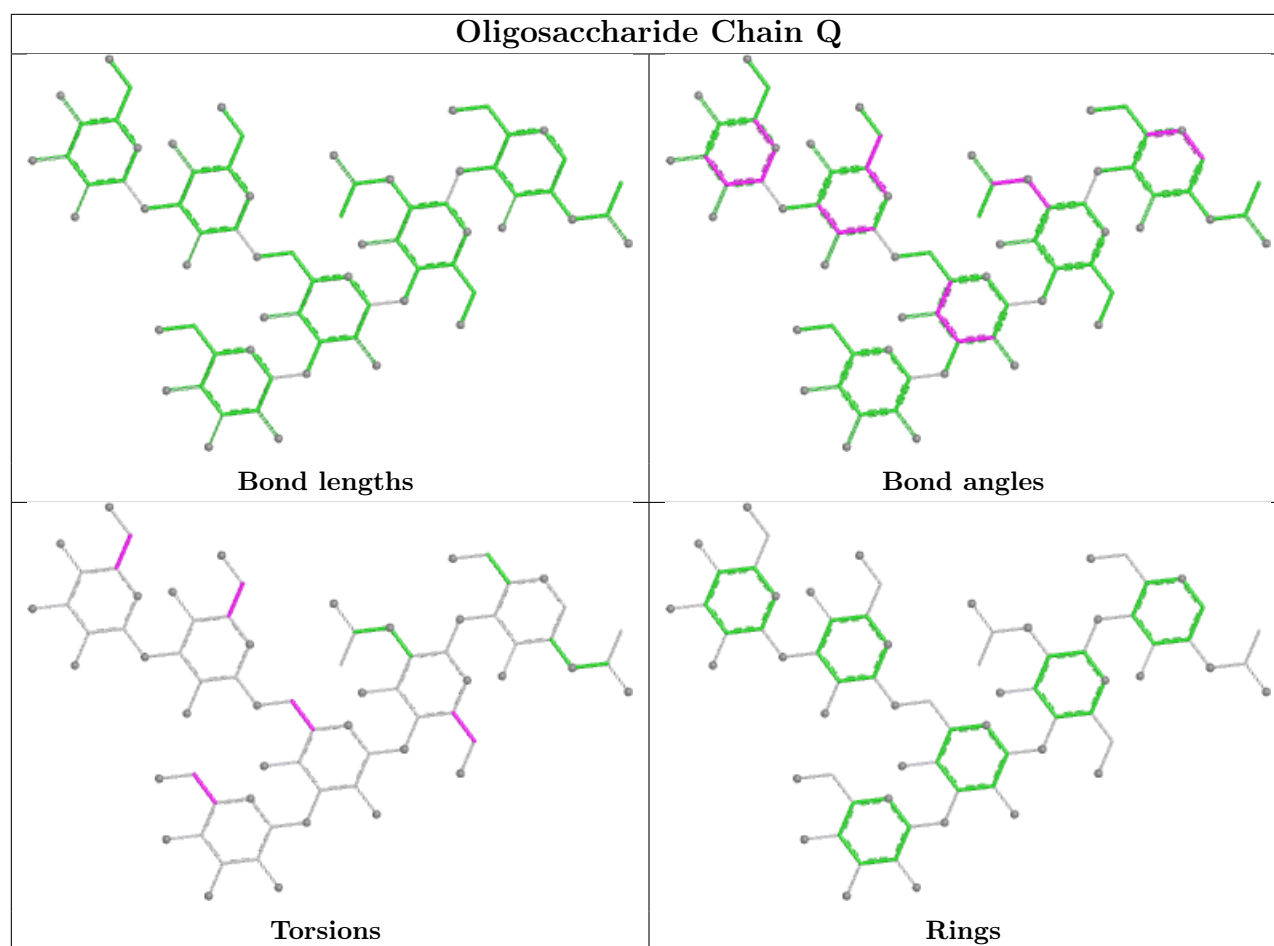












5.6 Ligand geometry [i](#)

4 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	1327	1	14,14,15	0.53	0	17,19,21	0.97	1 (5%)
7	NAG	A	1325	1	14,14,15	0.53	0	17,19,21	0.98	1 (5%)
7	NAG	A	1321	1	14,14,15	0.62	0	17,19,21	1.26	1 (5%)
7	NAG	B	1322	1	14,14,15	0.62	0	17,19,21	1.26	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	1327	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1325	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1321	1	-	1/6/23/26	0/1/1/1
7	NAG	B	1322	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1322	NAG	C4-C3-C2	3.33	115.90	111.02
7	A	1321	NAG	C4-C3-C2	3.30	115.85	111.02
7	A	1325	NAG	C4-C3-C2	2.24	114.30	111.02
7	B	1327	NAG	C4-C3-C2	2.23	114.28	111.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1327	NAG	C4-C5-C6-O6
7	A	1325	NAG	C4-C5-C6-O6
7	A	1321	NAG	C4-C5-C6-O6
7	B	1322	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	7

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Mol	Chain	Number of breaks
1	A	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1147:ASP	C	1148:PRO	N	3.75
1	A	1043:THR	C	1044:GLU	N	2.21
1	B	658:ASN	C	659:CYS	N	2.12
1	A	704:CYS	C	705:PRO	N	2.07
1	A	658:ASN	C	659:CYS	N	2.04
1	B	561:CYS	C	562:VAL	N	1.99
1	B	1147:ASP	C	1148:PRO	N	1.96
1	B	859:CYS	C	860:THR	N	1.76
1	A	510:VAL	C	511:GLU	N	1.75
1	B	1043:THR	C	1044:GLU	N	1.64
1	B	957:VAL	C	958:THR	N	1.61
1	B	510:VAL	C	511:GLU	N	1.19
1	A	859:CYS	C	860:THR	N	0.89

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	1171/1212 (96%)	0.38	91 (7%)	19	25	241, 248, 360, 360	0
1	B	1171/1212 (96%)	0.37	84 (7%)	21	27	243, 247, 397, 397	0
All	All	2342/2424 (96%)	0.38	175 (7%)	20	26	241, 248, 365, 397	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	672	SER	9.8
1	B	699	ASN	5.8
1	A	1089	GLU	5.7
1	A	1106	SER	5.6
1	A	967	SER	5.3
1	A	1198	THR	5.2
1	A	771	SER	4.9
1	B	1084	GLY	4.8
1	A	1205	LEU	4.8
1	B	700	MET	4.8
1	A	814	CYS	4.7
1	A	699	ASN	4.7
1	A	750	PRO	4.7
1	A	1087	GLU	4.6
1	B	547	ARG	4.5
1	A	1091	SER	4.5
1	A	996	GLY	4.5
1	A	1171	GLY	4.5
1	B	1085	GLY	4.4
1	B	1222	GLY	4.4
1	B	1052	ASP	4.4
1	A	1086	ILE	4.3
1	B	1173	ASN	4.2
1	A	342	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	487	ASP	4.2
1	B	271	ALA	4.2
1	A	264	GLN	4.2
1	A	859	CYS	4.0
1	B	741	GLU	3.9
1	B	1109	ASN	3.9
1	A	1182	SER	3.9
1	A	989	ASP	3.9
1	A	876	GLY	3.9
1	A	924	ASP	3.6
1	A	1199	VAL	3.6
1	B	1164	SER	3.4
1	B	674	PRO	3.4
1	B	1143	LEU	3.4
1	A	1149	VAL	3.4
1	A	1109	ASN	3.3
1	B	110	ASP	3.3
1	B	306	GLU	3.3
1	A	1054	GLU	3.3
1	B	552	GLN	3.3
1	B	927	THR	3.2
1	B	1044	GLU	3.2
1	B	675	CYS	3.2
1	B	1087	GLU	3.2
1	B	877	GLY	3.2
1	A	399	GLN	3.1
1	B	920	CYS	3.1
1	B	1122	ASP	3.1
1	A	487	ASP	3.1
1	B	90	ASN	3.1
1	A	1000	SER	3.1
1	B	923	GLY	3.1
1	B	168	ALA	3.1
1	B	791	ASN	3.0
1	A	1195	CYS	3.0
1	A	1110	PRO	3.0
1	B	614	HIS	3.0
1	B	673	PHE	3.0
1	B	836	SER	3.0
1	B	967	SER	3.0
1	A	748	GLY	3.0
1	A	476	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1078	ARG	3.0
1	B	817	CYS	2.9
1	B	921	GLU	2.9
1	A	299	GLY	2.9
1	B	1198	THR	2.9
1	A	852	ALA	2.8
1	A	1053	PRO	2.8
1	B	1108	ASP	2.8
1	A	1047	THR	2.8
1	A	1202	THR	2.8
1	B	546	GLU	2.8
1	B	415	GLY	2.7
1	B	676	HIS	2.7
1	A	168	ALA	2.7
1	A	1043	THR	2.7
1	A	557	ASP	2.7
1	A	1085	GLY	2.7
1	A	749	SER	2.7
1	B	1082	LYS	2.7
1	B	738	ARG	2.7
1	A	1069	THR	2.7
1	A	1019	PRO	2.7
1	B	246	TYR	2.6
1	B	1086	ILE	2.6
1	B	851	HIS	2.6
1	B	609	GLU	2.6
1	A	550	GLU	2.6
1	B	169	GLY	2.6
1	A	987	GLY	2.6
1	A	988	SER	2.6
1	A	978	GLY	2.6
1	B	1171	GLY	2.6
1	B	1072	ALA	2.6
1	B	513	CYS	2.6
1	B	1045	ASP	2.5
1	A	963	ARG	2.5
1	A	300	CYS	2.5
1	B	790	GLY	2.5
1	A	262	ASP	2.5
1	A	1206	CYS	2.5
1	B	814	CYS	2.5
1	A	1088	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	108	SER	2.4
1	A	1183	ARG	2.4
1	A	194	GLU	2.4
1	A	1185	ASN	2.4
1	A	955	THR	2.4
1	A	545	CYS	2.4
1	B	739	GLY	2.4
1	B	88	GLU	2.4
1	A	851	HIS	2.4
1	B	783	ASN	2.4
1	B	581	VAL	2.4
1	B	1070	ASN	2.3
1	A	320	GLN	2.3
1	A	1059	SER	2.3
1	B	1061	GLY	2.3
1	B	761	SER	2.3
1	B	1083	TYR	2.3
1	A	420	GLU	2.3
1	B	1053	PRO	2.3
1	A	923	GLY	2.3
1	B	905	CYS	2.3
1	B	769	SER	2.3
1	A	312	ASP	2.3
1	B	430	ASP	2.3
1	B	1203	GLN	2.3
1	A	1029	ASN	2.2
1	B	565	THR	2.2
1	A	825	GLU	2.2
1	B	1187	THR	2.2
1	A	1068	GLY	2.2
1	A	745	HIS	2.2
1	A	1203	GLN	2.2
1	B	1088	ARG	2.2
1	A	651	SER	2.2
1	A	857	SER	2.2
1	A	741	GLU	2.2
1	B	1007	ARG	2.2
1	A	90	ASN	2.2
1	A	1034	SER	2.2
1	A	522	CYS	2.2
1	A	579	PRO	2.1
1	B	1152	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1187	THR	2.1
1	A	551	PRO	2.1
1	B	745	HIS	2.1
1	B	579	PRO	2.1
1	A	51	HIS	2.1
1	A	531	GLY	2.1
1	B	201	SER	2.1
1	A	773	GLU	2.1
1	A	581	VAL	2.1
1	A	431	GLY	2.1
1	A	506	THR	2.1
1	A	1197	LEU	2.1
1	A	317	ARG	2.1
1	A	875	GLN	2.1
1	B	651	SER	2.1
1	B	752	ARG	2.0
1	B	92	LYS	2.0
1	B	165	GLY	2.0
1	A	674	PRO	2.0
1	B	1194	PRO	2.0
1	A	169	GLY	2.0
1	B	1097	ASP	2.0
1	B	611	GLY	2.0
1	B	835	CYS	2.0
1	A	540	SER	2.0

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	MAN	J	6	11/12	0.76	0.37	359,359,359,359	0
2	BMA	E	3	11/12	0.81	0.15	271,271,271,271	0
4	MAN	J	4	11/12	0.86	0.35	359,359,359,359	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MAN	Q	4	11/12	0.87	0.12	308,308,308,308	0
3	NAG	I	1	14/15	0.90	0.18	314,314,314,314	0
4	MAN	R	5	11/12	0.91	0.22	365,365,365,365	0
2	MAN	C	4	11/12	0.91	0.12	242,242,242,242	0
6	NAG	L	1	14/15	0.92	0.18	282,282,282,282	0
2	MAN	E	4	11/12	0.92	0.15	271,271,271,271	0
6	MAN	Q	6	11/12	0.92	0.15	308,308,308,308	0
4	MAN	R	7	11/12	0.93	0.18	365,365,365,365	0
4	BMA	J	3	11/12	0.93	0.32	359,359,359,359	0
3	BMA	D	3	11/12	0.94	0.14	271,271,271,271	0
5	BMA	P	3	11/12	0.94	0.08	270,270,270,270	0
3	NAG	I	2	14/15	0.94	0.14	314,314,314,314	0
6	NAG	L	2	14/15	0.94	0.13	282,282,282,282	0
6	NAG	Q	1	14/15	0.94	0.14	308,308,308,308	0
3	MAN	D	4	11/12	0.94	0.09	271,271,271,271	0
4	MAN	R	6	11/12	0.94	0.21	365,365,365,365	0
3	MAN	I	5	11/12	0.95	0.17	314,314,314,314	0
6	BMA	Q	3	11/12	0.95	0.09	308,308,308,308	0
3	BMA	I	3	11/12	0.95	0.11	314,314,314,314	0
6	MAN	L	4	11/12	0.95	0.12	282,282,282,282	0
4	NAG	R	1	14/15	0.96	0.25	365,365,365,365	0
4	BMA	R	3	11/12	0.96	0.30	365,365,365,365	0
2	MAN	M	4	11/12	0.96	0.11	282,282,282,282	0
3	MAN	D	5	11/12	0.96	0.10	271,271,271,271	0
4	MAN	F	7	11/12	0.96	0.09	271,271,271,271	0
5	BMA	H	3	11/12	0.96	0.09	248,248,248,248	0
4	MAN	J	7	11/12	0.96	0.17	359,359,359,359	0
4	MAN	N	4	11/12	0.97	0.07	282,282,282,282	0
6	MAN	L	5	11/12	0.97	0.18	282,282,282,282	0
6	MAN	L	6	11/12	0.97	0.24	282,282,282,282	0
2	BMA	M	3	11/12	0.97	0.12	282,282,282,282	0
2	NAG	O	1	14/15	0.97	0.15	270,270,270,270	0
2	BMA	O	3	11/12	0.97	0.07	270,270,270,270	0
4	BMA	N	3	11/12	0.97	0.05	282,282,282,282	0
4	NAG	J	2	14/15	0.98	0.18	359,359,359,359	0
2	BMA	K	3	11/12	0.98	0.16	243,243,243,243	0
2	MAN	K	4	11/12	0.98	0.13	243,243,243,243	0
5	NAG	G	1	14/15	0.98	0.10	248,248,248,248	0
5	BMA	G	3	11/12	0.98	0.04	248,248,248,248	0
5	NAG	H	1	14/15	0.98	0.15	248,248,248,248	0
5	NAG	H	2	14/15	0.98	0.16	248,248,248,248	0
4	MAN	J	5	11/12	0.98	0.18	359,359,359,359	0

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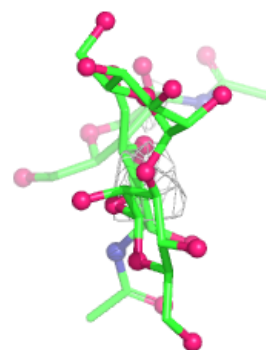
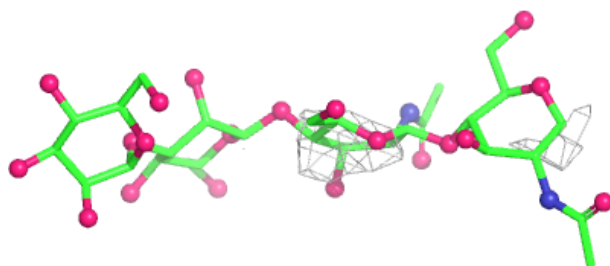
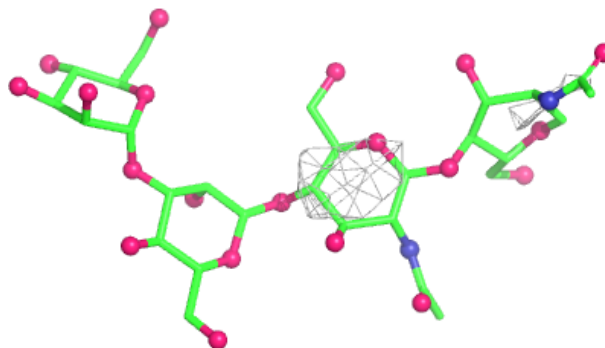
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	M	1	14/15	0.98	0.12	282,282,282,282	0
2	BMA	C	3	11/12	0.98	0.11	242,242,242,242	0
4	BMA	F	3	11/12	0.98	0.15	271,271,271,271	0
4	MAN	F	4	11/12	0.98	0.07	271,271,271,271	0
4	MAN	N	5	11/12	0.98	0.08	282,282,282,282	0
4	MAN	N	6	11/12	0.98	0.09	282,282,282,282	0
4	MAN	N	7	11/12	0.98	0.09	282,282,282,282	0
6	NAG	Q	2	14/15	0.98	0.17	308,308,308,308	0
4	MAN	F	6	11/12	0.98	0.11	271,271,271,271	0
2	NAG	K	1	14/15	0.98	0.11	243,243,243,243	0
4	MAN	R	4	11/12	0.98	0.23	365,365,365,365	0
2	MAN	O	4	11/12	0.99	0.05	270,270,270,270	0
5	NAG	G	2	14/15	0.99	0.08	248,248,248,248	0
4	NAG	F	1	14/15	0.99	0.10	271,271,271,271	0
4	NAG	N	1	14/15	0.99	0.13	282,282,282,282	0
4	NAG	N	2	14/15	0.99	0.08	282,282,282,282	0
4	NAG	F	2	14/15	0.99	0.14	271,271,271,271	0
5	NAG	P	1	14/15	0.99	0.09	270,270,270,270	0
5	NAG	P	2	14/15	0.99	0.19	270,270,270,270	0
3	NAG	D	2	14/15	0.99	0.11	271,271,271,271	0
2	NAG	M	2	14/15	0.99	0.14	282,282,282,282	0
4	MAN	F	5	11/12	0.99	0.12	271,271,271,271	0
6	BMA	L	3	11/12	0.99	0.13	282,282,282,282	0
2	NAG	K	2	14/15	0.99	0.17	243,243,243,243	0
2	NAG	C	2	14/15	0.99	0.12	242,242,242,242	0
4	NAG	R	2	14/15	0.99	0.13	365,365,365,365	0
4	NAG	J	1	14/15	0.99	0.12	359,359,359,359	0
2	NAG	E	1	14/15	0.99	0.17	271,271,271,271	0
2	NAG	O	2	14/15	0.99	0.17	270,270,270,270	0
2	NAG	E	2	14/15	0.99	0.14	271,271,271,271	0
6	MAN	Q	5	11/12	0.99	0.07	308,308,308,308	0
3	MAN	I	4	11/12	0.99	0.13	314,314,314,314	0
2	NAG	C	1	14/15	1.00	0.11	242,242,242,242	0
3	NAG	D	1	14/15	1.00	0.05	271,271,271,271	0

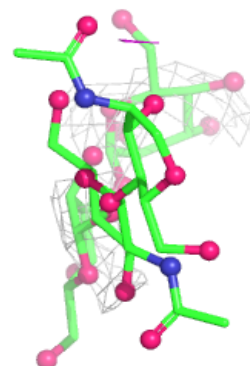
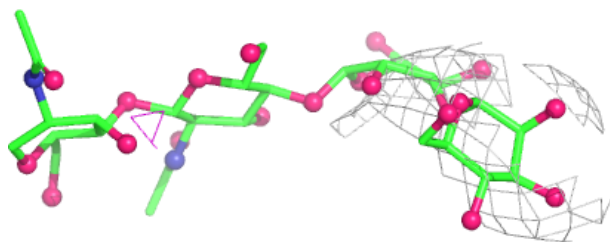
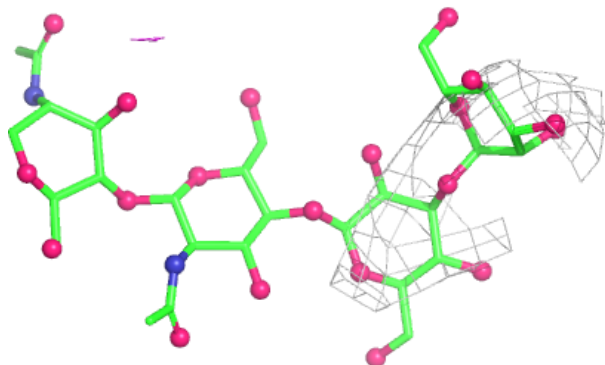
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

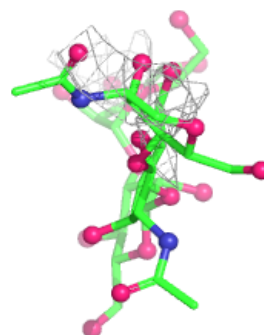
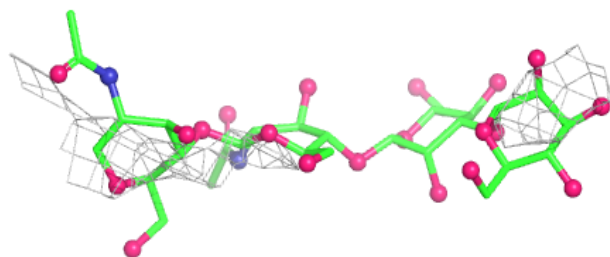
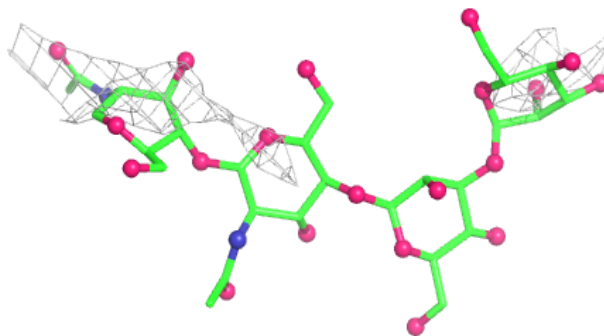
**Electron density around Chain E:**

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

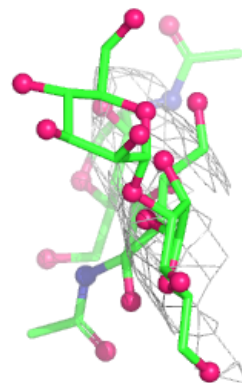
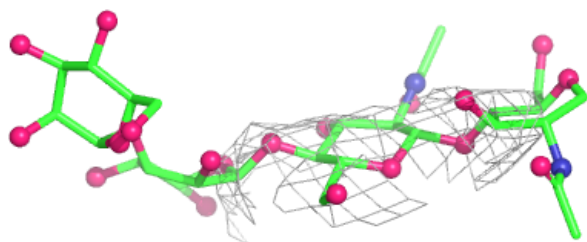
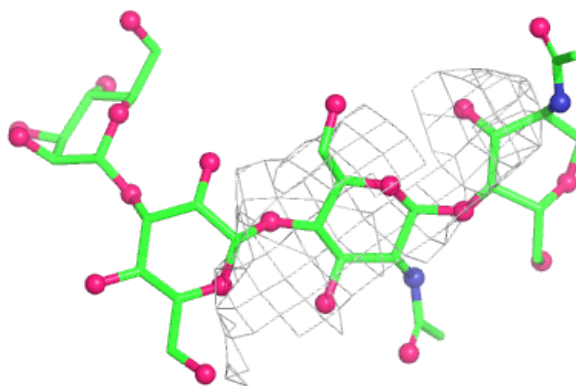


Electron density around Chain K:

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

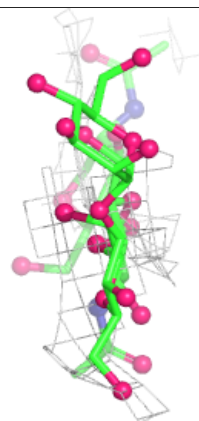
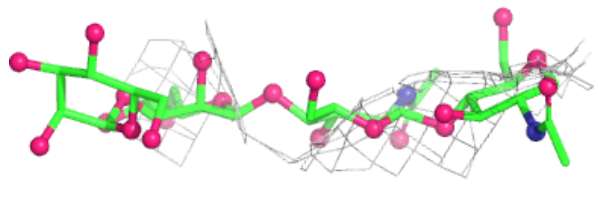
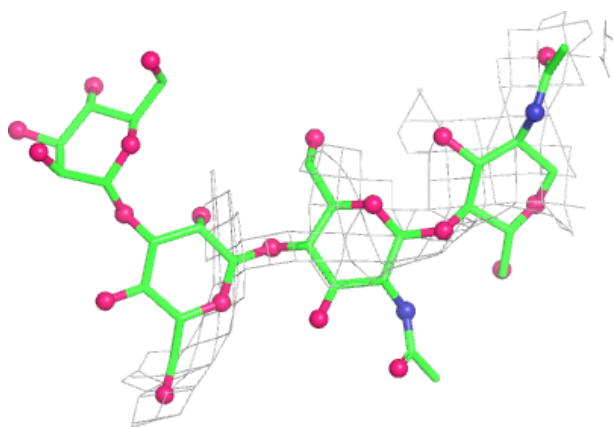
**Electron density around Chain M:**

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



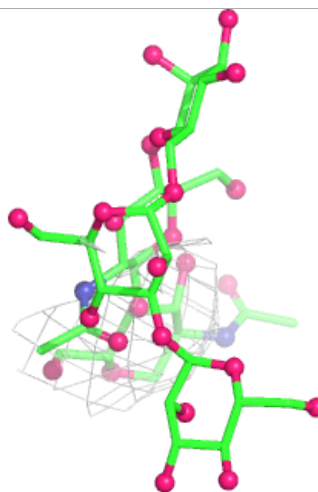
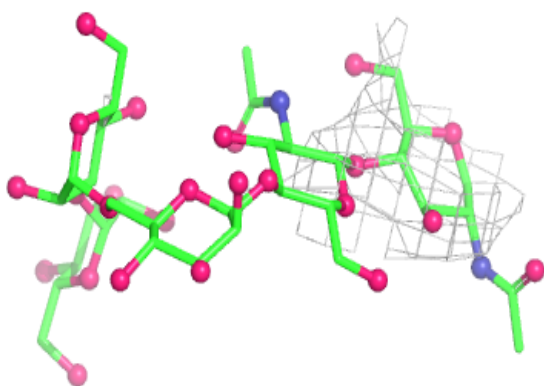
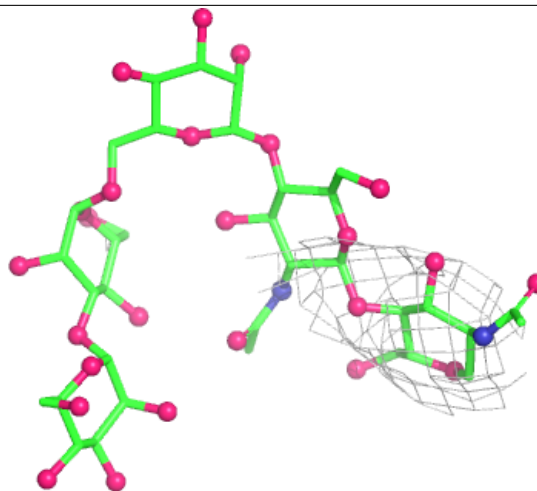
Electron density around Chain O:

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



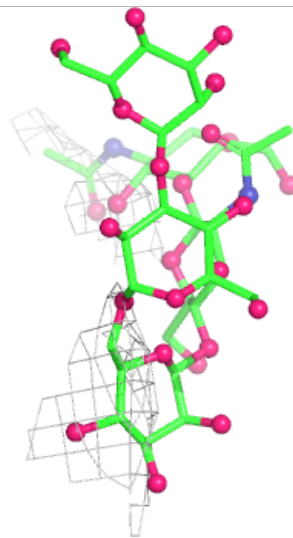
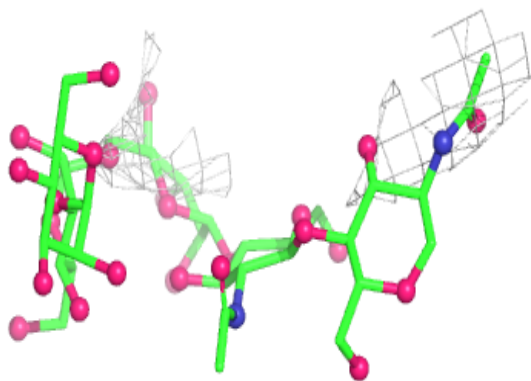
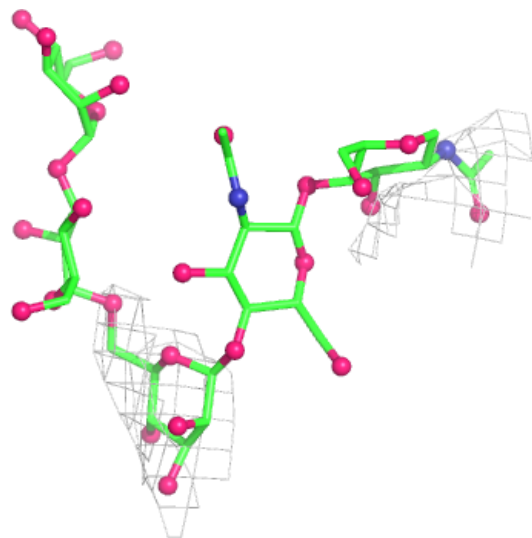
Electron density around Chain D:

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



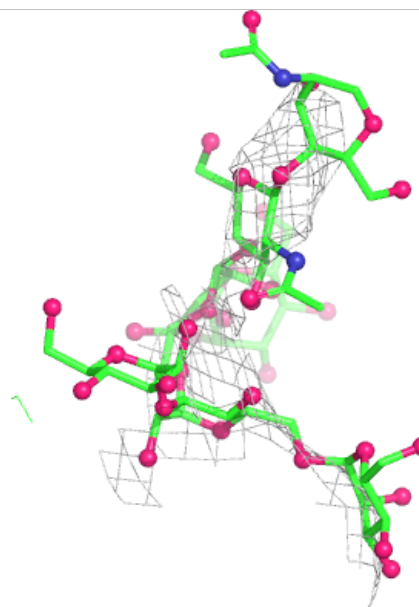
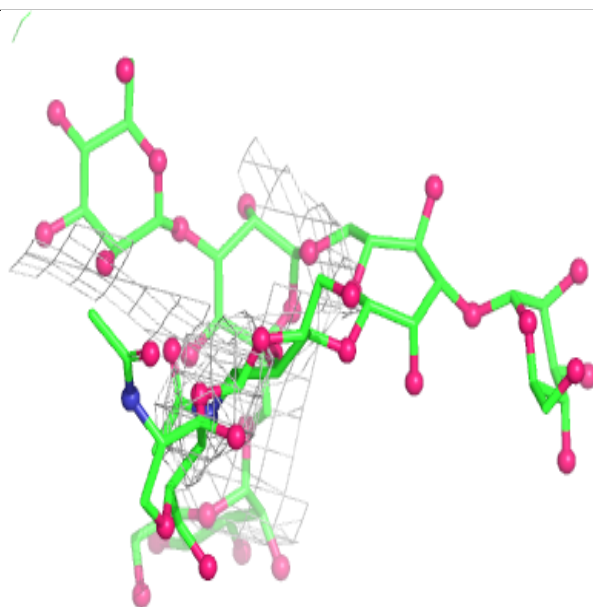
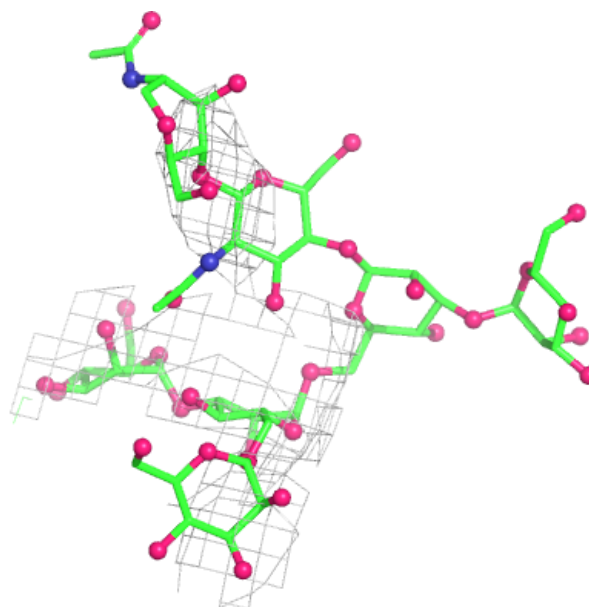
Electron density around Chain I:

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



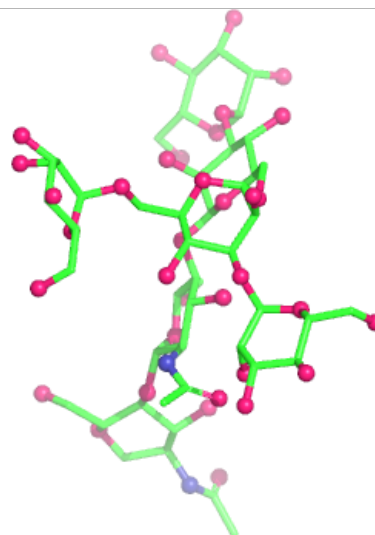
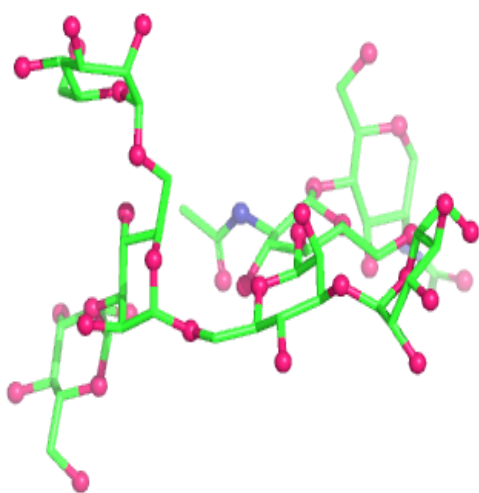
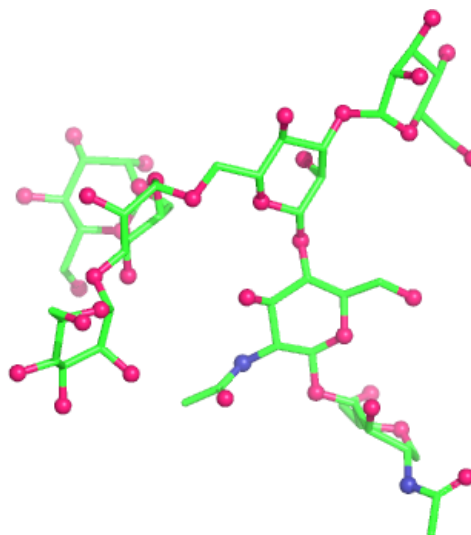
Electron density around Chain F:

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



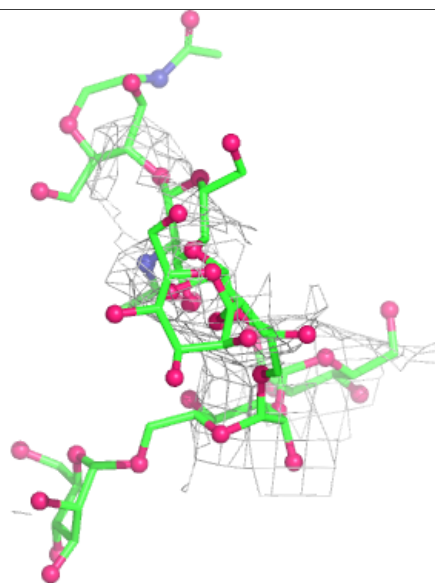
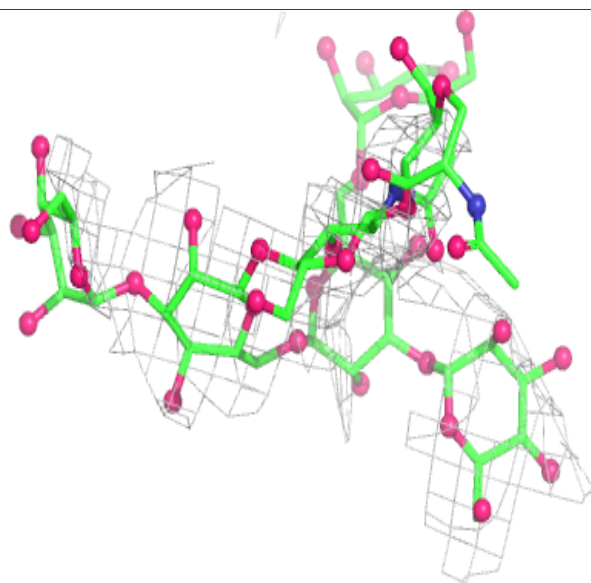
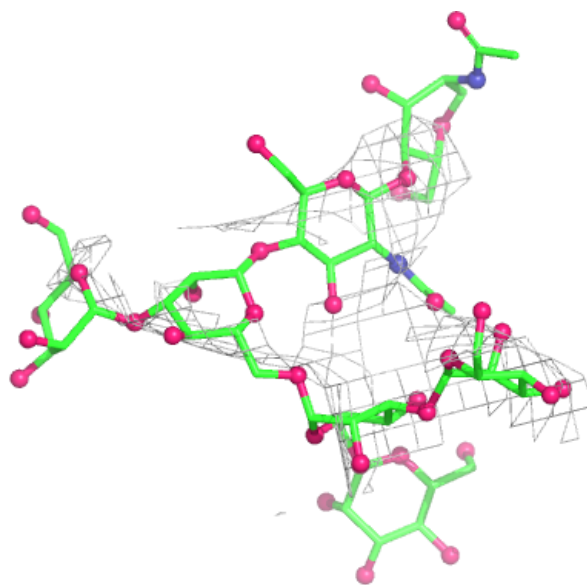
Electron density around Chain J:

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



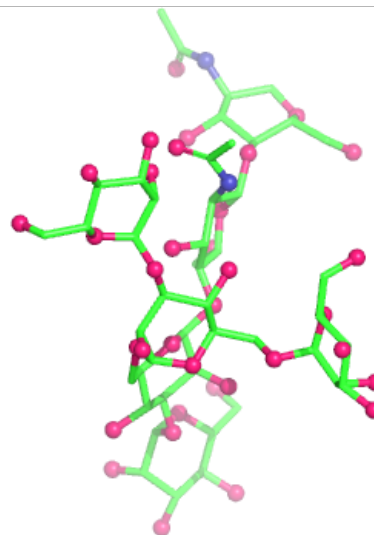
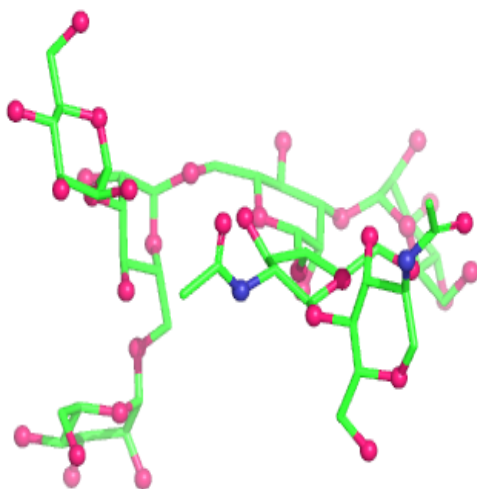
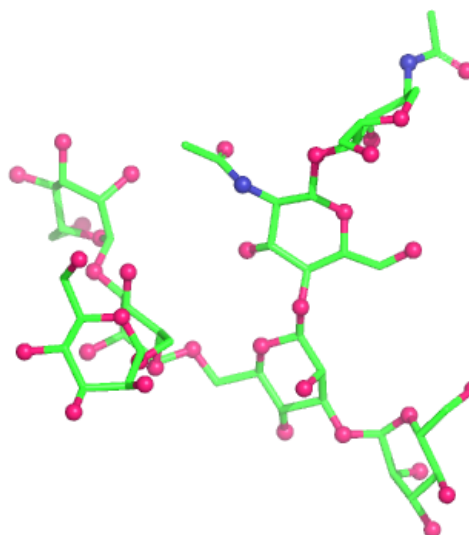
Electron density around Chain N:

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



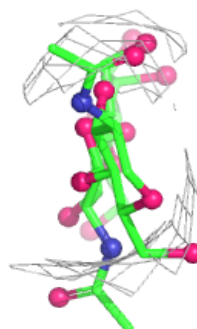
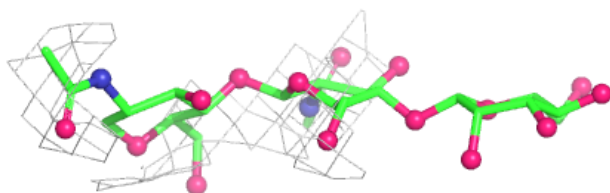
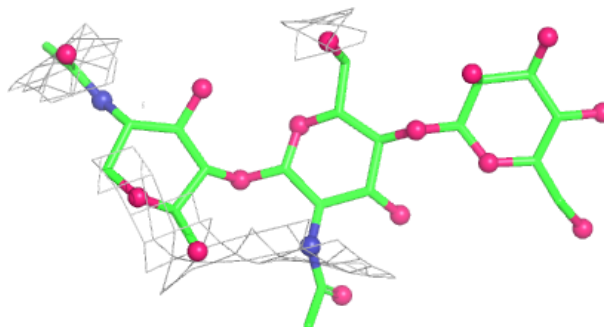
Electron density around Chain R:

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

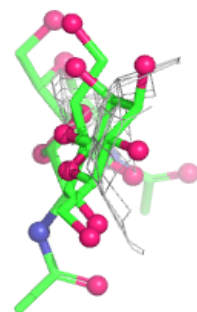
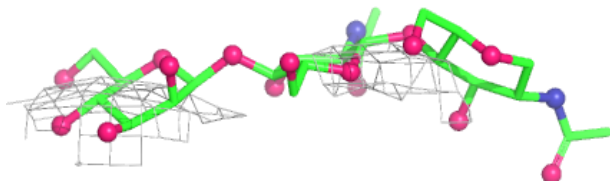
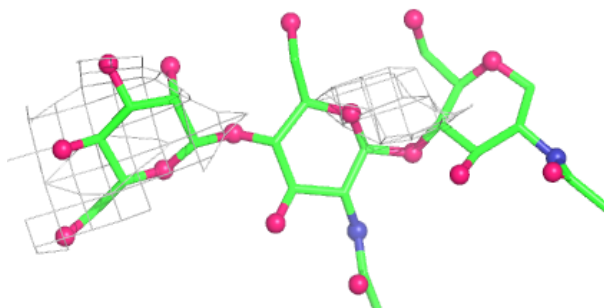


Electron density around Chain G:

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

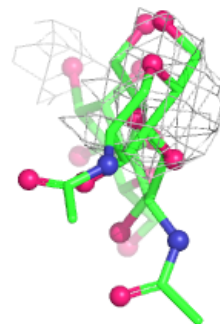
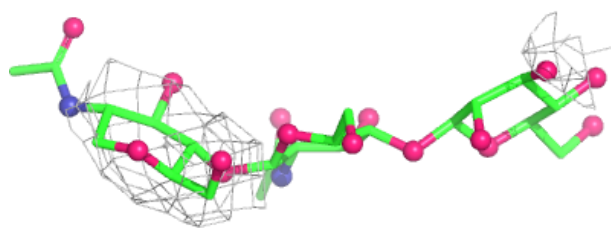
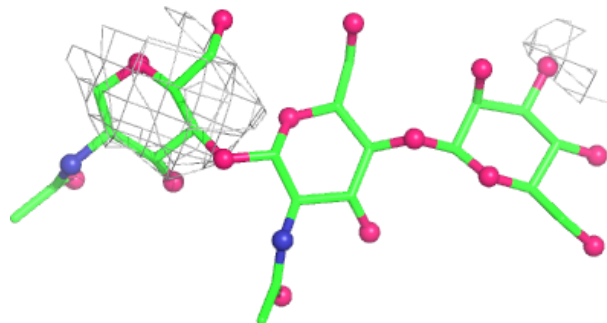
**Electron density around Chain H:**

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



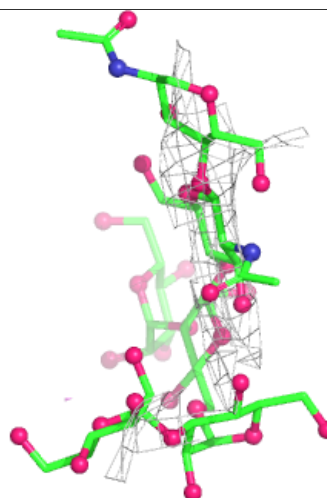
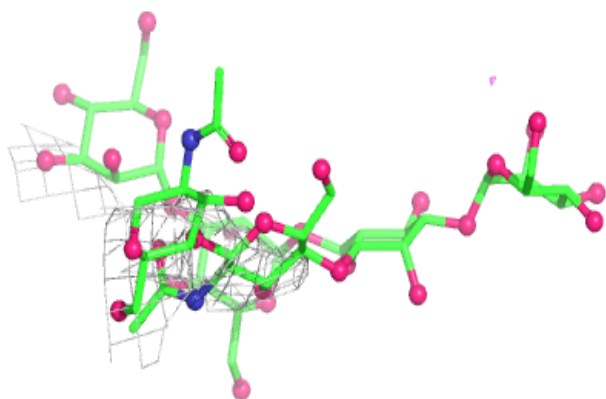
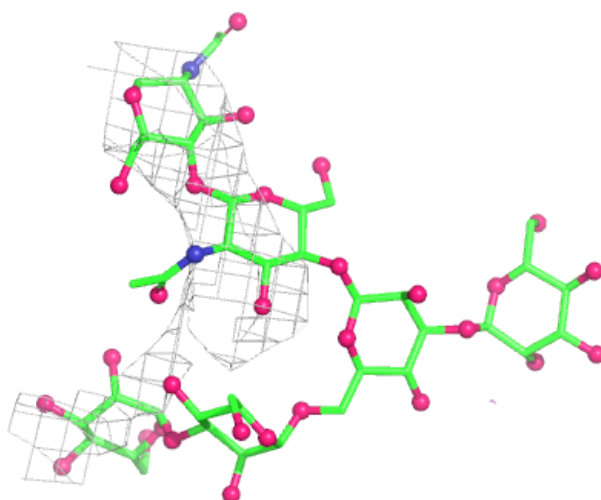
Electron density around Chain P:

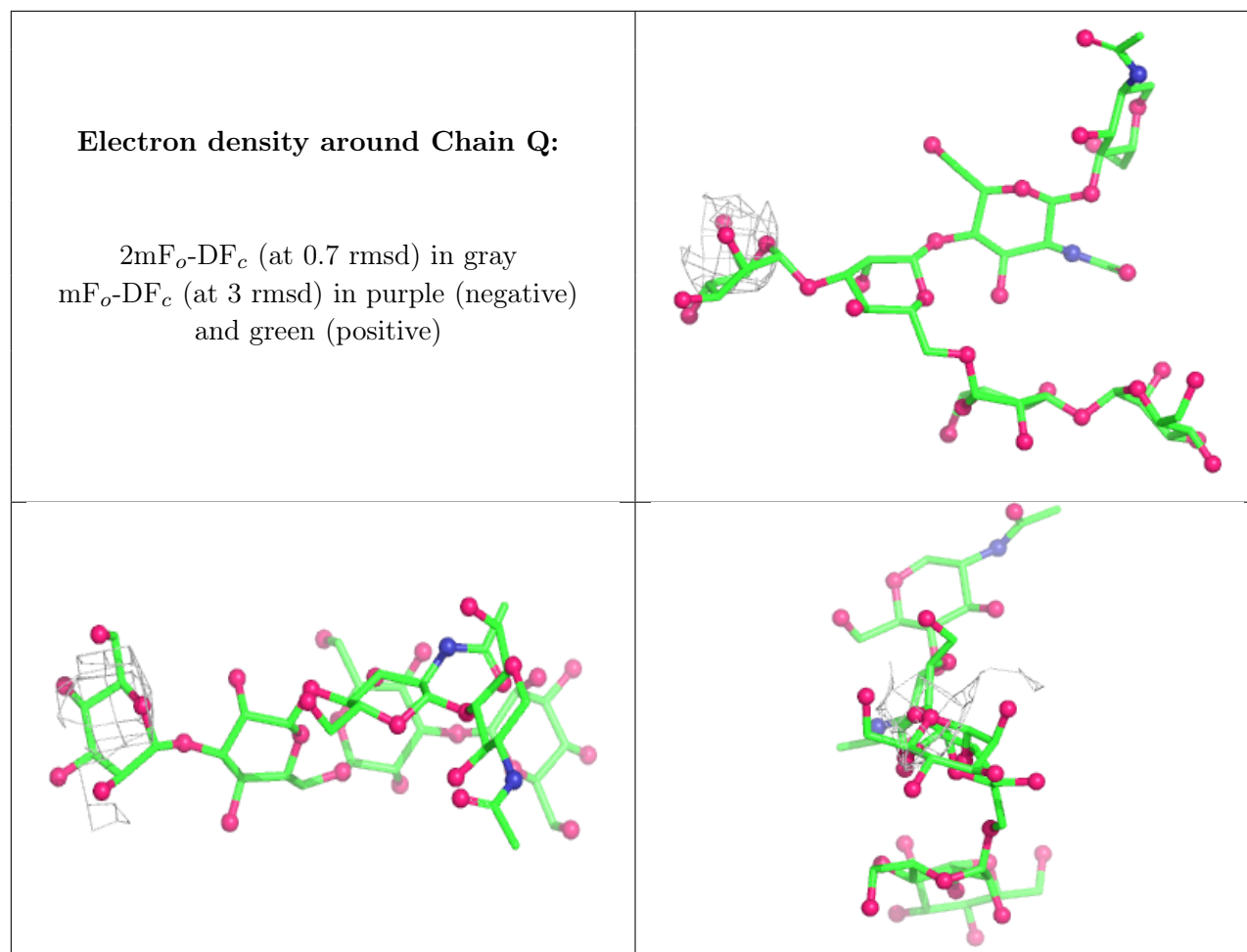
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain L:

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





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
7	NAG	A	1321	14/15	0.98	0.11	240,240,240,240	0
7	NAG	A	1325	14/15	0.98	0.11	248,248,248,248	0
7	NAG	B	1322	14/15	0.98	0.08	251,251,251,251	0
7	NAG	B	1327	14/15	0.98	0.18	270,270,270,270	0

6.5 Other polymers [i](#)

There are no such residues in this entry.