



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:34 PM UTC

PDB ID : 6PDX / pdb_00006pdx
Title : Crystal structure of C585 Fab in complex with influenza virus hemagglutinin from A/Switzerland/9715293/2013 (H3N2)
Authors : Qiu, Y.; Zhou, Y.
Deposited on : 2019-06-19
Resolution : 3.99 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

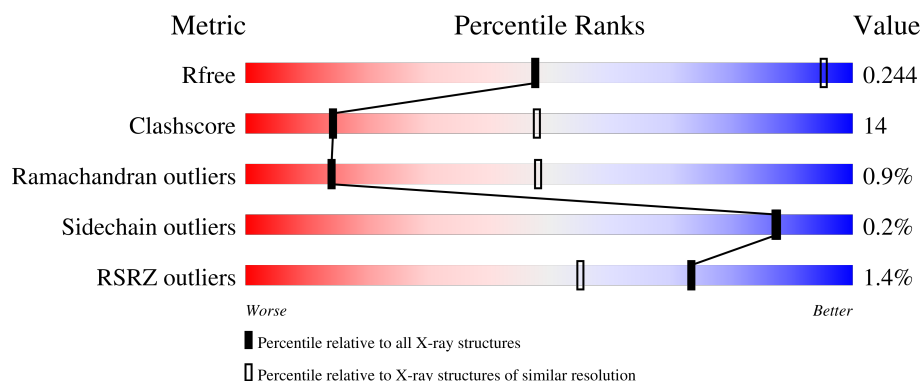
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.99 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	505	0% 75% 23% •
1	B	505	0% 74% 22% •
1	C	505	0% 75% 21% •
2	H	237	2% 70% 23% • 7%
2	M	237	0% 73% 19% • 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	O	237	
3	L	215	
3	N	215	
3	P	215	
4	D	3	
4	E	3	
4	G	3	
4	I	3	
4	J	3	
4	K	3	
4	Q	3	
4	R	3	
4	U	3	
4	W	3	
4	X	3	
4	Y	3	
4	Z	3	
5	F	2	
5	S	2	
5	T	2	
5	V	2	
5	a	2	

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	D	2	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20896 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	1	0
			3798	2364	673	742	19			
1	B	488	Total	C	N	O	S	0	0	0
			3684	2290	652	724	18			
1	C	487	Total	C	N	O	S	0	0	0
			3719	2313	651	737	18			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	505	SER	-	expression tag	UNP A0A1L3A363
B	505	SER	-	expression tag	UNP A0A1L3A363
C	505	SER	-	expression tag	UNP A0A1L3A363

- Molecule 2 is a protein called C585 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	0	0
			1559	981	265	308	5			
2	M	221	Total	C	N	O	S	0	0	0
			1547	974	261	306	6			
2	O	221	Total	C	N	O	S	0	0	0
			1575	998	263	308	6			

- Molecule 3 is a protein called C585 Fab light chain.

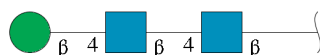
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1446	902	239	299	6			
3	N	213	Total	C	N	O	S	0	1	0
			1426	897	235	288	6			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	214	Total	C	N	O	S	0	0	0
			1481	936	242	298	5			

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



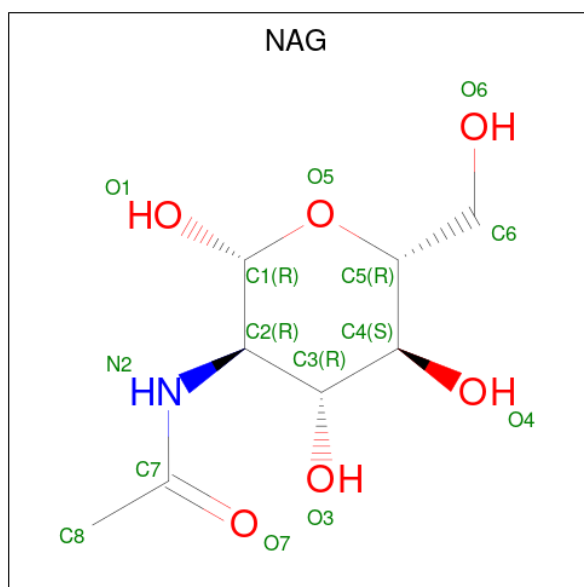
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O		0	0	0
			39	22	2	15				
4	E	3	Total	C	N	O		0	0	0
			39	22	2	15				
4	G	3	Total	C	N	O		0	0	0
			39	22	2	15				
4	I	3	Total	C	N	O		0	0	0
			39	22	2	15				
4	J	3	Total	C	N	O		0	0	0
			39	22	2	15				
4	K	3	Total	C	N	O		0	0	0
			39	22	2	15				
4	Q	3	Total	C	N	O		0	0	0
			39	22	2	15				
4	R	3	Total	C	N	O		0	0	0
			39	22	2	15				
4	U	3	Total	C	N	O		0	0	0
			39	22	2	15				
4	W	3	Total	C	N	O		0	0	0
			39	22	2	15				
4	X	3	Total	C	N	O		0	0	0
			39	22	2	15				
4	Y	3	Total	C	N	O		0	0	0
			39	22	2	15				
4	Z	3	Total	C	N	O		0	0	0
			39	22	2	15				

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	a	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

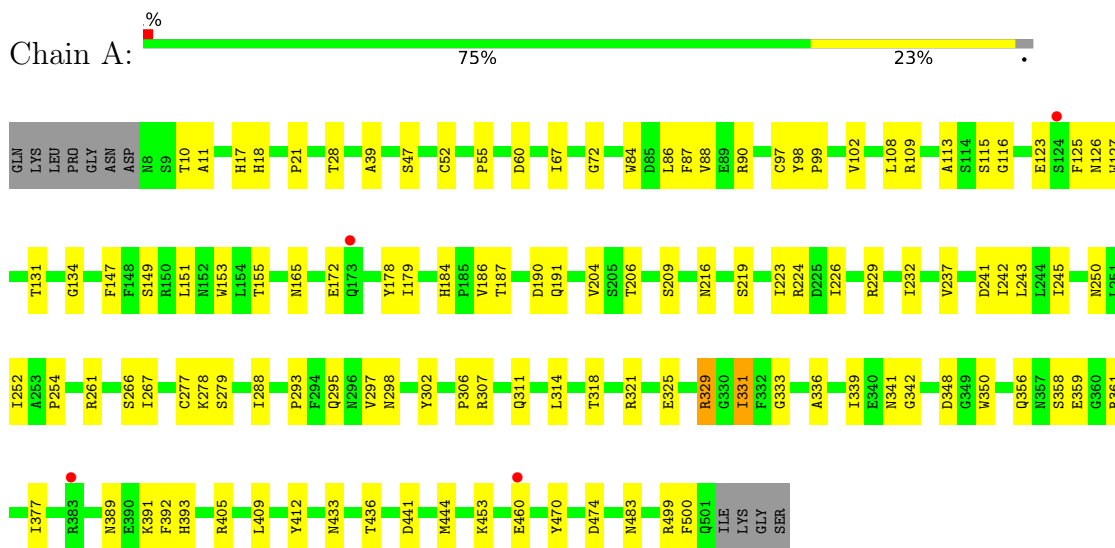


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

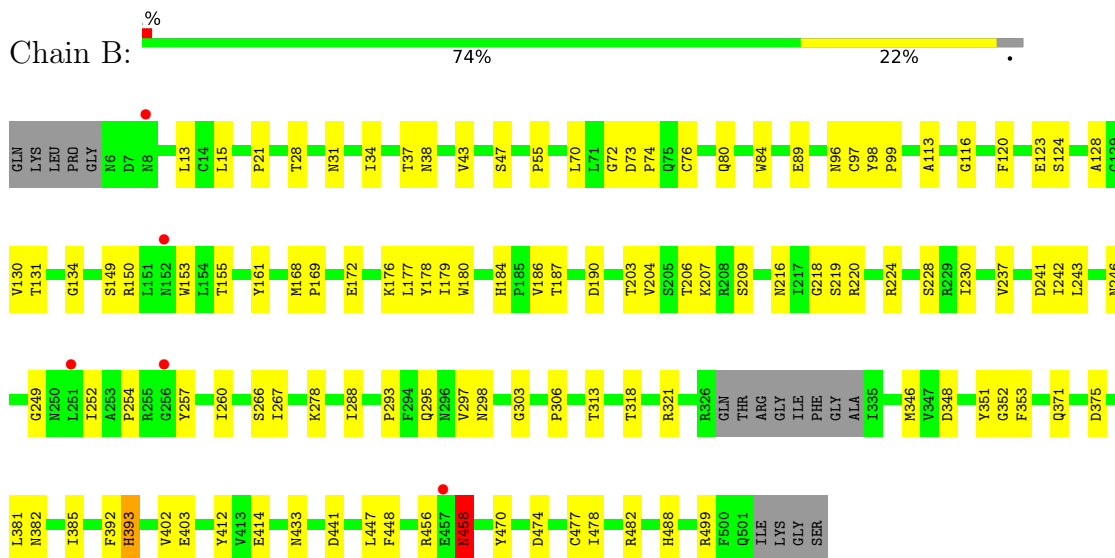
3 Residue-property plots

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.

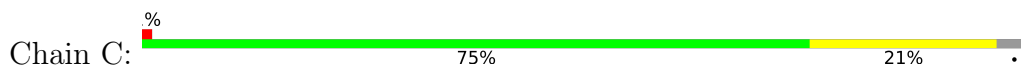
• Molecule 1: Hemagglutinin

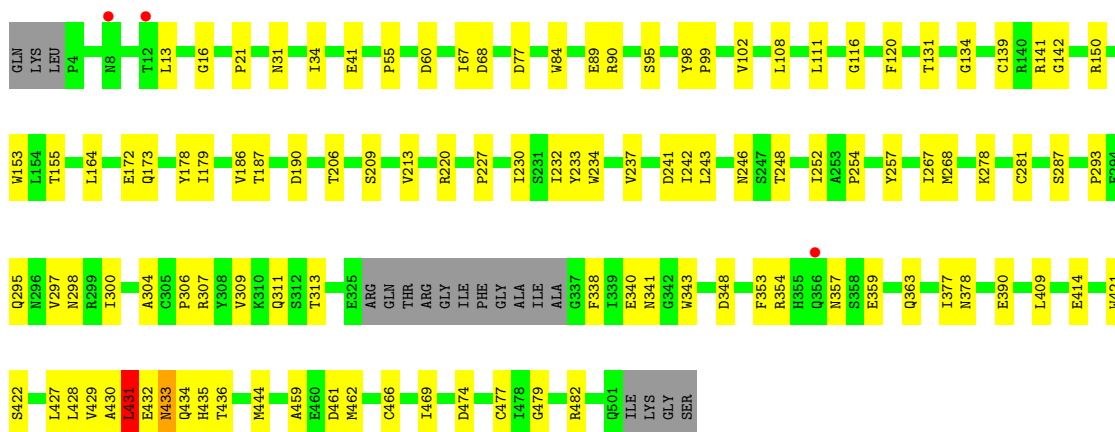


• Molecule 1: Hemagglutinin

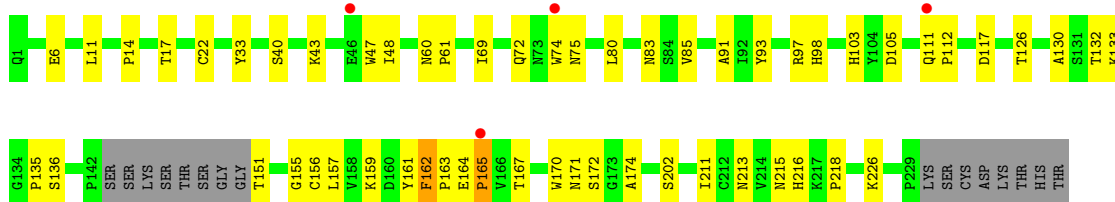


• Molecule 1: Hemagglutinin

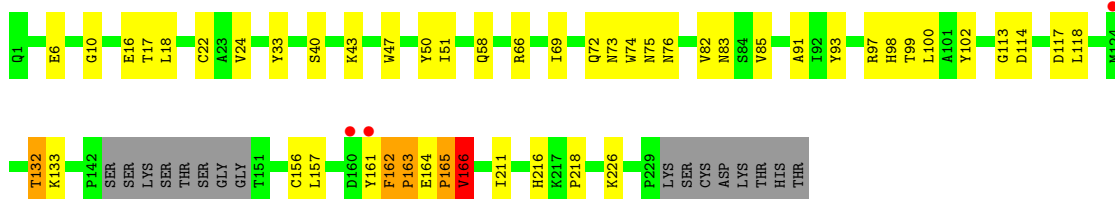
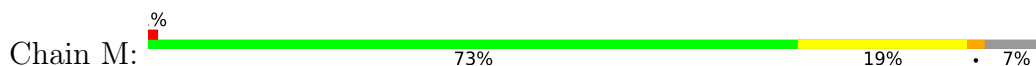




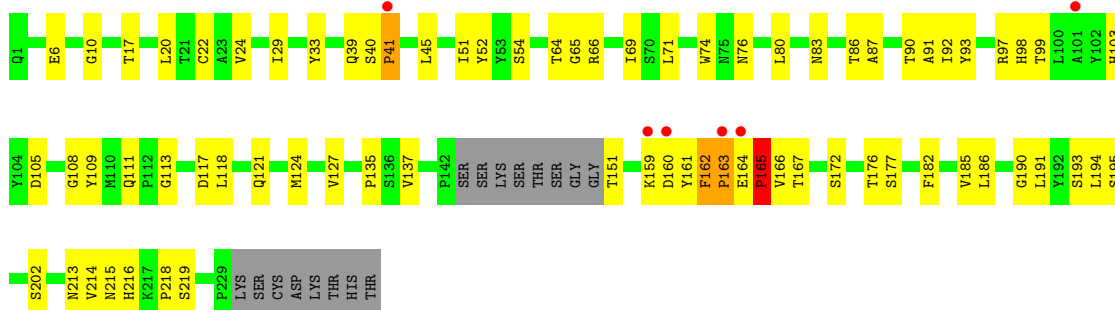
• Molecule 2: C585 Fab heavy chain



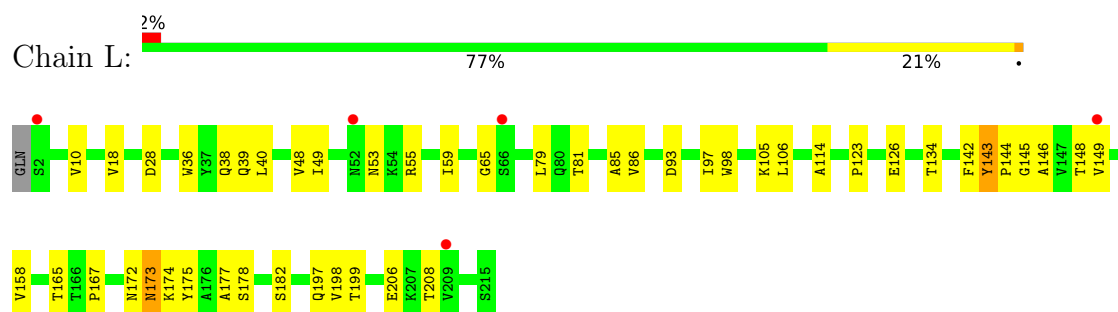
• Molecule 2: C585 Fab heavy chain



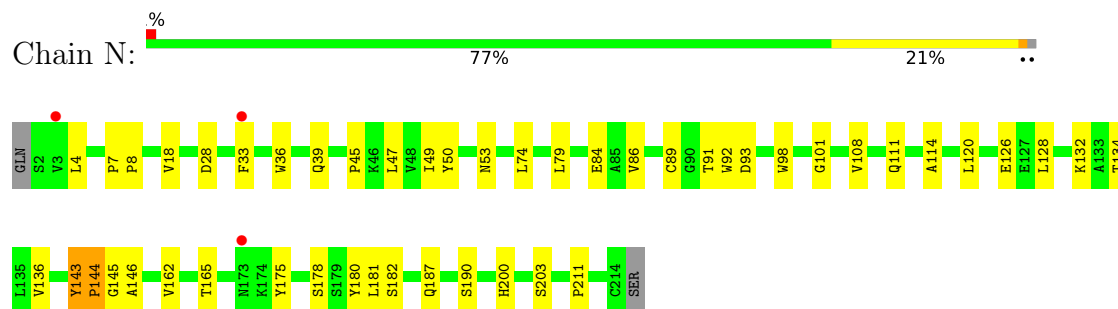
• Molecule 2: C585 Fab heavy chain



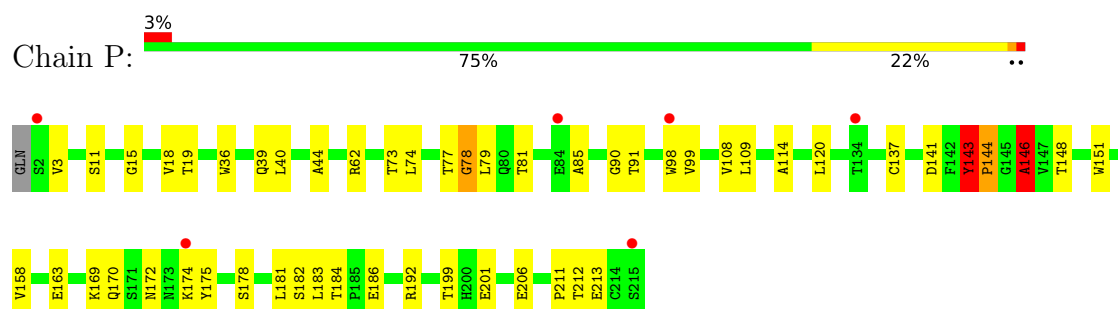
• Molecule 3: C585 Fab light chain



- Molecule 3: C585 Fab light chain



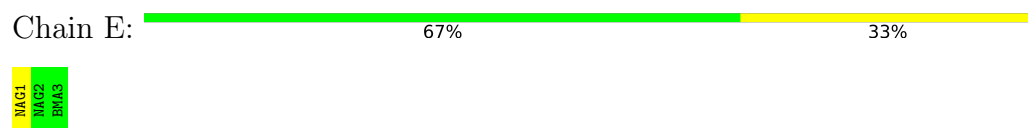
- Molecule 3: C585 Fab light chain



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



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



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

Chain G:  100%



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

Chain I:  100%



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

Chain J:  100%



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

Chain K:  67% 33%



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

Chain Q:  33% 33% 33%



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

Chain R:  67% 33%



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

Chain U:  33% 33% 33%

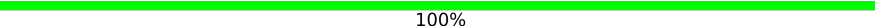


- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  67% 33%



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

Chain X:  100%

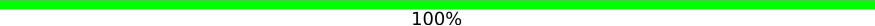


- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  67% 33%

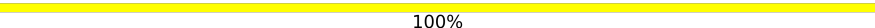


- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  100%

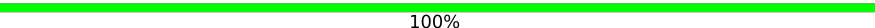


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%



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

Chain S:  100%



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

Chain T:  50% 50%



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

Chain V:  100%



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

Chain a:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	287.26Å 287.26Å 182.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.88 – 3.99 47.88 – 3.99	Depositor EDS
% Data completeness (in resolution range)	96.7 (47.88-3.99) 96.7 (47.88-3.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 4.00Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.212 , 0.241 0.216 , 0.244	Depositor DCC
R_{free} test set	3518 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	126.5	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 164.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.046 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20896	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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: BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.21	0/3880	0.43	2/5275 (0.0%)
1	B	0.17	0/3761	0.39	1/5126 (0.0%)
1	C	0.18	0/3798	0.42	5/5169 (0.1%)
2	H	0.24	0/1602	0.49	0/2210
2	M	0.34	1/1589 (0.1%)	0.62	5/2191 (0.2%)
2	O	0.51	3/1619 (0.2%)	0.74	9/2231 (0.4%)
3	L	0.24	0/1484	0.41	0/2050
3	N	0.26	1/1465 (0.1%)	0.46	1/2027 (0.0%)
3	P	0.34	1/1522 (0.1%)	0.59	4/2102 (0.2%)
All	All	0.27	6/20720 (0.0%)	0.49	27/28381 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	163	PRO	C-O	-6.83	1.15	1.23
2	O	40	SER	CA-CB	-6.75	1.45	1.53
2	O	165	PRO	C-O	-5.97	1.16	1.24
2	M	165	PRO	C-O	-5.72	1.17	1.23
3	P	144	PRO	N-CD	-5.46	1.40	1.47
3	N	144	PRO	C-O	-5.36	1.17	1.23

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	162	PHE	CA-CB-CG	-10.42	103.38	113.80
2	M	163	PRO	N-CD-CG	-8.25	90.82	103.20
2	O	41	PRO	N-CA-C	-7.31	99.02	110.50
2	O	163	PRO	N-CA-CB	-7.04	97.04	103.31
1	B	458	ASN	N-CA-C	7.03	125.78	110.80
2	M	165	PRO	CB-CA-C	-7.01	102.42	111.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	144	PRO	N-CD-CG	-7.01	92.69	103.20
1	C	433	ASN	CA-C-O	-6.88	113.82	120.90
1	C	431	LEU	N-CA-C	-6.83	103.77	111.14
2	O	41	PRO	CB-CA-C	-6.83	104.12	111.56
3	P	146	ALA	CA-C-N	-6.74	113.57	122.94
3	P	146	ALA	C-N-CA	-6.74	113.57	122.94
2	O	159	LYS	N-CA-C	6.54	120.12	109.59
1	C	433	ASN	O-C-N	6.51	129.06	122.03
2	O	162	PHE	CB-CA-C	-6.41	97.54	110.17
2	O	165	PRO	CB-CA-C	-6.24	101.26	111.56
1	C	433	ASN	CA-CB-CG	-6.24	106.36	112.60
2	O	165	PRO	N-CA-CB	-6.19	96.75	103.25
3	N	144	PRO	N-CA-C	-6.17	100.81	110.50
2	O	163	PRO	N-CD-CG	-6.13	94.01	103.20
2	O	163	PRO	CB-CA-C	-5.75	104.04	111.46
1	C	430	ALA	O-C-N	5.73	128.19	122.12
2	M	163	PRO	N-CA-CB	-5.55	97.43	103.25
1	A	329	ARG	CB-CA-C	-5.37	102.20	110.26
1	A	483	ASN	N-CA-C	5.24	116.99	111.28
2	M	161	TYR	CA-C-O	-5.23	115.45	121.47
3	P	143	TYR	N-CA-CB	5.12	119.48	110.37

There are no chirality outliers.

There are no planarity outliers.

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	3798	0	3560	90	0
1	B	3684	0	3364	79	0
1	C	3719	0	3432	77	0
2	H	1559	0	1379	65	0
2	M	1547	0	1371	44	0
2	O	1575	0	1425	74	0
3	L	1446	0	1255	39	0
3	N	1426	0	1260	47	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	1481	0	1347	50	0
4	D	39	0	34	9	0
4	E	39	0	34	0	0
4	G	39	0	34	0	0
4	I	39	0	34	0	0
4	J	39	0	34	4	0
4	K	39	0	34	1	0
4	Q	39	0	34	2	0
4	R	39	0	34	1	0
4	U	39	0	34	4	0
4	W	39	0	34	2	0
4	X	39	0	34	0	0
4	Y	39	0	34	2	0
4	Z	39	0	34	0	0
5	F	28	0	25	0	0
5	S	28	0	25	0	0
5	T	28	0	25	0	0
5	V	28	0	25	0	0
5	a	28	0	25	1	0
6	B	14	0	13	0	0
All	All	20896	0	18973	560	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (560) 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)
2:O:163:PRO:HG3	2:O:216:HIS:CE1	1.13	1.65
2:O:163:PRO:CG	2:O:216:HIS:NE2	1.68	1.53
2:O:163:PRO:CG	2:O:216:HIS:CE1	1.95	1.48
2:O:163:PRO:HG3	2:O:216:HIS:NE2	1.14	1.41
3:N:143:TYR:CD2	3:N:144:PRO:HG3	1.66	1.29
2:H:132:THR:HA	2:H:162:PHE:CD1	1.68	1.28
1:C:429:VAL:O	1:C:433:ASN:ND2	1.68	1.26
3:N:143:TYR:HD2	3:N:144:PRO:CG	1.51	1.23
2:M:163:PRO:HD2	2:M:216:HIS:NE2	1.55	1.20
1:A:131:THR:HB	1:A:155:THR:CG2	1.72	1.18
2:H:163:PRO:HG2	2:H:216:HIS:CE1	1.82	1.15
2:H:163:PRO:HG2	2:H:216:HIS:NE2	1.66	1.09
2:O:163:PRO:HG2	2:O:216:HIS:NE2	1.69	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:143:TYR:HB3	3:N:144:PRO:CD	1.84	1.07
1:A:131:THR:HB	1:A:155:THR:HG22	1.34	1.07
3:N:143:TYR:CB	3:N:144:PRO:HD3	1.82	1.06
3:P:143:TYR:HB3	3:P:144:PRO:HD3	1.42	0.99
2:H:163:PRO:CG	2:H:216:HIS:CE1	2.45	0.99
2:M:163:PRO:HD2	2:M:216:HIS:HE2	0.82	0.97
3:N:143:TYR:HB3	3:N:144:PRO:HD3	0.96	0.96
2:H:162:PHE:HB3	2:H:163:PRO:CD	1.97	0.94
3:P:143:TYR:HD2	3:P:144:PRO:HG3	1.30	0.94
2:M:163:PRO:CD	2:M:216:HIS:HE2	1.77	0.93
3:N:143:TYR:HD2	3:N:144:PRO:HG3	0.77	0.92
2:O:163:PRO:HG3	2:O:216:HIS:HE1	1.22	0.91
2:H:111:GLN:HB3	2:H:112:PRO:HD2	1.56	0.87
2:H:132:THR:HA	2:H:162:PHE:HD1	1.34	0.87
1:A:131:THR:HB	1:A:155:THR:HG23	1.55	0.86
1:B:456:ARG:NH2	1:B:488:HIS:NE2	2.23	0.85
2:H:132:THR:CA	2:H:162:PHE:CD1	2.57	0.85
2:O:162:PHE:H	2:O:163:PRO:HD2	1.43	0.84
2:H:74:TRP:CZ3	4:D:2:NAG:H2	2.13	0.83
3:L:199:THR:HA	3:L:206:GLU:HB3	1.61	0.83
1:B:161:TYR:HE2	1:B:249:GLY:HA2	1.44	0.83
2:O:162:PHE:N	2:O:163:PRO:HD2	1.91	0.83
2:H:151:THR:N	2:H:202:SER:HG	1.77	0.83
3:N:162:VAL:HG21	3:N:181:LEU:HA	1.61	0.82
3:P:146:ALA:HB1	3:P:201:GLU:CB	2.11	0.81
2:H:74:TRP:CZ3	4:D:2:NAG:H4	2.16	0.80
2:H:74:TRP:CE3	4:D:2:NAG:H2	2.16	0.80
1:C:428:LEU:O	1:C:432:GLU:HB2	1.82	0.80
1:B:206:THR:HG23	1:B:209:SER:H	1.44	0.80
1:B:237:VAL:HG21	1:B:243:LEU:HB2	1.64	0.80
3:N:143:TYR:CD2	3:N:144:PRO:CG	2.43	0.79
2:M:163:PRO:CD	2:M:216:HIS:NE2	2.42	0.79
3:L:143:TYR:HB3	3:L:144:PRO:HD3	1.63	0.79
2:O:163:PRO:CG	2:O:216:HIS:HE1	1.83	0.78
3:P:181:LEU:HG	3:P:183:LEU:HD21	1.66	0.77
3:P:143:TYR:CD2	3:P:144:PRO:HG3	2.17	0.77
2:H:162:PHE:HB3	2:H:163:PRO:HD2	1.66	0.77
1:B:470:TYR:HD2	1:B:499:ARG:HG2	1.49	0.76
2:H:74:TRP:CH2	4:D:2:NAG:H4	2.20	0.76
3:P:169:LYS:HG2	3:P:175:TYR:CE1	2.20	0.76
3:P:91:THR:N	3:P:98:TRP:CZ3	2.53	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:TYR:N	1:C:139:CYS:SG	2.58	0.75
3:P:3:VAL:HG22	3:P:99:VAL:HG21	1.68	0.75
3:P:169:LYS:CG	3:P:175:TYR:HE1	1.99	0.75
1:A:499:ARG:CD	1:A:500:PHE:CE1	2.71	0.73
2:H:163:PRO:CG	2:H:216:HIS:NE2	2.45	0.72
2:H:163:PRO:HG2	2:H:216:HIS:HE2	1.52	0.72
3:P:181:LEU:HG	3:P:183:LEU:CD2	2.20	0.71
3:N:143:TYR:CB	3:N:144:PRO:CD	2.52	0.71
2:H:162:PHE:CB	2:H:163:PRO:CD	2.68	0.70
1:B:402:VAL:HG11	1:C:111:LEU:HD13	1.73	0.70
2:H:162:PHE:HB3	2:H:163:PRO:HD3	1.73	0.70
2:M:163:PRO:HD2	2:M:216:HIS:CE1	2.26	0.70
2:O:163:PRO:CB	2:O:216:HIS:NE2	2.54	0.70
1:B:47:SER:HB2	1:B:288:ILE:HG22	1.71	0.70
3:N:143:TYR:O	3:N:175:TYR:CD2	2.45	0.70
1:A:97:CYS:SG	1:A:98:TYR:N	2.65	0.70
1:A:499:ARG:HD2	1:A:500:PHE:CE1	2.26	0.69
1:A:87:PHE:HB3	1:A:267:ILE:HG22	1.73	0.69
2:O:161:TYR:HE2	2:O:194:LEU:H	1.39	0.68
1:B:31:ASN:HD21	1:B:34:ILE:HB	1.59	0.68
1:B:458:ASN:N	1:B:458:ASN:OD1	2.26	0.68
2:O:92:ILE:HG22	2:O:124:MET:HG2	1.75	0.68
4:D:1:NAG:H62	4:D:2:NAG:H83	1.75	0.67
1:A:131:THR:CB	1:A:155:THR:CG2	2.63	0.67
1:B:206:THR:CG2	1:B:209:SER:H	2.08	0.67
1:A:125:PHE:O	1:A:127:TRP:N	2.27	0.66
3:N:143:TYR:CD2	3:N:144:PRO:N	2.63	0.66
2:H:164:GLU:N	2:H:165:PRO:HD2	2.10	0.66
3:L:148:THR:HG23	3:L:199:THR:HB	1.77	0.66
1:C:429:VAL:C	1:C:433:ASN:ND2	2.51	0.66
2:O:163:PRO:CD	2:O:216:HIS:CE1	2.77	0.66
3:L:28:ASP:HA	3:L:93:ASP:HA	1.75	0.66
3:N:47:LEU:HD21	3:N:50:TYR:HB3	1.77	0.66
1:A:331:ILE:HD13	1:A:331:ILE:N	2.11	0.65
3:N:143:TYR:CD2	3:N:144:PRO:CD	2.78	0.65
1:C:462:MET:HE2	1:C:466:CYS:HB3	1.79	0.65
2:H:163:PRO:HG3	2:H:216:HIS:CE1	2.33	0.64
1:A:499:ARG:HD2	1:A:500:PHE:CZ	2.33	0.64
3:N:143:TYR:O	3:N:175:TYR:HD2	1.78	0.64
1:C:16:GLY:HA2	1:C:338:PHE:HB3	1.79	0.64
1:A:99:PRO:HB3	1:A:223:ILE:HD11	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:132:THR:HA	2:H:162:PHE:CG	2.27	0.64
1:A:295:GLN:NE2	1:A:298:ASN:O	2.28	0.64
2:O:10:GLY:HA3	2:O:218:PRO:HB3	1.80	0.64
1:C:295:GLN:NE2	1:C:298:ASN:O	2.28	0.64
3:P:120:LEU:HD13	3:P:211:PRO:HD3	1.79	0.64
1:C:433:ASN:O	1:C:436:THR:N	2.31	0.63
3:P:143:TYR:CB	3:P:144:PRO:HD3	2.18	0.63
2:O:39:GLN:O	2:O:91:ALA:HB1	1.98	0.63
1:A:409:LEU:HD12	1:C:409:LEU:HD21	1.79	0.63
1:B:31:ASN:ND2	1:B:34:ILE:HB	2.12	0.63
1:C:55:PRO:HD3	1:C:278:LYS:HA	1.81	0.63
3:L:18:VAL:HG13	3:L:79:LEU:HD11	1.79	0.63
3:N:36:TRP:CG	3:N:74:LEU:HD12	2.33	0.63
1:C:340:GLU:OE1	1:C:341:ASN:ND2	2.31	0.63
1:A:206:THR:HG23	1:A:209:SER:H	1.64	0.63
2:M:10:GLY:HA3	2:M:218:PRO:HB3	1.81	0.63
2:O:91:ALA:HB3	2:O:93:TYR:HE1	1.64	0.62
1:A:86:LEU:HB2	1:A:302:TYR:HE2	1.64	0.62
2:H:155:GLY:HA2	2:H:170:TRP:HH2	1.63	0.62
3:N:143:TYR:HD2	3:N:144:PRO:CD	2.11	0.62
3:P:169:LYS:HG3	3:P:175:TYR:HE1	1.65	0.62
2:O:163:PRO:CD	2:O:216:HIS:HE1	2.12	0.62
2:H:133:LYS:H	2:H:162:PHE:HB2	1.65	0.62
1:A:125:PHE:HB2	1:A:127:TRP:CE2	2.33	0.62
1:B:161:TYR:CE2	1:B:249:GLY:HA2	2.32	0.62
2:H:132:THR:HG22	2:H:162:PHE:CE1	2.35	0.62
2:H:163:PRO:HG3	2:H:216:HIS:HE1	1.65	0.61
3:L:36:TRP:HB2	3:L:49:ILE:HB	1.81	0.61
3:P:40:LEU:HD23	3:P:85:ALA:HB2	1.82	0.61
2:M:74:TRP:CZ2	4:U:2:NAG:H2	2.35	0.61
3:P:169:LYS:CG	3:P:175:TYR:CE1	2.80	0.61
2:M:163:PRO:CD	2:M:216:HIS:CE1	2.84	0.61
1:C:230:ILE:HD13	1:C:252:ILE:HD13	1.83	0.60
2:H:172:SER:N	2:H:213:ASN:OD1	2.34	0.60
3:N:18:VAL:HG13	3:N:79:LEU:HD11	1.84	0.60
3:P:120:LEU:HD22	3:P:211:PRO:HG3	1.82	0.60
2:H:133:LYS:N	2:H:162:PHE:HB2	2.17	0.60
5:a:2:NAG:H3	5:a:2:NAG:H83	1.84	0.60
3:P:170:GLN:HG3	3:P:172:ASN:H	1.67	0.59
3:P:81:THR:HA	3:P:108:VAL:HG21	1.83	0.59
2:H:6:GLU:HG3	2:H:22:CYS:SG	2.42	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:144:PRO:C	3:L:146:ALA:H	2.11	0.59
4:J:2:NAG:H3	4:J:3:BMA:O5	2.03	0.59
1:B:177:LEU:HB2	1:B:260:ILE:HD11	1.84	0.59
2:M:51:ILE:HB	2:M:69:ILE:HG21	1.85	0.59
1:A:460:GLU:OE1	1:B:456:ARG:NH1	2.36	0.58
2:H:132:THR:CA	2:H:162:PHE:HD1	2.09	0.58
3:N:120:LEU:HD13	3:N:211:PRO:HD3	1.84	0.58
1:A:325:GLU:HA	1:A:341:ASN:HB2	1.85	0.58
1:A:131:THR:CB	1:A:155:THR:HG22	2.23	0.58
2:M:50:TYR:CE1	2:M:58:GLN:HB2	2.38	0.58
2:O:124:MET:SD	2:O:164:GLU:HG2	2.44	0.58
3:N:84:GLU:HG3	3:N:108:VAL:HG12	1.85	0.58
1:A:97:CYS:O	1:A:224:ARG:NH2	2.21	0.58
2:O:166:VAL:O	2:O:166:VAL:HG13	2.02	0.58
1:C:172:GLU:N	1:C:172:GLU:OE1	2.36	0.58
1:C:429:VAL:C	1:C:433:ASN:HD22	2.08	0.58
2:O:163:PRO:HG2	2:O:216:HIS:CE1	2.18	0.58
2:H:17:THR:HG22	2:H:83:ASN:HB3	1.84	0.58
1:A:359:GLU:N	1:A:359:GLU:OE1	2.36	0.57
3:N:165:THR:HG22	3:N:178:SER:H	1.69	0.57
3:L:55:ARG:NH1	3:L:59:ILE:O	2.37	0.57
1:C:427:LEU:O	1:C:431:LEU:HB2	2.04	0.57
3:P:192:ARG:O	3:P:212:THR:HG23	2.04	0.57
2:H:163:PRO:HG3	2:H:218:PRO:HB2	1.86	0.57
3:P:11:SER:HB2	3:P:109:LEU:HD11	1.87	0.57
2:H:211:ILE:HA	2:H:226:LYS:HA	1.85	0.57
1:B:15:LEU:HD11	1:B:448:PHE:HD1	1.69	0.57
1:B:70:LEU:HD21	1:B:179:ILE:HG13	1.86	0.57
2:O:51:ILE:HB	2:O:69:ILE:HG21	1.87	0.57
4:K:2:NAG:O7	4:K:2:NAG:O3	2.20	0.57
2:M:18:LEU:HB3	2:M:82:VAL:HG13	1.86	0.56
2:M:166:VAL:HG23	2:M:166:VAL:O	2.05	0.56
3:N:111:GLN:HB2	3:N:143:TYR:CE1	2.40	0.56
2:O:162:PHE:C	2:O:162:PHE:CD2	2.83	0.56
2:H:163:PRO:CD	2:H:216:HIS:HE2	2.17	0.56
3:L:126:GLU:OE1	3:L:126:GLU:N	2.37	0.56
1:A:339:ILE:HD12	1:A:339:ILE:H	1.70	0.56
1:B:89:GLU:HG3	1:B:267:ILE:HD11	1.88	0.56
3:P:90:GLY:C	3:P:98:TRP:CZ3	2.83	0.56
3:P:143:TYR:HB3	3:P:144:PRO:CD	2.26	0.56
1:A:98:TYR:HD1	1:A:147:PHE:HE1	1.54	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:LYS:NZ	1:C:461:ASP:OD2	2.34	0.56
1:B:184:HIS:O	1:B:228:SER:OG	2.22	0.56
2:M:211:ILE:HA	2:M:226:LYS:HA	1.88	0.56
1:C:186:VAL:HG13	1:C:187:THR:HG22	1.87	0.56
2:M:40:SER:HB2	2:M:43:LYS:HB2	1.87	0.56
2:M:74:TRP:HE1	4:U:2:NAG:H83	1.71	0.56
3:P:199:THR:HA	3:P:206:GLU:HA	1.88	0.56
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.86	0.55
2:H:132:THR:HG22	2:H:162:PHE:HE1	1.70	0.55
1:B:172:GLU:OE1	1:B:172:GLU:N	2.39	0.55
1:B:203:THR:N	1:B:246:ASN:O	2.39	0.55
1:A:241:ASP:OD1	1:A:242:ILE:N	2.38	0.55
2:H:111:GLN:HB3	2:H:112:PRO:CD	2.35	0.55
1:B:266:SER:HB2	1:B:393:HIS:HB2	1.89	0.55
1:A:67:ILE:HD12	1:A:108:LEU:HD23	1.88	0.55
1:A:499:ARG:HG2	1:A:500:PHE:CE1	2.42	0.55
2:H:163:PRO:HD2	2:H:216:HIS:HE2	1.72	0.55
3:P:90:GLY:C	3:P:98:TRP:HZ3	2.13	0.55
3:L:167:PRO:HA	3:L:177:ALA:HB2	1.89	0.55
1:B:187:THR:HG23	1:B:190:ASP:H	1.72	0.55
2:H:163:PRO:CG	2:H:216:HIS:HE2	2.12	0.55
1:A:102:VAL:HG23	1:A:232:ILE:O	2.07	0.54
3:N:162:VAL:HG22	3:N:180:TYR:O	2.07	0.54
1:A:356:GLN:HB2	1:A:361:ARG:HD3	1.89	0.54
1:A:460:GLU:OE1	1:A:470:TYR:OH	2.23	0.54
1:A:18:HIS:N	1:A:350:TRP:O	2.41	0.54
1:A:307:ARG:NH2	1:A:389:ASN:OD1	2.39	0.54
2:O:216:HIS:CD2	2:O:218:PRO:HD2	2.42	0.54
2:O:29:ILE:HD11	2:O:71:LEU:HB2	1.90	0.54
2:O:91:ALA:HB3	2:O:93:TYR:CE1	2.43	0.54
2:O:216:HIS:HD1	2:O:219:SER:HG	1.54	0.54
3:P:143:TYR:CB	3:P:144:PRO:CD	2.85	0.54
3:L:149:VAL:HG22	3:L:198:VAL:HG13	1.90	0.54
1:B:207:LYS:CB	1:B:241:ASP:OD1	2.56	0.54
2:M:162:PHE:CD2	2:M:162:PHE:C	2.85	0.54
3:L:123:PRO:HB3	3:L:134:THR:H	1.72	0.53
1:C:459:ALA:HB2	1:C:469:ILE:HD13	1.90	0.53
2:O:6:GLU:N	2:O:6:GLU:OE1	2.41	0.53
1:A:165:ASN:HB2	4:J:1:NAG:H83	1.91	0.53
2:M:91:ALA:HB3	2:M:93:TYR:HE1	1.73	0.53
1:B:124:SER:OG	2:M:73:ASN:OD1	2.22	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:134:THR:HG22	3:N:182:SER:HA	1.88	0.53
2:H:130:ALA:HB3	2:H:162:PHE:CZ	2.44	0.53
1:C:428:LEU:O	1:C:432:GLU:CB	2.55	0.53
2:H:74:TRP:CZ3	4:D:2:NAG:C4	2.90	0.53
3:L:40:LEU:HD23	3:L:85:ALA:HB2	1.91	0.53
1:A:266:SER:HB2	1:A:393:HIS:HB2	1.89	0.53
2:M:162:PHE:HD2	2:M:163:PRO:HG3	1.72	0.53
2:O:185:VAL:HG21	3:P:163:GLU:HB3	1.90	0.53
1:B:295:GLN:NE2	1:B:298:ASN:O	2.38	0.53
1:B:98:TYR:CG	1:B:99:PRO:HD2	2.44	0.53
2:O:74:TRP:CE3	4:W:2:NAG:H2	2.44	0.53
1:A:302:TYR:HE1	1:A:392:PHE:CD1	2.27	0.53
1:C:281:CYS:O	1:C:287:SER:OG	2.20	0.53
1:A:98:TYR:CE2	1:A:226:ILE:HG12	2.44	0.53
1:A:172:GLU:N	1:A:172:GLU:OE1	2.41	0.52
4:Q:1:NAG:O3	4:Q:2:NAG:O5	2.23	0.52
1:A:55:PRO:HD3	1:A:278:LYS:HA	1.91	0.52
1:A:333:GLY:O	1:A:361:ARG:NH2	2.42	0.52
3:L:38:GLN:HB3	3:L:48:VAL:HG21	1.91	0.52
1:C:354:ARG:HG2	1:C:363:GLN:HB2	1.91	0.52
1:C:431:LEU:C	1:C:431:LEU:HD23	2.34	0.52
1:A:499:ARG:HG2	1:A:500:PHE:CD1	2.44	0.52
2:H:47:TRP:CG	3:L:98:TRP:HB3	2.45	0.52
1:C:433:ASN:ND2	1:C:433:ASN:H	2.08	0.52
2:M:133:LYS:H	2:M:162:PHE:HB2	1.75	0.52
2:M:156:CYS:C	2:M:157:LEU:HD12	2.34	0.52
3:P:148:THR:HG1	3:P:199:THR:HG1	1.57	0.52
3:L:134:THR:HG22	3:L:182:SER:HA	1.91	0.52
2:M:97:ARG:HH21	2:M:118:LEU:HD22	1.73	0.52
1:B:179:ILE:O	1:B:254:PRO:HB3	2.10	0.52
1:C:102:VAL:HG23	1:C:232:ILE:O	2.10	0.52
2:M:6:GLU:N	2:M:6:GLU:OE1	2.43	0.52
3:N:143:TYR:CD2	3:N:144:PRO:CA	2.93	0.52
1:C:248:THR:HG23	4:Y:1:NAG:H82	1.91	0.52
1:A:325:GLU:OE2	1:A:329:ARG:HG3	2.10	0.52
1:B:37:THR:OG1	1:B:38:ASN:N	2.42	0.52
1:A:321:ARG:NH1	1:A:441:ASP:OD2	2.28	0.51
3:L:143:TYR:CB	3:L:144:PRO:HD3	2.38	0.51
1:B:73:ASP:HB3	1:B:76:CYS:SG	2.50	0.51
3:P:212:THR:HG22	3:P:213:GLU:N	2.25	0.51
1:B:218:GLY:O	1:B:220:ARG:NH1	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LEU:HB2	1:A:302:TYR:CE2	2.45	0.51
1:A:109:ARG:CZ	1:A:267:ILE:HD11	2.40	0.51
2:H:91:ALA:HB3	2:H:93:TYR:HE1	1.75	0.51
2:H:105:ASP:HB3	2:H:111:GLN:HG3	1.92	0.51
1:A:47:SER:HB2	1:A:288:ILE:HG22	1.91	0.51
1:B:295:GLN:OE1	1:B:297:VAL:N	2.43	0.51
1:A:98:TYR:HD2	1:A:99:PRO:CD	2.23	0.51
1:A:348:ASP:OD1	1:A:348:ASP:N	2.38	0.51
1:B:80:GLN:HB2	1:B:150:ARG:NH2	2.26	0.51
3:N:143:TYR:CG	3:N:144:PRO:N	2.77	0.51
1:A:311:GLN:HG2	1:A:314:LEU:HD21	1.92	0.51
3:L:143:TYR:HD2	3:L:144:PRO:CD	2.24	0.51
3:L:142:PHE:O	3:L:175:TYR:HB2	2.11	0.51
1:C:474:ASP:N	1:C:477:CYS:SG	2.84	0.51
2:H:61:PRO:HD3	3:L:97:ILE:HD13	1.93	0.50
1:C:68:ASP:OD2	1:C:95:SER:OG	2.28	0.50
1:C:173:GLN:HG2	2:O:108:GLY:HA2	1.93	0.50
1:C:179:ILE:O	1:C:254:PRO:HB3	2.11	0.50
1:B:186:VAL:HG13	1:B:187:THR:HG22	1.92	0.50
1:A:28:THR:HG22	1:A:433:ASN:HB3	1.93	0.50
1:A:377:ILE:HD12	1:A:436:THR:HG23	1.92	0.50
2:O:105:ASP:HB3	2:O:111:GLN:HG2	1.93	0.50
3:P:141:ASP:HA	3:P:174:LYS:HB3	1.92	0.50
1:A:60:ASP:HA	1:A:88:VAL:HG23	1.93	0.50
3:L:143:TYR:CD2	3:L:144:PRO:CD	2.94	0.50
1:C:246:ASN:CG	4:Y:1:NAG:H83	2.37	0.50
4:Q:1:NAG:H83	4:R:1:NAG:H82	1.94	0.50
1:A:98:TYR:HD2	1:A:99:PRO:HD2	1.75	0.50
1:B:84:TRP:CE2	1:B:116:GLY:HA2	2.46	0.50
1:A:186:VAL:HG23	1:A:219:SER:HA	1.93	0.50
2:M:99:THR:O	2:M:113:GLY:HA3	2.12	0.50
1:B:474:ASP:N	1:B:477:CYS:SG	2.85	0.50
3:N:187:GLN:HA	3:N:190:SER:HB3	1.94	0.50
1:A:277:CYS:SG	1:A:278:LYS:N	2.84	0.50
3:L:53:ASN:ND2	3:L:53:ASN:O	2.45	0.50
1:C:433:ASN:ND2	1:C:433:ASN:N	2.60	0.50
2:O:54:SER:HB2	2:O:109:TYR:CD2	2.47	0.50
2:H:17:THR:HA	2:H:83:ASN:HA	1.94	0.50
3:L:114:ALA:HB3	3:L:143:TYR:N	2.27	0.50
2:H:33:TYR:HB2	2:H:98:HIS:HB2	1.93	0.49
1:B:55:PRO:HD3	1:B:278:LYS:HA	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:TYR:CE1	1:C:257:TYR:HB3	2.47	0.49
2:M:47:TRP:CG	3:N:98:TRP:HB3	2.47	0.49
1:A:237:VAL:HG21	1:A:243:LEU:HB2	1.95	0.49
3:P:184:THR:HG22	3:P:186:GLU:H	1.77	0.49
3:L:81:THR:O	3:L:173:ASN:ND2	2.44	0.49
1:B:207:LYS:HB2	1:B:241:ASP:OD1	2.10	0.49
1:A:60:ASP:OD2	1:A:90:ARG:NH2	2.44	0.49
1:B:131:THR:OG1	1:B:155:THR:OG1	2.22	0.49
2:M:66:ARG:O	2:M:82:VAL:HA	2.13	0.49
2:H:163:PRO:CG	2:H:216:HIS:HE1	2.10	0.49
1:B:123:GLU:HB3	1:B:168:MET:HE3	1.94	0.49
3:N:36:TRP:HB2	3:N:49:ILE:HB	1.94	0.49
1:C:187:THR:HG23	1:C:190:ASP:H	1.78	0.49
1:C:431:LEU:C	1:C:431:LEU:CD2	2.85	0.49
2:O:24:VAL:HG12	2:O:76:ASN:O	2.13	0.49
1:A:499:ARG:CG	1:A:500:PHE:CE1	2.96	0.49
2:M:163:PRO:C	2:M:165:PRO:HD2	2.38	0.49
3:N:200:HIS:HB3	3:N:203:SER:CB	2.43	0.49
2:O:151:THR:N	2:O:202:SER:HG	2.10	0.49
1:B:134:GLY:HA3	1:B:153:TRP:HB3	1.95	0.49
2:O:17:THR:HA	2:O:83:ASN:HA	1.95	0.49
2:O:163:PRO:HG2	2:O:163:PRO:O	2.13	0.49
2:H:6:GLU:N	2:H:6:GLU:OE1	2.46	0.48
1:C:206:THR:HG23	1:C:209:SER:H	1.78	0.48
3:P:18:VAL:HG13	3:P:79:LEU:HD11	1.94	0.48
1:A:113:ALA:HB1	1:A:267:ILE:HG23	1.95	0.48
3:L:39:GLN:HB3	3:L:86:VAL:HG23	1.94	0.48
1:C:309:VAL:HG12	1:C:311:GLN:H	1.77	0.48
1:A:186:VAL:HG13	1:A:187:THR:HG22	1.94	0.48
2:H:69:ILE:HG12	2:H:80:LEU:HD13	1.93	0.48
1:C:309:VAL:HG13	1:C:422:SER:HA	1.95	0.48
2:O:135:PRO:HB3	2:O:161:TYR:HB3	1.95	0.48
2:M:24:VAL:HG12	2:M:76:ASN:O	2.12	0.48
2:O:39:GLN:HA	2:O:45:LEU:HD23	1.94	0.48
1:A:84:TRP:CZ2	1:A:116:GLY:HA2	2.48	0.48
2:H:103:HIS:O	2:H:103:HIS:ND1	2.47	0.48
3:N:144:PRO:C	3:N:146:ALA:H	2.21	0.48
2:O:182:PHE:CD2	3:P:178:SER:HB3	2.48	0.48
4:D:1:NAG:H62	4:D:2:NAG:C8	2.44	0.48
3:L:10:VAL:HG23	3:L:106:LEU:HD23	1.95	0.48
1:B:456:ARG:CZ	1:B:488:HIS:NE2	2.75	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:128:LEU:HA	3:N:132:LYS:O	2.13	0.48
1:C:429:VAL:HG13	1:C:433:ASN:HD21	1.78	0.48
2:O:160:ASP:HA	2:O:191:LEU:HB3	1.96	0.48
1:C:304:ALA:HA	1:C:390:GLU:HA	1.96	0.48
1:C:348:ASP:N	1:C:348:ASP:OD1	2.46	0.48
1:A:184:HIS:CE1	1:A:216:ASN:H	2.32	0.47
1:B:96:ASN:HA	1:B:224:ARG:CZ	2.43	0.47
3:N:33:PHE:O	3:N:91:THR:OG1	2.30	0.47
3:N:39:GLN:HB2	3:N:45:PRO:HB3	1.95	0.47
3:N:39:GLN:HB3	3:N:86:VAL:HG23	1.94	0.47
1:C:429:VAL:O	1:C:433:ASN:N	2.39	0.47
2:H:74:TRP:CD1	2:H:75:ASN:N	2.82	0.47
1:A:84:TRP:CE2	1:A:116:GLY:HA2	2.49	0.47
1:B:84:TRP:HZ2	1:B:113:ALA:HA	1.79	0.47
1:B:381:LEU:O	1:B:385:ILE:HG22	2.14	0.47
2:O:90:THR:HB	2:O:127:VAL:HG23	1.97	0.47
2:O:162:PHE:N	2:O:163:PRO:CD	2.71	0.47
1:B:43:VAL:HB	1:B:313:THR:HA	1.96	0.47
1:B:184:HIS:CE1	1:B:216:ASN:H	2.32	0.47
1:B:478:ILE:HG22	1:B:482:ARG:HH11	1.80	0.47
1:C:77:ASP:CG	1:C:141:ARG:HH21	2.21	0.47
1:C:108:LEU:HD23	1:C:234:TRP:CD2	2.49	0.47
2:M:100:LEU:H	2:M:100:LEU:HD23	1.80	0.47
3:N:53:ASN:OD1	3:N:53:ASN:N	2.47	0.47
1:C:241:ASP:OD1	1:C:242:ILE:N	2.41	0.47
2:O:162:PHE:CD2	2:O:162:PHE:O	2.68	0.47
2:O:167:THR:OG1	2:O:215:ASN:HB3	2.15	0.47
1:B:28:THR:HG22	1:B:433:ASN:HB3	1.95	0.47
1:C:16:GLY:C	1:C:444:MET:HE1	2.39	0.47
1:C:67:ILE:HD12	1:C:108:LEU:HD12	1.96	0.47
2:O:103:HIS:O	2:O:103:HIS:ND1	2.47	0.47
2:O:162:PHE:O	2:O:162:PHE:CG	2.67	0.47
3:P:212:THR:HG22	3:P:213:GLU:O	2.15	0.47
2:H:40:SER:HB2	2:H:43:LYS:HB2	1.95	0.47
1:C:429:VAL:CG1	1:C:433:ASN:HD21	2.27	0.47
1:C:13:LEU:HD11	1:C:353:PHE:HB3	1.97	0.47
1:B:38:ASN:OD1	1:B:318:THR:OG1	2.32	0.47
2:M:97:ARG:NH2	2:M:118:LEU:HD22	2.29	0.47
2:O:69:ILE:HG12	2:O:80:LEU:HD13	1.95	0.47
4:D:1:NAG:O3	4:D:1:NAG:H83	2.15	0.47
1:A:412:TYR:OH	1:B:414:GLU:OE1	2.32	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ASP:OD1	1:A:474:ASP:N	2.42	0.46
3:P:146:ALA:CB	3:P:201:GLU:CB	2.91	0.46
1:A:52:CYS:HB2	1:A:279:SER:HB3	1.97	0.46
3:N:120:LEU:HD13	3:N:211:PRO:CD	2.45	0.46
3:P:36:TRP:CE2	3:P:74:LEU:HB2	2.50	0.46
1:A:18:HIS:HB2	1:A:350:TRP:HA	1.97	0.46
1:B:371:GLN:NE2	1:B:375:ASP:OD1	2.46	0.46
1:C:295:GLN:OE1	1:C:297:VAL:N	2.49	0.46
2:O:66:ARG:HH12	2:O:86:THR:HG22	1.80	0.46
1:B:293:PRO:C	1:B:306:PRO:HB3	2.40	0.46
2:H:135:PRO:HA	2:H:161:TYR:HB3	1.98	0.46
2:O:64:THR:C	2:O:66:ARG:H	2.23	0.46
3:P:114:ALA:HB3	3:P:143:TYR:N	2.31	0.46
1:A:39:ALA:HA	1:A:318:THR:HG23	1.97	0.46
1:C:343:TRP:CE2	1:C:354:ARG:HD2	2.51	0.46
4:J:2:NAG:C1	4:J:2:NAG:C8	2.94	0.46
2:M:17:THR:HA	2:M:83:ASN:HA	1.97	0.46
2:O:172:SER:N	2:O:213:ASN:OD1	2.48	0.46
1:A:391:LYS:HA	1:A:391:LYS:HD2	1.64	0.45
1:B:98:TYR:CD1	1:B:99:PRO:HD2	2.51	0.45
2:M:6:GLU:HG3	2:M:22:CYS:HB2	1.98	0.45
1:C:479:GLY:HA2	1:C:482:ARG:HG2	1.97	0.45
3:L:143:TYR:HD2	3:L:144:PRO:HG3	1.81	0.45
2:M:162:PHE:CD1	2:M:162:PHE:O	2.68	0.45
3:L:143:TYR:CD2	3:L:144:PRO:HD3	2.51	0.45
3:L:172:ASN:O	3:L:174:LYS:N	2.50	0.45
2:O:41:PRO:O	2:O:41:PRO:HG2	2.15	0.45
2:H:171:ASN:HB2	2:H:174:ALA:HB3	1.99	0.45
1:B:169:PRO:HA	1:B:242:ILE:HG22	1.97	0.45
3:N:36:TRP:NE1	3:N:89:CYS:HB3	2.31	0.45
2:O:86:THR:OG1	2:O:87:ALA:N	2.50	0.45
2:H:72:GLN:NE2	2:H:74:TRP:CZ2	2.85	0.45
2:H:156:CYS:C	2:H:157:LEU:HD12	2.41	0.45
2:M:72:GLN:HG3	2:M:75:ASN:OD1	2.16	0.45
3:P:19:THR:HG23	3:P:73:THR:HG23	1.99	0.45
3:P:62:ARG:HG3	3:P:77:THR:O	2.17	0.45
2:H:74:TRP:CG	2:H:75:ASN:N	2.84	0.45
3:L:143:TYR:HD2	3:L:144:PRO:HD3	1.81	0.45
2:O:6:GLU:HG3	2:O:22:CYS:HB2	1.98	0.45
2:O:33:TYR:CE1	2:O:52:TYR:HB2	2.52	0.45
2:O:182:PHE:HB2	2:O:195:SER:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:143:TYR:HD2	3:P:144:PRO:CG	2.17	0.45
1:A:109:ARG:NE	1:A:267:ILE:HD11	2.32	0.45
1:A:115:SER:HA	1:A:261:ARG:O	2.17	0.45
1:A:179:ILE:O	1:A:254:PRO:HB3	2.17	0.45
2:O:74:TRP:CZ3	4:W:2:NAG:H2	2.52	0.45
1:A:325:GLU:HG2	1:A:342:GLY:O	2.18	0.44
3:L:143:TYR:HB3	3:L:144:PRO:CD	2.40	0.44
1:B:382:ASN:HA	1:B:385:ILE:HG22	2.00	0.44
2:O:161:TYR:CE2	2:O:193:SER:HA	2.52	0.44
1:A:293:PRO:C	1:A:306:PRO:HB3	2.42	0.44
1:B:303:GLY:HA2	1:B:392:PHE:HE1	1.81	0.44
2:H:14:PRO:HA	2:H:85:VAL:HG23	1.98	0.44
1:B:176:LYS:HE3	1:B:257:TYR:CG	2.53	0.44
2:M:33:TYR:HB2	2:M:98:HIS:HB2	2.00	0.44
1:C:237:VAL:HG21	1:C:243:LEU:HB2	1.99	0.44
2:H:48:ILE:O	2:H:60:ASN:N	2.43	0.44
1:C:41:GLU:OE1	1:C:313:THR:OG1	2.34	0.44
1:C:131:THR:OG1	1:C:155:THR:OG1	2.33	0.44
1:B:178:TYR:CE1	1:B:257:TYR:HB3	2.53	0.44
2:M:162:PHE:O	2:M:162:PHE:CG	2.68	0.44
2:O:161:TYR:OH	2:O:194:LEU:CB	2.65	0.44
1:B:74:PRO:HD2	1:B:97:CYS:HB2	2.00	0.44
3:P:170:GLN:HG2	3:P:174:LYS:O	2.18	0.44
1:B:321:ARG:HH12	1:B:441:ASP:CG	2.24	0.44
1:A:295:GLN:OE1	1:A:297:VAL:N	2.50	0.44
1:C:164:LEU:O	1:C:246:ASN:HA	2.17	0.44
4:J:1:NAG:H4	4:J:2:NAG:H82	1.98	0.44
1:A:405:ARG:HH22	1:B:403:GLU:CD	2.24	0.43
1:C:220:ARG:HB2	1:C:227:PRO:O	2.18	0.43
1:C:293:PRO:C	1:C:306:PRO:HB3	2.42	0.43
2:O:176:THR:HG23	2:O:177:SER:H	1.82	0.43
1:B:180:TRP:CE2	1:B:204:VAL:HG21	2.53	0.43
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.99	0.43
3:P:181:LEU:O	3:P:183:LEU:HD23	2.18	0.43
1:B:230:ILE:HD13	1:B:252:ILE:HD13	2.00	0.43
2:O:97:ARG:HH21	2:O:118:LEU:HD22	1.83	0.43
4:D:2:NAG:O7	4:D:2:NAG:C3	2.66	0.43
1:B:470:TYR:CD2	1:B:499:ARG:HG2	2.40	0.43
2:M:114:ASP:HA	3:N:92:TRP:HE1	1.83	0.43
3:P:182:SER:O	3:P:183:LEU:HD22	2.17	0.43
2:O:97:ARG:O	2:O:117:ASP:N	2.38	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:MET:HE1	1:B:351:TYR:C	2.43	0.43
1:B:412:TYR:OH	1:C:414:GLU:OE1	2.28	0.43
1:C:31:ASN:HB2	1:C:34:ILE:HG13	2.01	0.43
2:H:155:GLY:HA2	2:H:170:TRP:CH2	2.48	0.43
1:B:128:ALA:O	1:B:130:VAL:HG13	2.17	0.43
1:A:10:THR:OG1	1:A:11:ALA:N	2.52	0.43
1:A:191:GLN:OE1	1:A:250:ASN:ND2	2.43	0.43
3:L:165:THR:HG22	3:L:178:SER:H	1.84	0.43
1:C:60:ASP:OD2	1:C:90:ARG:NH2	2.48	0.43
3:L:145:GLY:O	3:L:167:PRO:HG2	2.19	0.43
3:N:143:TYR:CG	3:N:144:PRO:CD	3.02	0.43
1:A:72:GLY:HA3	1:A:149:SER:OG	2.18	0.43
2:H:136:SER:OG	2:H:159:LYS:O	2.29	0.43
1:B:72:GLY:HA3	1:B:149:SER:OG	2.19	0.43
2:M:164:GLU:N	2:M:165:PRO:HD2	2.34	0.43
2:H:97:ARG:O	2:H:117:ASP:N	2.35	0.42
1:C:307:ARG:HD3	1:C:421:TRP:CE2	2.54	0.42
1:A:125:PHE:HB2	1:A:127:TRP:CZ2	2.54	0.42
1:C:98:TYR:CD1	1:C:99:PRO:HD2	2.54	0.42
1:C:428:LEU:O	1:C:432:GLU:N	2.43	0.42
2:M:47:TRP:HZ2	2:M:50:TYR:HD1	1.66	0.42
2:O:137:VAL:HG11	2:O:214:VAL:HG21	2.00	0.42
1:B:348:ASP:OD1	1:B:348:ASP:N	2.52	0.42
1:C:431:LEU:HD23	1:C:431:LEU:O	2.20	0.42
3:P:151:TRP:HB2	3:P:158:VAL:HG11	1.99	0.42
2:H:132:THR:CB	2:H:162:PHE:HD1	2.32	0.42
1:C:84:TRP:CZ2	1:C:116:GLY:HA2	2.54	0.42
2:O:20:LEU:CD1	2:O:93:TYR:HD2	2.33	0.42
3:P:137:CYS:HB2	3:P:151:TRP:CH2	2.55	0.42
3:P:15:GLY:C	3:P:78:GLY:HA2	2.44	0.42
2:O:33:TYR:HB2	2:O:98:HIS:HB2	2.02	0.42
3:L:86:VAL:HG12	3:L:105:LYS:HA	2.01	0.42
1:B:346:MET:HE1	1:B:352:GLY:HA3	2.02	0.42
2:M:16:GLU:H	2:M:85:VAL:HG12	1.84	0.42
1:C:357:ASN:HD21	1:C:359:GLU:HB2	1.84	0.42
2:O:20:LEU:HD11	2:O:93:TYR:HD2	1.84	0.42
1:A:358:SER:OG	1:A:359:GLU:OE1	2.28	0.42
1:B:13:LEU:HD11	1:B:353:PHE:HB3	2.02	0.42
1:B:15:LEU:HD11	1:B:448:PHE:CD1	2.52	0.42
2:O:121:GLN:HA	3:P:44:ALA:HB2	2.02	0.42
1:A:99:PRO:HB2	1:A:229:ARG:HD3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:HD13	1:A:252:ILE:HD12	2.01	0.42
3:L:144:PRO:C	3:L:146:ALA:N	2.74	0.42
1:B:207:LYS:HB3	1:B:241:ASP:OD1	2.19	0.42
2:M:74:TRP:CE2	4:U:2:NAG:H2	2.55	0.42
3:P:151:TRP:CE3	3:P:181:LEU:HD22	2.55	0.42
1:B:186:VAL:HG23	1:B:219:SER:HA	2.02	0.41
1:B:353:PHE:CZ	1:B:447:LEU:HD11	2.55	0.41
2:M:102:TYR:HD1	2:M:102:TYR:HA	1.75	0.41
3:N:143:TYR:O	3:N:175:TYR:CE2	2.73	0.41
2:O:20:LEU:HD23	2:O:20:LEU:HA	1.92	0.41
3:N:36:TRP:CD1	3:N:74:LEU:HD12	2.56	0.41
3:N:136:VAL:HG22	3:N:180:TYR:CD2	2.55	0.41
1:C:98:TYR:HD2	1:C:230:ILE:HD12	1.86	0.41
1:C:120:PHE:CE2	1:C:150:ARG:HD2	2.55	0.41
1:A:17:HIS:HB3	1:A:444:MET:SD	2.61	0.41
3:L:53:ASN:HB3	3:L:65:GLY:O	2.20	0.41
1:B:120:PHE:CE2	1:B:150:ARG:HD2	2.55	0.41
1:C:89:GLU:HG3	1:C:267:ILE:HD11	2.02	0.41
2:O:64:THR:O	2:O:66:ARG:N	2.54	0.41
2:O:216:HIS:HD2	2:O:218:PRO:HD2	1.82	0.41
2:M:132:THR:HA	2:M:162:PHE:CB	2.51	0.41
2:M:97:ARG:O	2:M:117:ASP:N	2.39	0.41
3:N:28:ASP:HA	3:N:93:ASP:HA	2.02	0.41
2:O:186:LEU:HD11	2:O:190:GLY:HA2	2.03	0.41
2:H:167:THR:OG1	2:H:215:ASN:HB3	2.21	0.41
3:L:197:GLN:HA	3:L:208:THR:OG1	2.20	0.41
3:N:4:LEU:HB3	3:N:101:GLY:HA2	2.02	0.41
1:A:113:ALA:CB	1:A:267:ILE:HG23	2.51	0.41
3:L:143:TYR:CB	3:L:144:PRO:CD	2.99	0.41
1:C:84:TRP:CE2	1:C:116:GLY:HA2	2.56	0.41
1:C:300:ILE:HD13	1:C:300:ILE:HA	1.91	0.41
3:L:143:TYR:CD2	3:L:144:PRO:N	2.89	0.41
1:B:176:LYS:HE3	1:B:257:TYR:CD1	2.56	0.41
1:C:213:VAL:HG11	1:C:233:TYR:CE1	2.56	0.41
1:C:268:MET:HE3	1:C:268:MET:HB2	1.94	0.41
1:C:433:ASN:HD22	1:C:433:ASN:H	1.68	0.41
2:O:99:THR:O	2:O:113:GLY:HA3	2.20	0.41
2:O:167:THR:HG1	2:O:215:ASN:HB3	1.86	0.41
4:U:2:NAG:H62	4:U:3:BMA:O5	2.20	0.41
1:A:187:THR:HG23	1:A:190:ASP:H	1.85	0.41
2:H:162:PHE:CD1	2:H:163:PRO:HD3	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:PHE:HE2	1:B:150:ARG:HD2	1.86	0.41
1:B:303:GLY:HA2	1:B:392:PHE:CE1	2.55	0.41
2:O:39:GLN:NE2	3:P:39:GLN:HE22	2.19	0.41
3:P:120:LEU:HD13	3:P:211:PRO:CD	2.48	0.41
1:A:329:ARG:NH2	1:A:336:ALA:HB2	2.36	0.40
1:A:204:VAL:HG22	1:A:245:ILE:HG23	2.03	0.40
1:A:123:GLU:OE1	1:A:178:TYR:OH	2.35	0.40
2:H:11:LEU:HA	2:H:126:THR:O	2.21	0.40
3:N:7:PRO:HA	3:N:8:PRO:HD3	1.98	0.40
3:N:114:ALA:HB3	3:N:143:TYR:N	2.37	0.40
1:C:433:ASN:C	1:C:435:HIS:N	2.78	0.40
2:O:41:PRO:O	2:O:41:PRO:CG	2.68	0.40
3:P:212:THR:CG2	3:P:213:GLU:N	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	493/505 (98%)	468 (95%)	23 (5%)	2 (0%)	30	65
1	B	484/505 (96%)	459 (95%)	22 (4%)	3 (1%)	21	57
1	C	483/505 (96%)	453 (94%)	25 (5%)	5 (1%)	12	45
2	H	217/237 (92%)	199 (92%)	16 (7%)	2 (1%)	14	48
2	M	217/237 (92%)	201 (93%)	14 (6%)	2 (1%)	14	48
2	O	217/237 (92%)	202 (93%)	13 (6%)	2 (1%)	14	48
3	L	212/215 (99%)	191 (90%)	18 (8%)	3 (1%)	9	39
3	N	212/215 (99%)	194 (92%)	16 (8%)	2 (1%)	14	48
3	P	212/215 (99%)	194 (92%)	15 (7%)	3 (1%)	9	39
All	All	2747/2871 (96%)	2561 (93%)	162 (6%)	24 (1%)	14	48

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
3	N	143	TYR
3	P	146	ALA
2	H	162	PHE
2	M	132	THR
2	M	166	VAL
3	N	145	GLY
2	O	65	GLY
3	L	173	ASN
1	B	458	ASN
1	C	21	PRO
3	L	143	TYR
1	B	21	PRO
1	C	434	GLN
2	O	165	PRO
3	P	78	GLY
1	A	21	PRO
1	B	393	HIS
1	C	378	ASN
2	H	165	PRO
1	C	142	GLY
3	P	143	TYR
3	L	158	VAL
1	C	377	ILE

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	405/440 (92%)	404 (100%)	1 (0%)	87	87
1	B	382/440 (87%)	381 (100%)	1 (0%)	86	85
1	C	395/440 (90%)	394 (100%)	1 (0%)	86	85
2	H	154/200 (77%)	154 (100%)	0	100	100
2	M	152/200 (76%)	151 (99%)	1 (1%)	76	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	O	159/200 (80%)	158 (99%)	1 (1%)	78	81
3	L	141/181 (78%)	141 (100%)	0	100	100
3	N	137/181 (76%)	137 (100%)	0	100	100
3	P	152/181 (84%)	152 (100%)	0	100	100
All	All	2077/2463 (84%)	2072 (100%)	5 (0%)	87	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	331	ILE
1	B	458	ASN
2	M	166	VAL
1	C	431	LEU
2	O	165	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	341	ASN
1	A	371	GLN
1	A	394	GLN
2	H	73	ASN
2	H	103	HIS
3	L	38	GLN
1	B	96	ASN
1	B	121	ASN
1	B	216	ASN
1	B	363	GLN
1	B	389	ASN
1	C	56	HIS
1	C	341	ASN
1	C	363	GLN
2	O	39	GLN
3	P	38	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

49 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$
4	NAG	D	1	4,1	14,14,15	2.99	8 (57%)	17,19,21	4.16	9 (52%)
4	NAG	D	2	4	14,14,15	1.66	4 (28%)	17,19,21	4.06	10 (58%)
4	BMA	D	3	4	11,11,12	1.31	2 (18%)	15,15,17	2.77	8 (53%)
4	NAG	E	1	4,1	14,14,15	0.28	0	17,19,21	0.68	1 (5%)
4	NAG	E	2	4	14,14,15	0.21	0	17,19,21	0.45	0
4	BMA	E	3	4	11,11,12	0.57	0	15,15,17	0.74	0
5	NAG	F	1	5,1	14,14,15	0.57	0	17,19,21	0.87	1 (5%)
5	NAG	F	2	5	14,14,15	0.37	0	17,19,21	0.68	1 (5%)
4	NAG	G	1	4,1	14,14,15	0.34	0	17,19,21	0.59	0
4	NAG	G	2	4	14,14,15	0.19	0	17,19,21	0.66	0
4	BMA	G	3	4	11,11,12	0.64	0	15,15,17	0.69	0
4	NAG	I	1	4,1	14,14,15	0.38	0	17,19,21	0.67	0
4	NAG	I	2	4	14,14,15	0.20	0	17,19,21	0.39	0
4	BMA	I	3	4	11,11,12	0.51	0	15,15,17	0.69	0
4	NAG	J	1	4,1	14,14,15	0.59	0	17,19,21	1.04	2 (11%)
4	NAG	J	2	4	14,14,15	1.37	2 (14%)	17,19,21	2.71	5 (29%)
4	BMA	J	3	4	11,11,12	1.08	1 (9%)	15,15,17	1.10	1 (6%)
4	NAG	K	1	4,1	14,14,15	0.47	0	17,19,21	0.64	0
4	NAG	K	2	4	14,14,15	0.32	0	17,19,21	0.76	1 (5%)
4	BMA	K	3	4	11,11,12	0.70	0	15,15,17	0.68	0
4	NAG	Q	1	4,1	14,14,15	0.23	0	17,19,21	0.40	0
4	NAG	Q	2	4	14,14,15	0.23	0	17,19,21	0.61	1 (5%)
4	BMA	Q	3	4	11,11,12	0.61	0	15,15,17	0.66	0
4	NAG	R	1	4,1	14,14,15	0.42	0	17,19,21	0.62	0
4	NAG	R	2	4	14,14,15	0.24	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMA	R	3	4	11,11,12	0.62	0	15,15,17	0.68	0
5	NAG	S	1	5,1	14,14,15	0.30	0	17,19,21	0.37	0
5	NAG	S	2	5	14,14,15	0.48	0	17,19,21	0.48	0
5	NAG	T	1	5,1	14,14,15	0.48	0	17,19,21	0.52	0
5	NAG	T	2	5	14,14,15	1.60	2 (14%)	17,19,21	1.39	1 (5%)
4	NAG	U	1	4,1	14,14,15	0.30	0	17,19,21	0.54	0
4	NAG	U	2	4	14,14,15	0.21	0	17,19,21	0.60	0
4	BMA	U	3	4	11,11,12	1.09	1 (9%)	15,15,17	0.96	0
5	NAG	V	1	5,1	14,14,15	0.25	0	17,19,21	0.46	0
5	NAG	V	2	5	14,14,15	0.23	0	17,19,21	0.52	0
4	NAG	W	1	4,1	14,14,15	0.37	0	17,19,21	0.52	0
4	NAG	W	2	4	14,14,15	0.22	0	17,19,21	0.79	1 (5%)
4	BMA	W	3	4	11,11,12	0.78	0	15,15,17	0.81	0
4	NAG	X	1	4,1	14,14,15	0.17	0	17,19,21	0.61	0
4	NAG	X	2	4	14,14,15	0.24	0	17,19,21	0.65	0
4	BMA	X	3	4	11,11,12	0.63	0	15,15,17	0.73	0
4	NAG	Y	1	4,1	14,14,15	0.23	0	17,19,21	0.48	0
4	NAG	Y	2	4	14,14,15	0.26	0	17,19,21	0.52	0
4	BMA	Y	3	4	11,11,12	0.65	0	15,15,17	0.69	0
4	NAG	Z	1	4,1	14,14,15	0.25	0	17,19,21	0.67	0
4	NAG	Z	2	4	14,14,15	0.32	0	17,19,21	0.39	0
4	BMA	Z	3	4	11,11,12	0.56	0	15,15,17	0.82	0
5	NAG	a	1	5,1	14,14,15	0.17	0	17,19,21	0.83	0
5	NAG	a	2	5	14,14,15	0.60	1 (7%)	17,19,21	1.39	2 (11%)

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

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	2	4	-	4/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	0/1/1/1
4	NAG	I	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	BMA	I	3	4	-	0/2/19/22	0/1/1/1
4	NAG	J	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	J	2	4	-	3/6/23/26	0/1/1/1
4	BMA	J	3	4	-	2/2/19/22	0/1/1/1
4	NAG	K	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	K	2	4	-	1/6/23/26	0/1/1/1
4	BMA	K	3	4	-	2/2/19/22	0/1/1/1
4	NAG	Q	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	BMA	Q	3	4	-	1/2/19/22	0/1/1/1
4	NAG	R	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
4	BMA	R	3	4	-	0/2/19/22	0/1/1/1
5	NAG	S	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	S	2	5	-	3/6/23/26	0/1/1/1
5	NAG	T	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	T	2	5	-	0/6/23/26	0/1/1/1
4	NAG	U	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	U	2	4	-	4/6/23/26	0/1/1/1
4	BMA	U	3	4	-	2/2/19/22	0/1/1/1
5	NAG	V	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	V	2	5	-	0/6/23/26	0/1/1/1
4	NAG	W	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1
4	BMA	W	3	4	-	0/2/19/22	0/1/1/1
4	NAG	X	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	X	2	4	-	4/6/23/26	0/1/1/1
4	BMA	X	3	4	-	1/2/19/22	0/1/1/1
4	NAG	Y	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	0/6/23/26	0/1/1/1
4	BMA	Y	3	4	-	2/2/19/22	0/1/1/1
4	NAG	Z	1	4,1	-	3/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	Z	2	4	-	0/6/23/26	0/1/1/1
4	BMA	Z	3	4	-	0/2/19/22	0/1/1/1
5	NAG	a	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	a	2	5	-	6/6/23/26	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	NAG	C1-C2	-5.68	1.44	1.52
4	D	1	NAG	O5-C1	-5.10	1.35	1.43
4	D	1	NAG	C2-N2	-4.76	1.38	1.46
5	T	2	NAG	O5-C1	4.40	1.51	1.43
5	T	2	NAG	C1-C2	3.96	1.57	1.52
4	J	2	NAG	C1-C2	3.67	1.57	1.52
4	D	1	NAG	C3-C2	-3.52	1.45	1.52
4	D	2	NAG	C2-N2	-3.26	1.40	1.46
4	J	2	NAG	O5-C1	-2.95	1.38	1.43
4	J	3	BMA	C1-C2	2.94	1.59	1.52
4	D	2	NAG	C1-C2	-2.87	1.48	1.52
4	D	1	NAG	O5-C5	-2.68	1.38	1.43
4	D	3	BMA	C4-C5	-2.65	1.47	1.53
4	U	3	BMA	C1-C2	2.58	1.58	1.52
4	D	1	NAG	C4-C5	-2.44	1.47	1.53
4	D	1	NAG	C4-C3	-2.20	1.46	1.52
4	D	2	NAG	C3-C2	-2.18	1.47	1.52
4	D	2	NAG	C4-C3	-2.10	1.46	1.52
4	D	3	BMA	C4-C3	-2.06	1.47	1.52
4	D	1	NAG	O4-C4	-2.06	1.37	1.43
5	a	2	NAG	C1-C2	2.03	1.55	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	NAG	C2-N2-C7	-11.40	107.62	122.90
4	D	2	NAG	C3-C4-C5	-9.90	92.28	110.23
4	J	2	NAG	C2-N2-C7	8.21	133.90	122.90
4	D	1	NAG	O5-C1-C2	-7.59	99.55	111.29
4	D	2	NAG	O4-C4-C5	6.61	125.60	109.32
4	D	2	NAG	C4-C3-C2	-6.53	101.45	111.02
4	D	3	BMA	C1-O5-C5	5.57	119.65	112.19
4	D	2	NAG	C8-C7-N2	-5.51	106.97	116.12
4	J	2	NAG	C1-C2-N2	5.47	119.06	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	NAG	C4-C3-C2	-5.33	103.20	111.02
4	D	2	NAG	O5-C1-C2	-5.24	103.18	111.29
5	T	2	NAG	C1-O5-C5	5.17	119.11	112.19
4	D	3	BMA	C1-C2-C3	4.59	116.33	109.64
5	a	2	NAG	C2-N2-C7	4.56	129.01	122.90
4	D	3	BMA	C3-C4-C5	-4.29	102.45	110.23
4	D	1	NAG	O4-C4-C3	-3.84	101.33	110.38
4	D	1	NAG	O3-C3-C4	-3.79	101.45	110.38
4	D	1	NAG	O5-C5-C4	-3.78	101.62	110.83
4	D	1	NAG	O3-C3-C2	-3.78	101.55	109.40
4	D	2	NAG	O7-C7-N2	3.43	128.05	121.98
4	D	3	BMA	O3-C3-C4	-3.16	102.94	110.38
4	D	3	BMA	O4-C4-C3	-3.13	103.00	110.38
4	J	3	BMA	C1-C2-C3	3.11	114.17	109.64
4	J	2	NAG	C4-C3-C2	3.10	115.56	111.02
4	D	1	NAG	C3-C4-C5	-2.99	104.81	110.23
4	J	1	NAG	C2-N2-C7	2.88	126.76	122.90
4	D	2	NAG	C2-N2-C7	-2.82	119.12	122.90
4	D	3	BMA	O3-C3-C2	2.79	115.75	110.05
5	F	1	NAG	C1-O5-C5	2.50	115.53	112.19
4	D	2	NAG	O3-C3-C2	2.41	114.40	109.40
4	D	3	BMA	O5-C5-C4	-2.37	105.05	110.83
4	K	2	NAG	C2-N2-C7	2.37	126.07	122.90
4	D	3	BMA	O5-C5-C6	2.33	112.20	107.66
5	a	2	NAG	C1-C2-N2	2.30	114.06	110.43
4	E	1	NAG	C1-O5-C5	2.25	115.21	112.19
4	J	2	NAG	O4-C4-C3	2.24	115.65	110.38
4	D	2	NAG	O3-C3-C4	2.22	115.61	110.38
4	W	2	NAG	C1-O5-C5	2.06	114.95	112.19
4	D	1	NAG	C1-O5-C5	-2.05	109.44	112.19
4	J	2	NAG	C1-O5-C5	-2.01	109.49	112.19
4	Q	2	NAG	C1-O5-C5	2.01	114.88	112.19
5	F	2	NAG	C1-O5-C5	2.01	114.88	112.19
4	J	1	NAG	C1-C2-N2	2.01	113.60	110.43
4	D	2	NAG	O6-C6-C5	-2.01	104.50	111.33

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	J	1	NAG	C1-C2-N2-C7
4	J	2	NAG	C1-C2-N2-C7
5	a	1	NAG	C1-C2-N2-C7
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	U	2	NAG	O5-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
4	U	3	BMA	O5-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	Y	3	BMA	O5-C5-C6-O6
4	D	3	BMA	C4-C5-C6-O6
4	J	3	BMA	O5-C5-C6-O6
5	S	2	NAG	O5-C5-C6-O6
5	a	2	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
5	S	2	NAG	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	J	3	BMA	C4-C5-C6-O6
5	a	2	NAG	C4-C5-C6-O6
4	G	3	BMA	C4-C5-C6-O6
4	U	3	BMA	C4-C5-C6-O6
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
4	Q	1	NAG	C8-C7-N2-C2
4	Q	1	NAG	O7-C7-N2-C2
4	U	2	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	U	2	NAG	O7-C7-N2-C2
4	Y	1	NAG	C8-C7-N2-C2
4	Y	1	NAG	O7-C7-N2-C2
5	F	1	NAG	C8-C7-N2-C2
5	F	1	NAG	O7-C7-N2-C2
5	a	2	NAG	C8-C7-N2-C2
5	a	2	NAG	O7-C7-N2-C2
4	K	3	BMA	O5-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
5	a	1	NAG	O5-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
5	V	1	NAG	O5-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	Q	3	BMA	O5-C5-C6-O6
4	X	3	BMA	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	K	2	NAG	C3-C2-N2-C7
4	Z	1	NAG	O5-C5-C6-O6
5	T	1	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	K	3	BMA	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	W	1	NAG	C4-C5-C6-O6
4	D	2	NAG	C1-C2-N2-C7
4	G	2	NAG	C1-C2-N2-C7
4	X	1	NAG	C1-C2-N2-C7
5	F	2	NAG	C1-C2-N2-C7
4	X	2	NAG	C4-C5-C6-O6
4	Y	3	BMA	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
5	a	1	NAG	C4-C5-C6-O6
4	D	2	NAG	C3-C2-N2-C7

Continued on next page...

Continued from previous page...

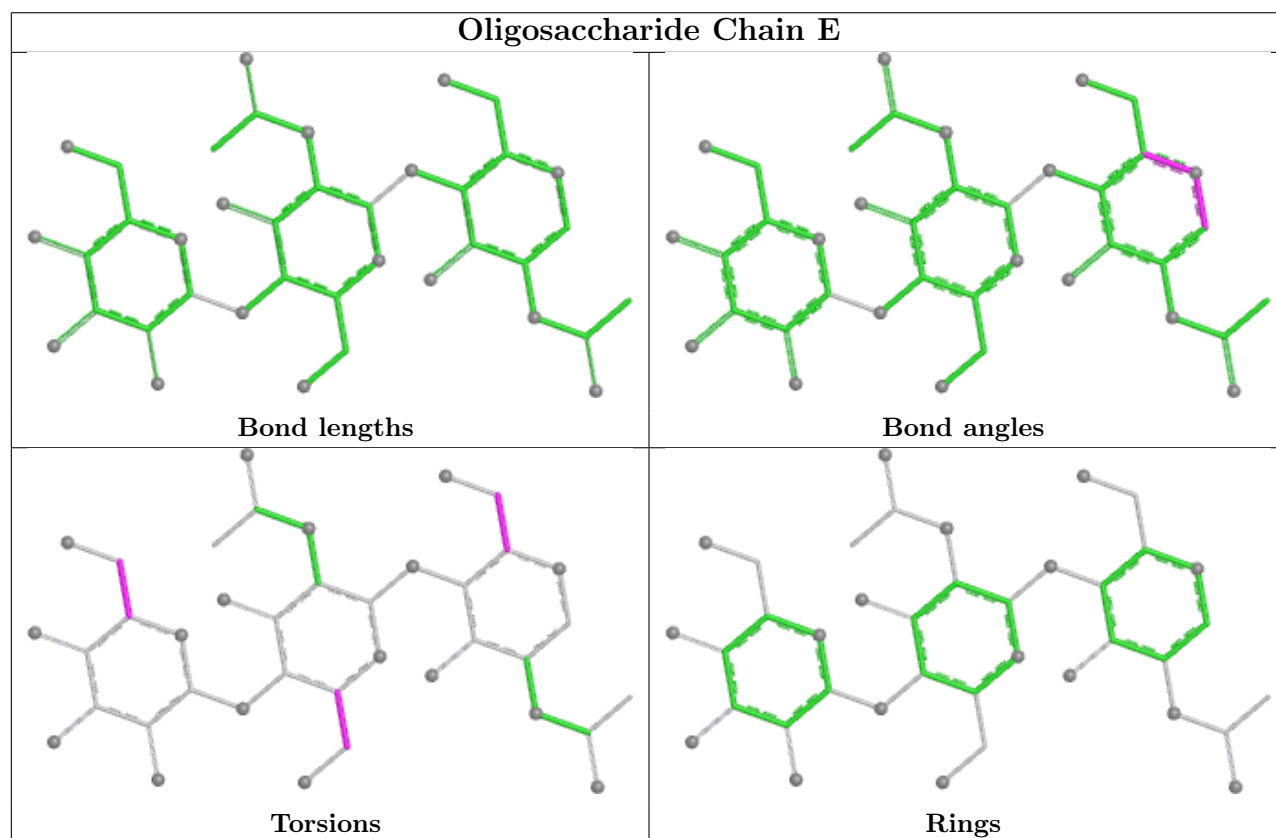
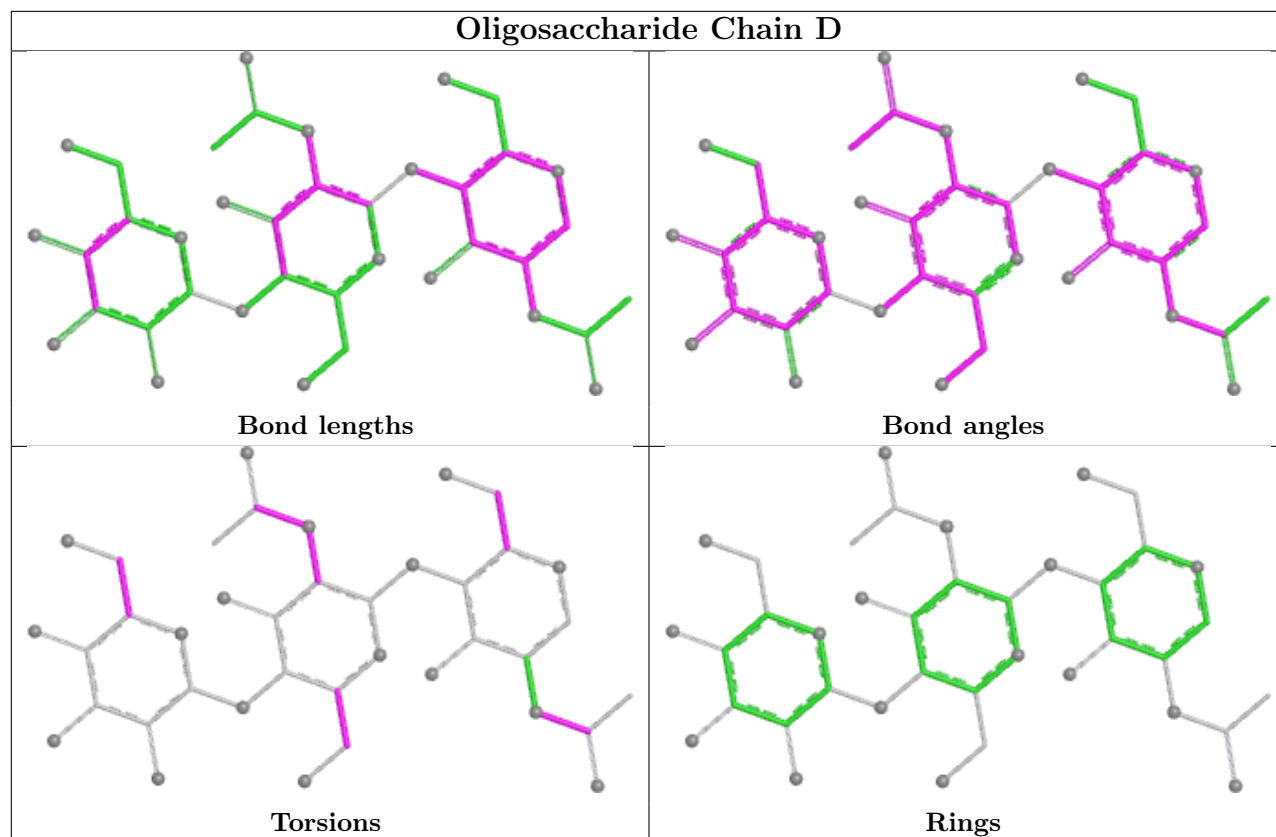
Mol	Chain	Res	Type	Atoms
4	W	2	NAG	C3-C2-N2-C7
4	X	1	NAG	C3-C2-N2-C7
4	X	2	NAG	C3-C2-N2-C7
4	Z	1	NAG	C3-C2-N2-C7
5	F	2	NAG	C3-C2-N2-C7
5	a	2	NAG	C3-C2-N2-C7
5	V	1	NAG	C4-C5-C6-O6
4	X	2	NAG	C1-C2-N2-C7
4	Z	1	NAG	C1-C2-N2-C7
5	a	2	NAG	C1-C2-N2-C7
4	G	2	NAG	C3-C2-N2-C7
4	K	1	NAG	C3-C2-N2-C7
5	S	2	NAG	C3-C2-N2-C7
4	I	2	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6

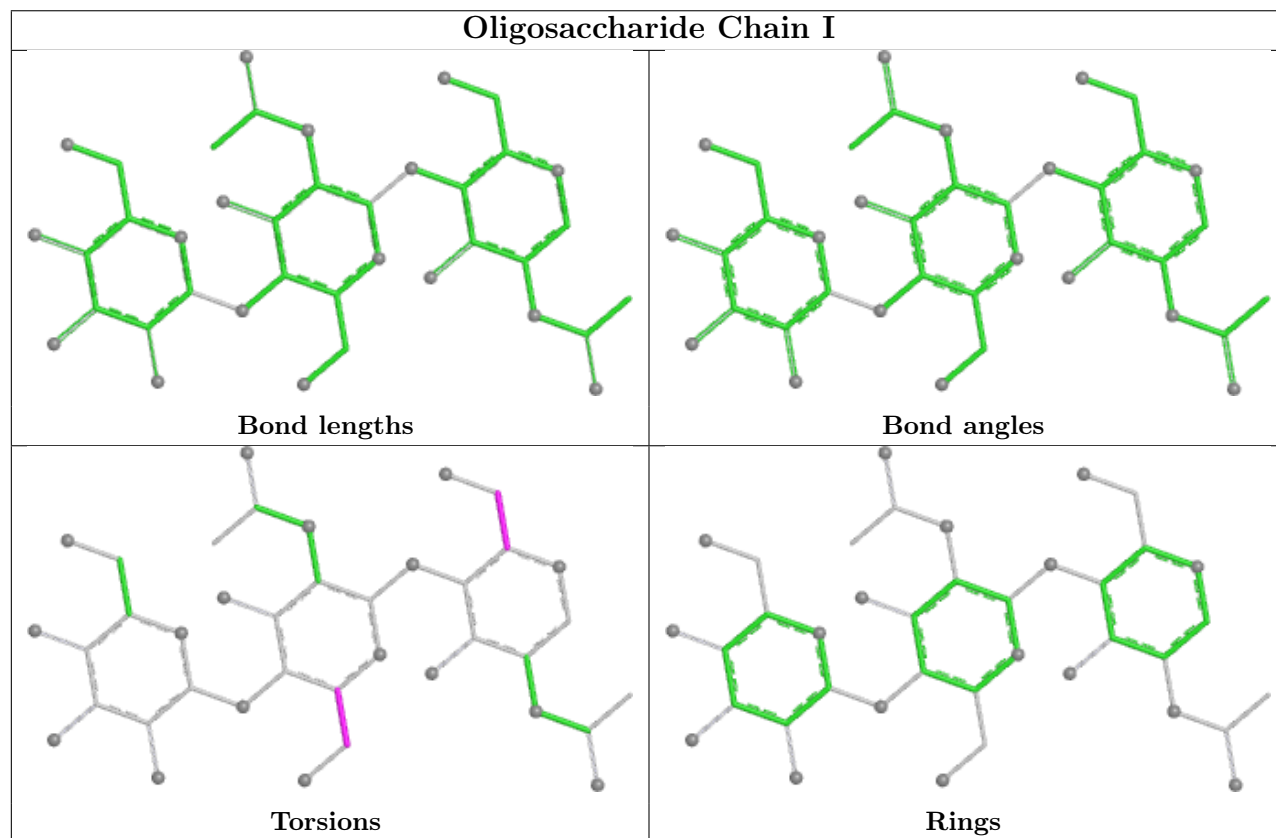
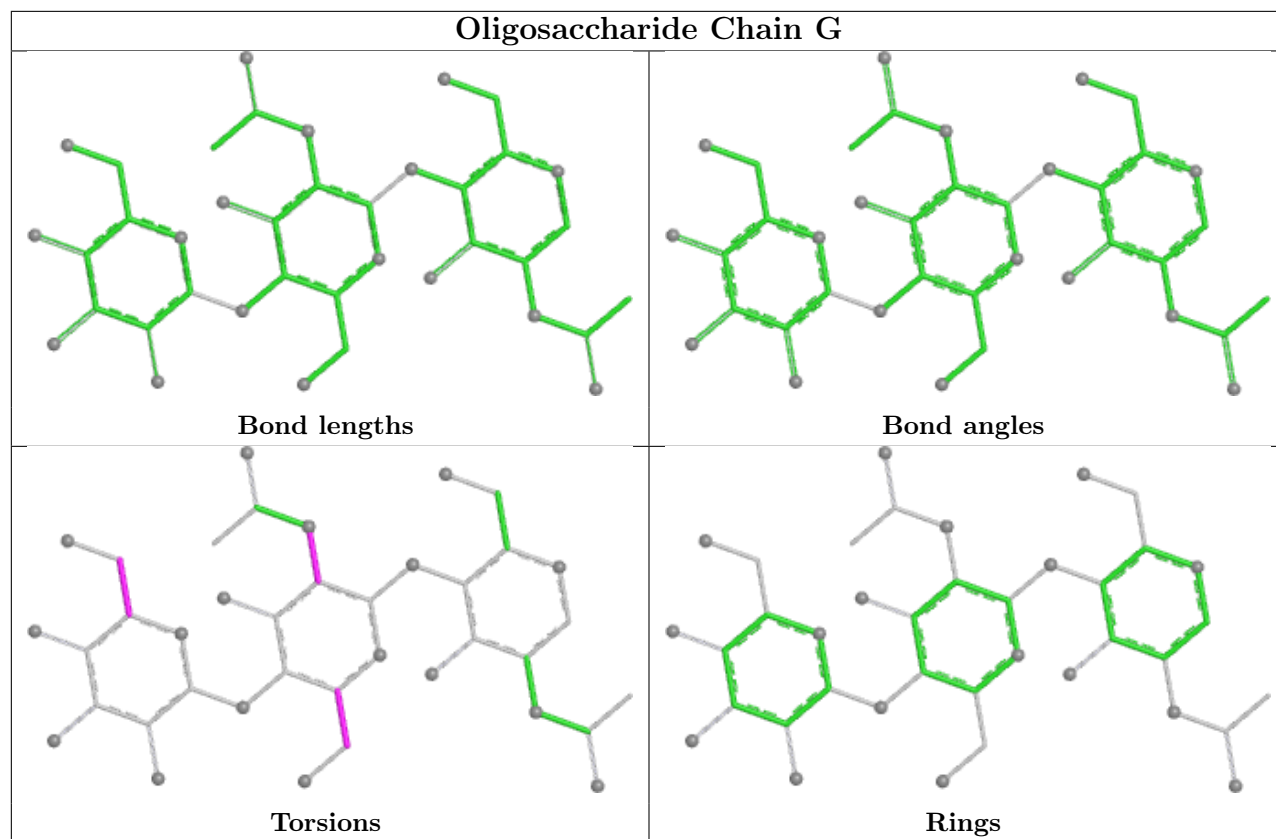
There are no ring outliers.

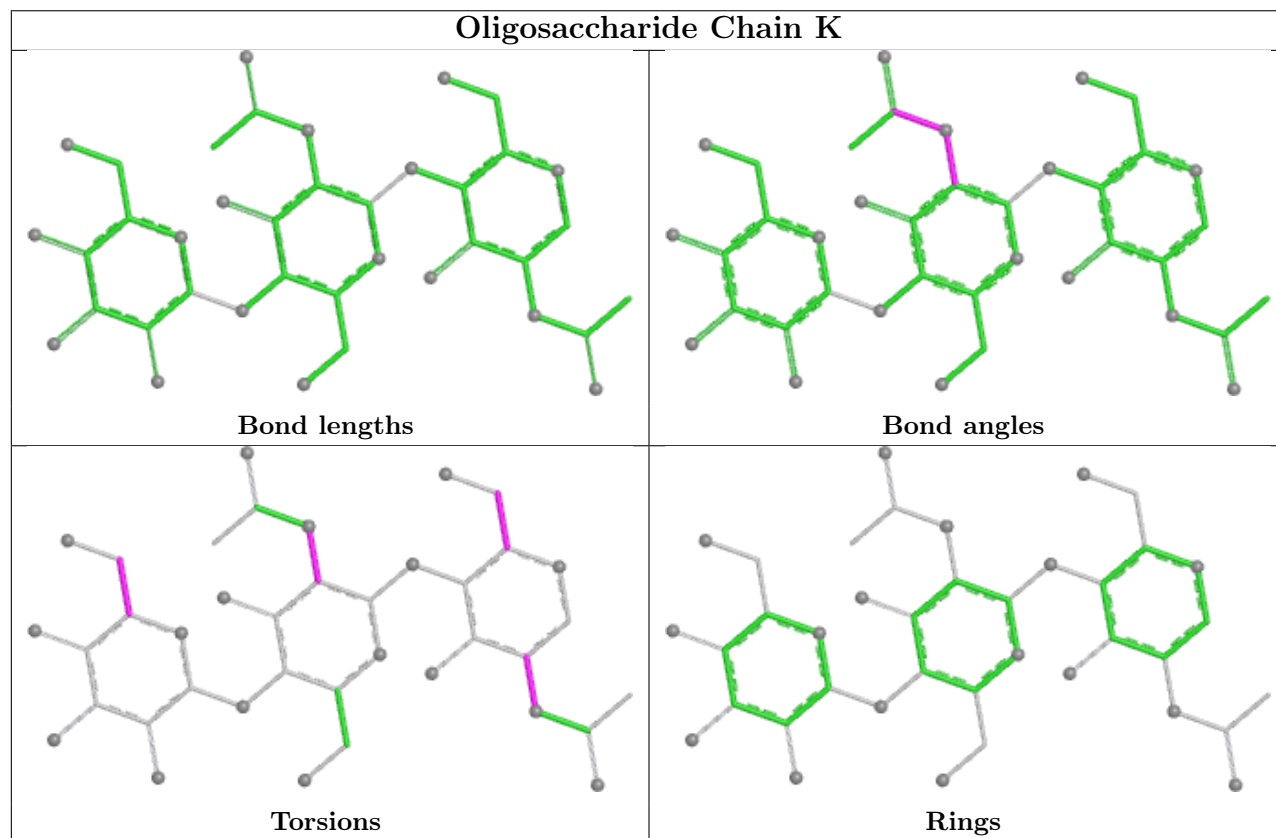
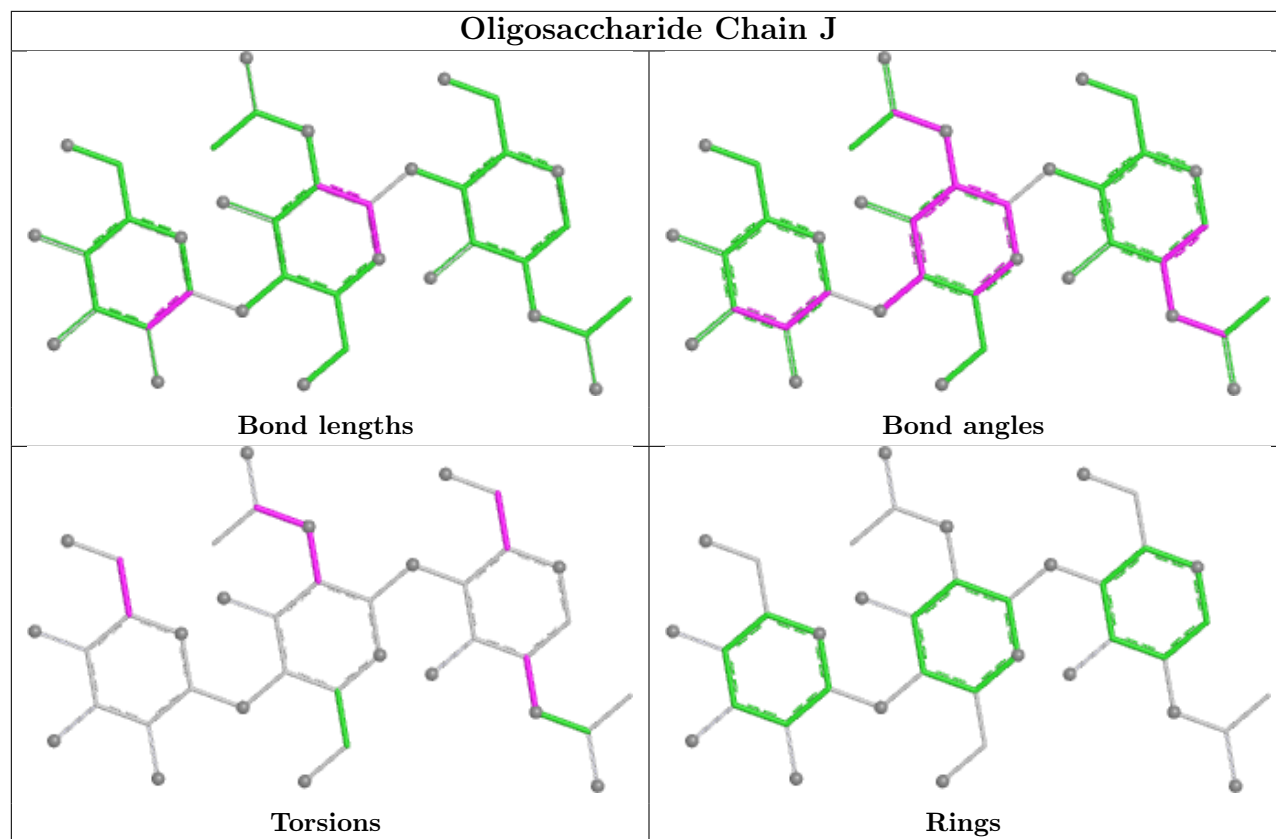
14 monomers are involved in 25 short contacts:

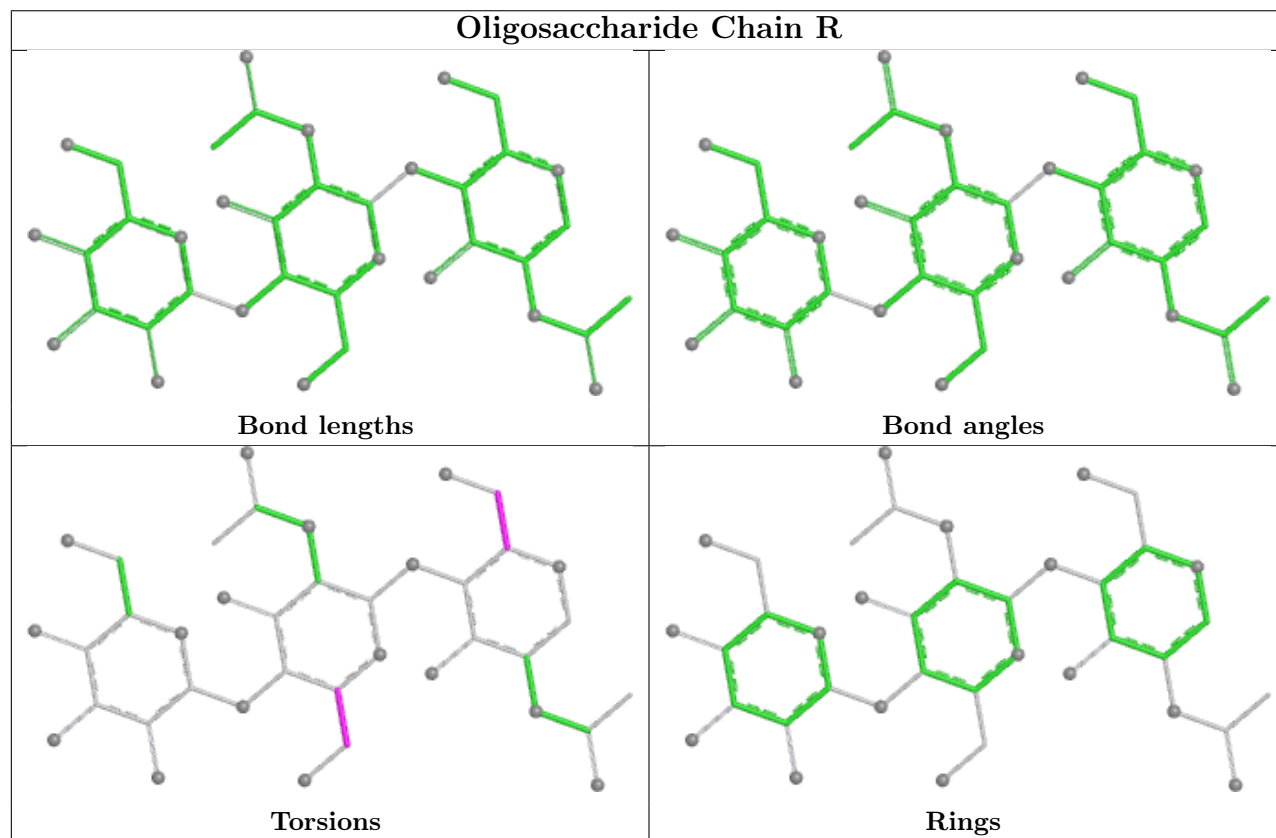
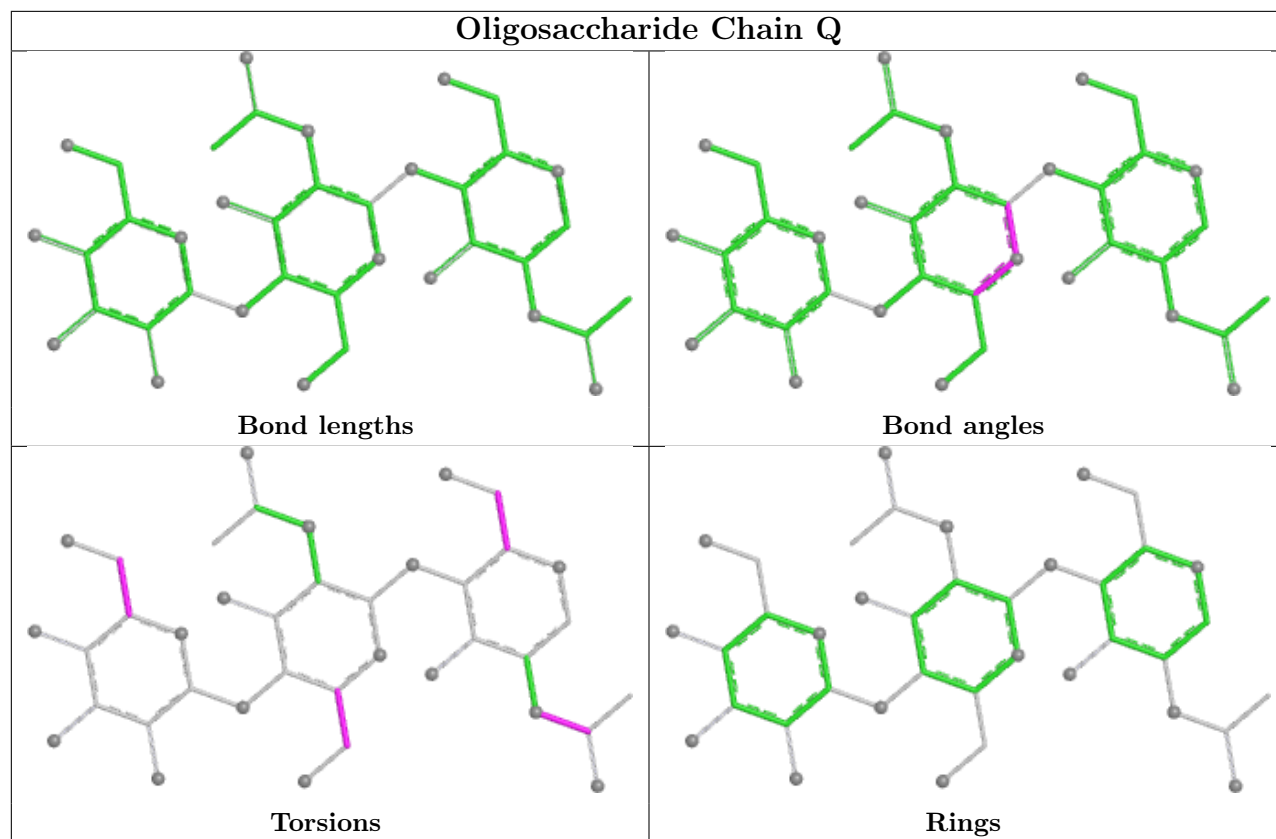
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	a	2	NAG	1	0
4	Y	1	NAG	2	0
4	U	2	NAG	4	0
4	R	1	NAG	1	0
4	Q	1	NAG	2	0
4	J	1	NAG	2	0
4	J	3	BMA	1	0
4	W	2	NAG	2	0
4	J	2	NAG	3	0
4	D	2	NAG	8	0
4	Q	2	NAG	1	0
4	U	3	BMA	1	0
4	D	1	NAG	3	0
4	K	2	NAG	1	0

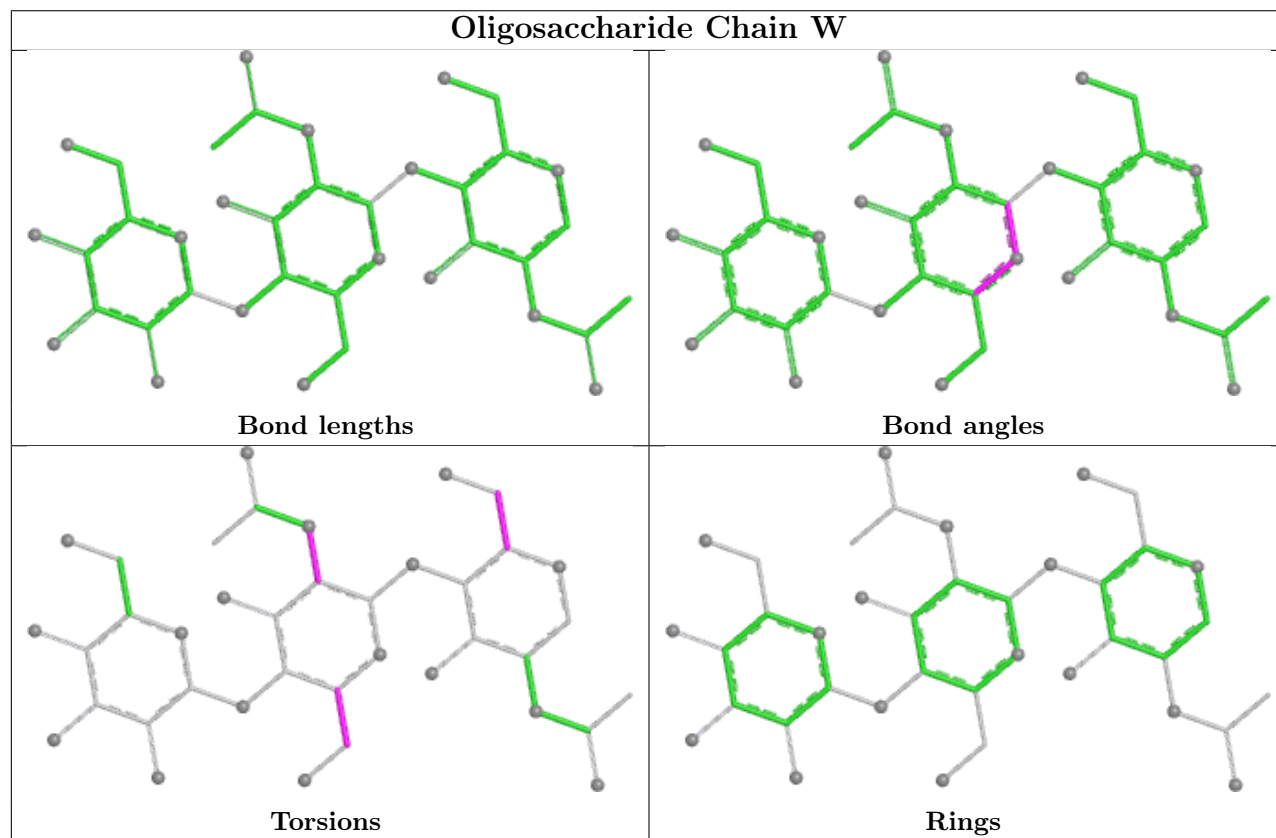
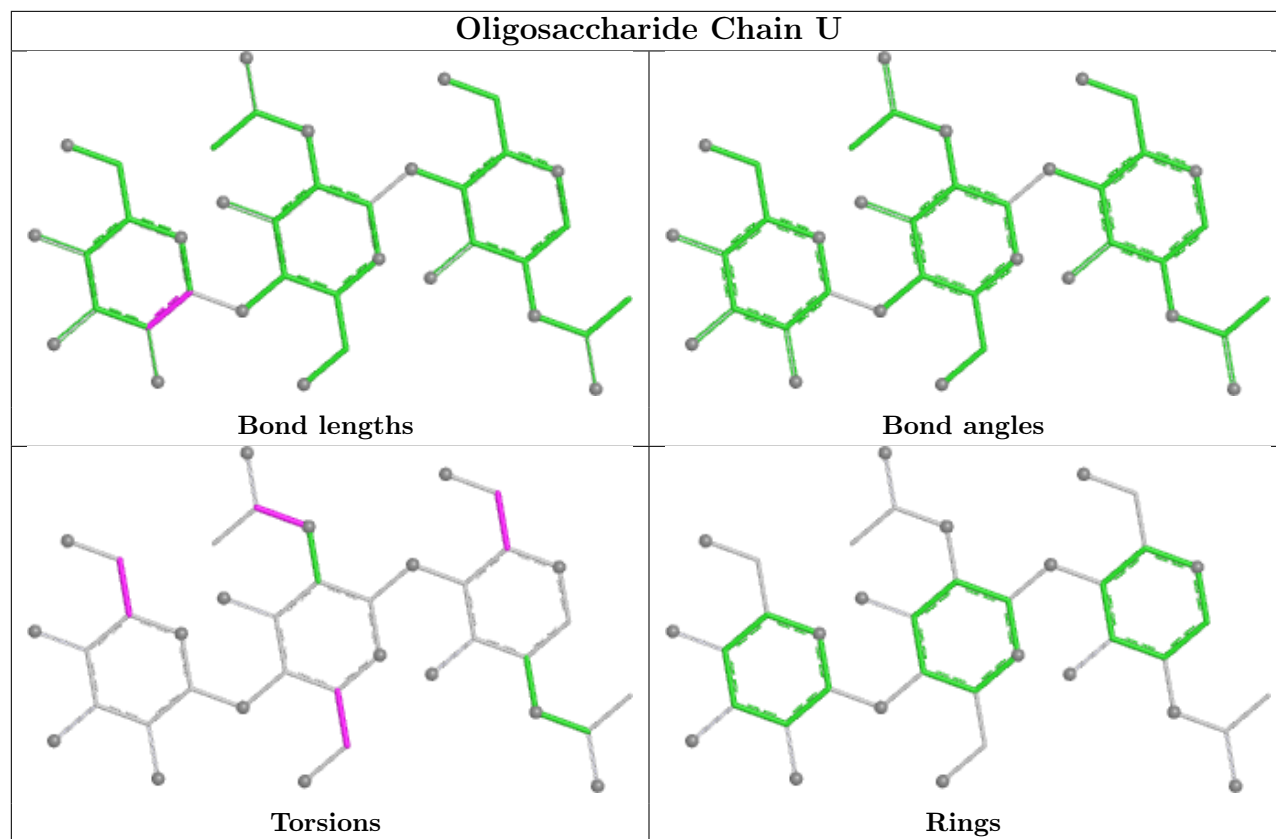
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

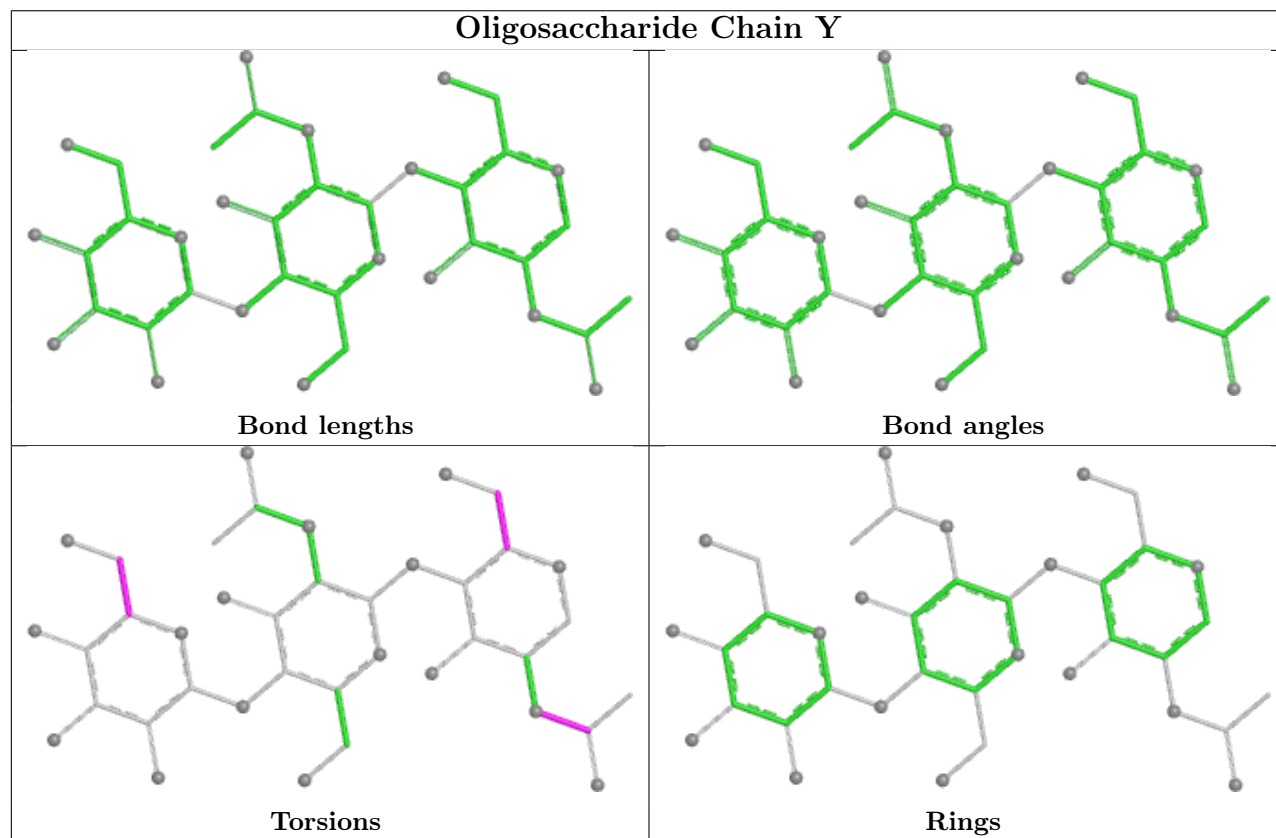
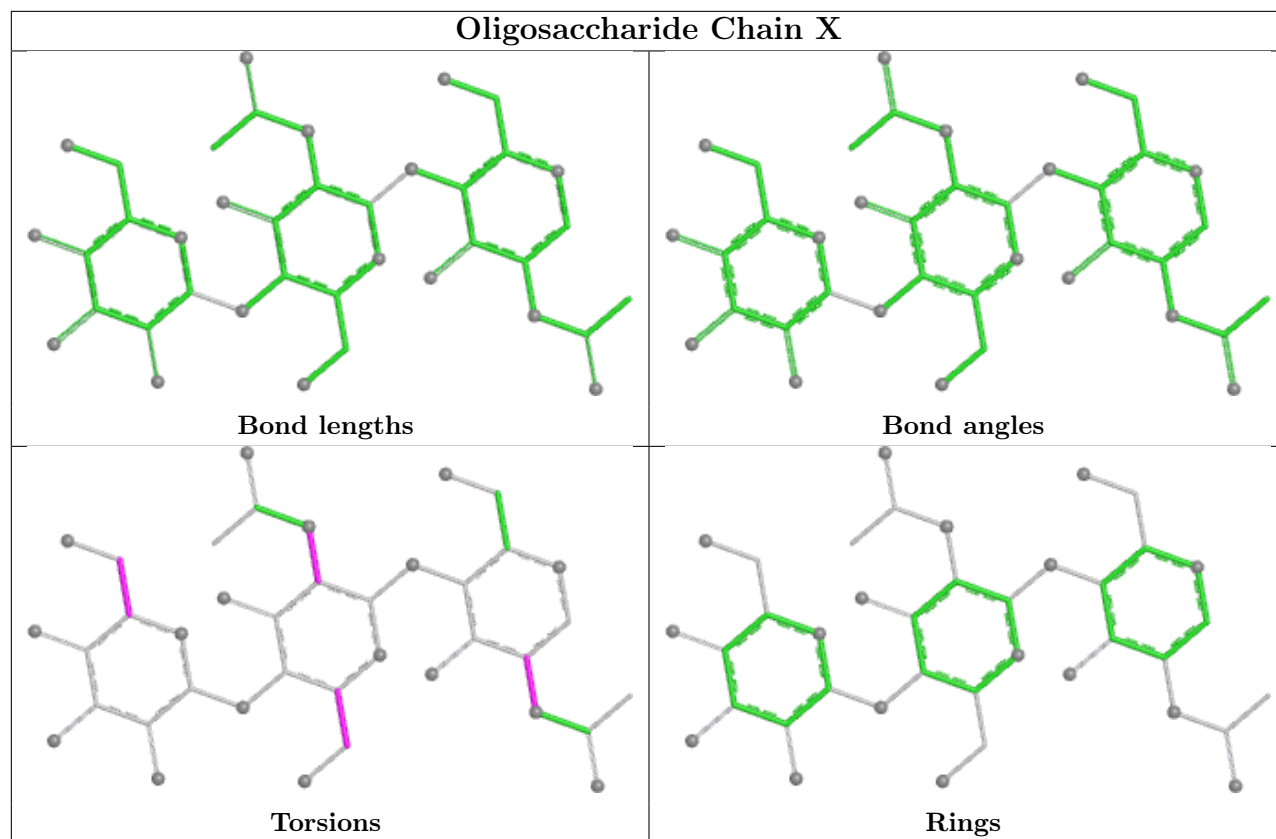


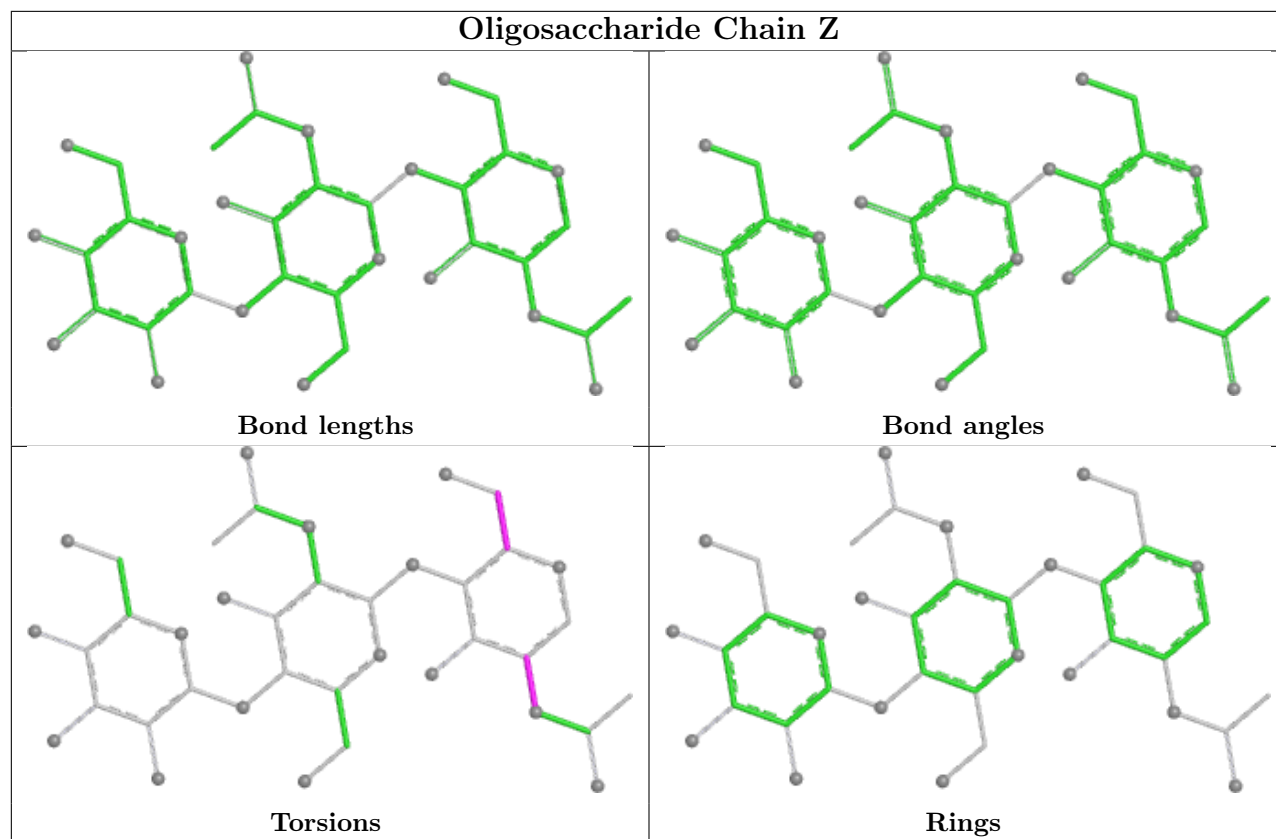


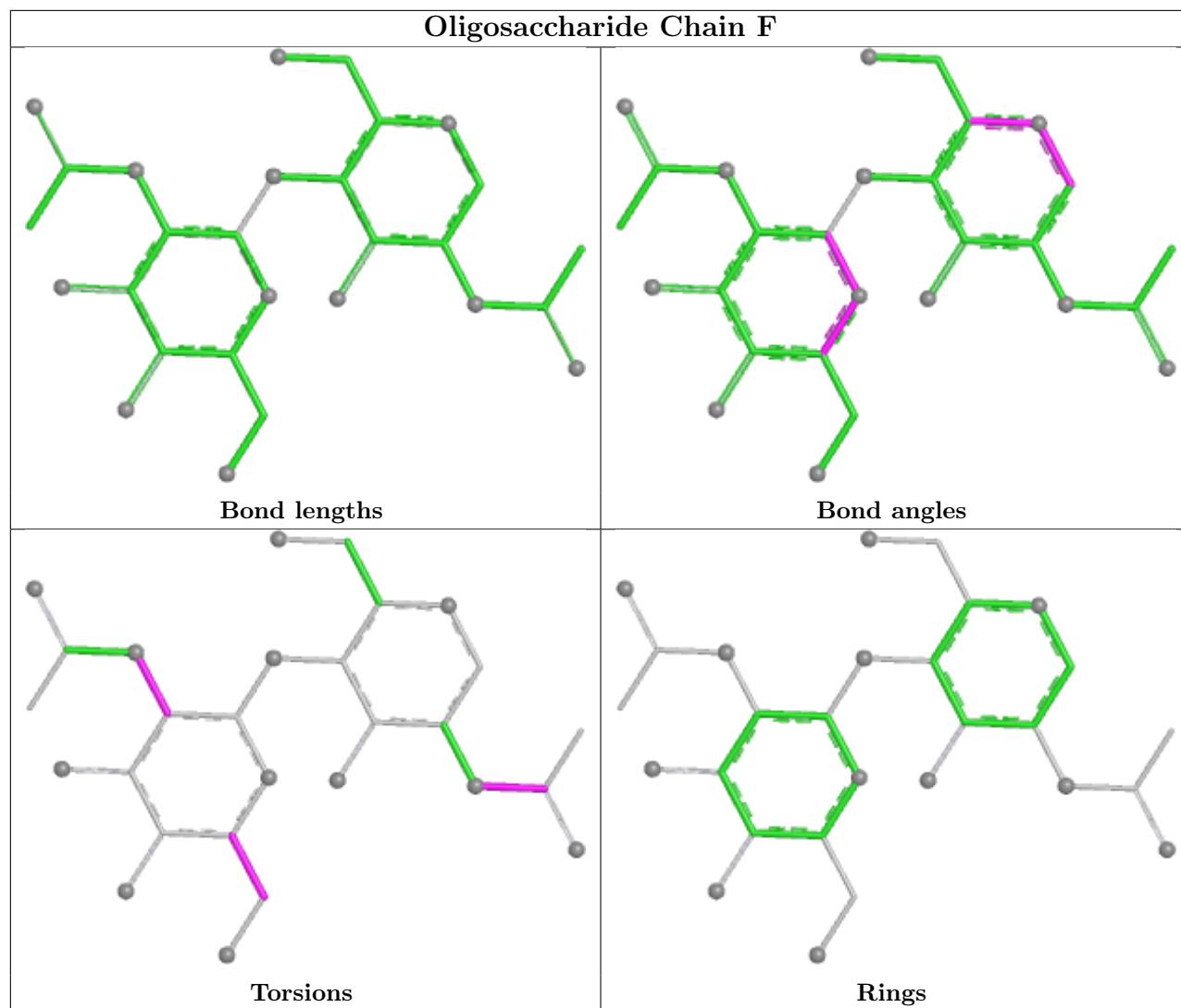


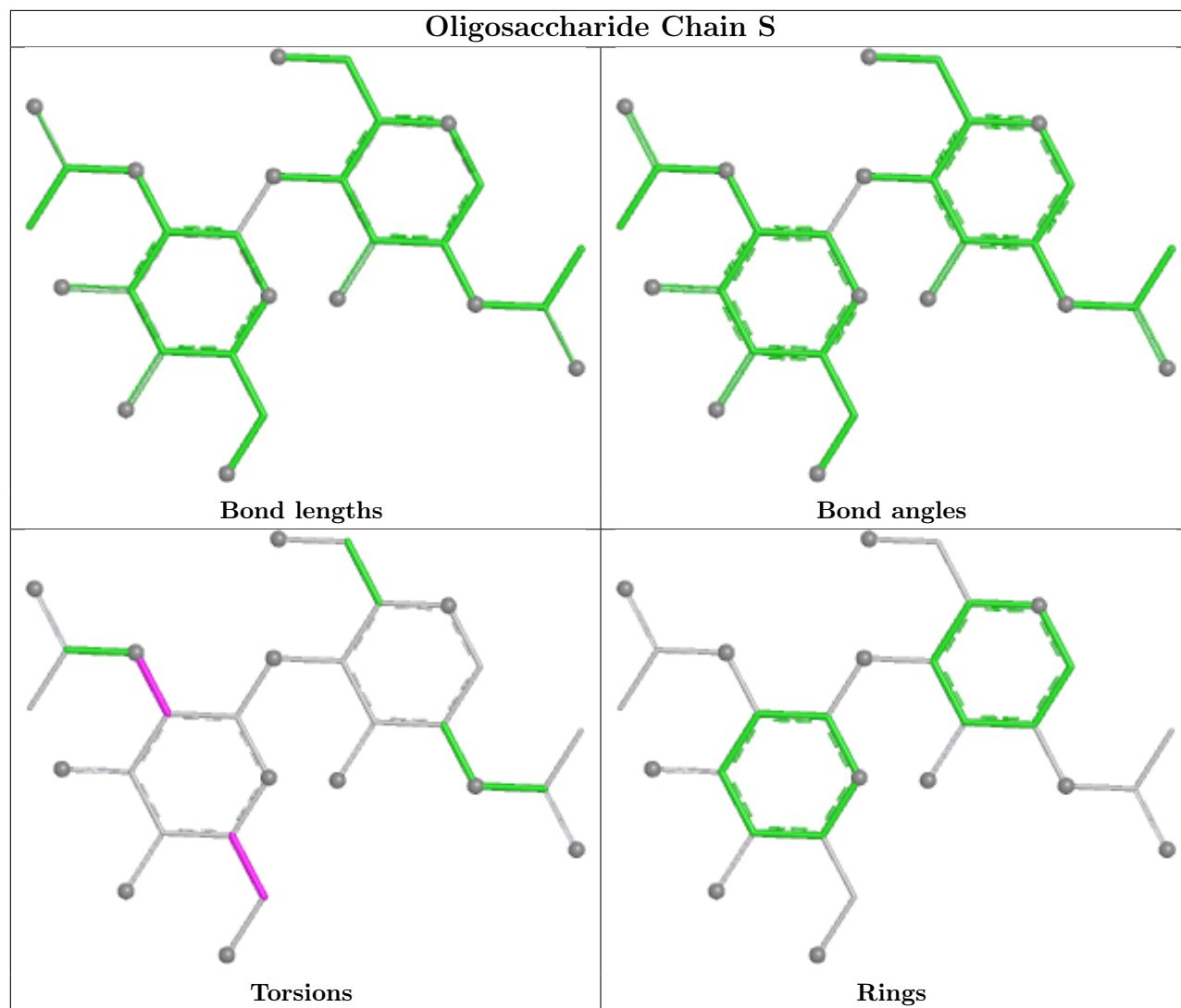


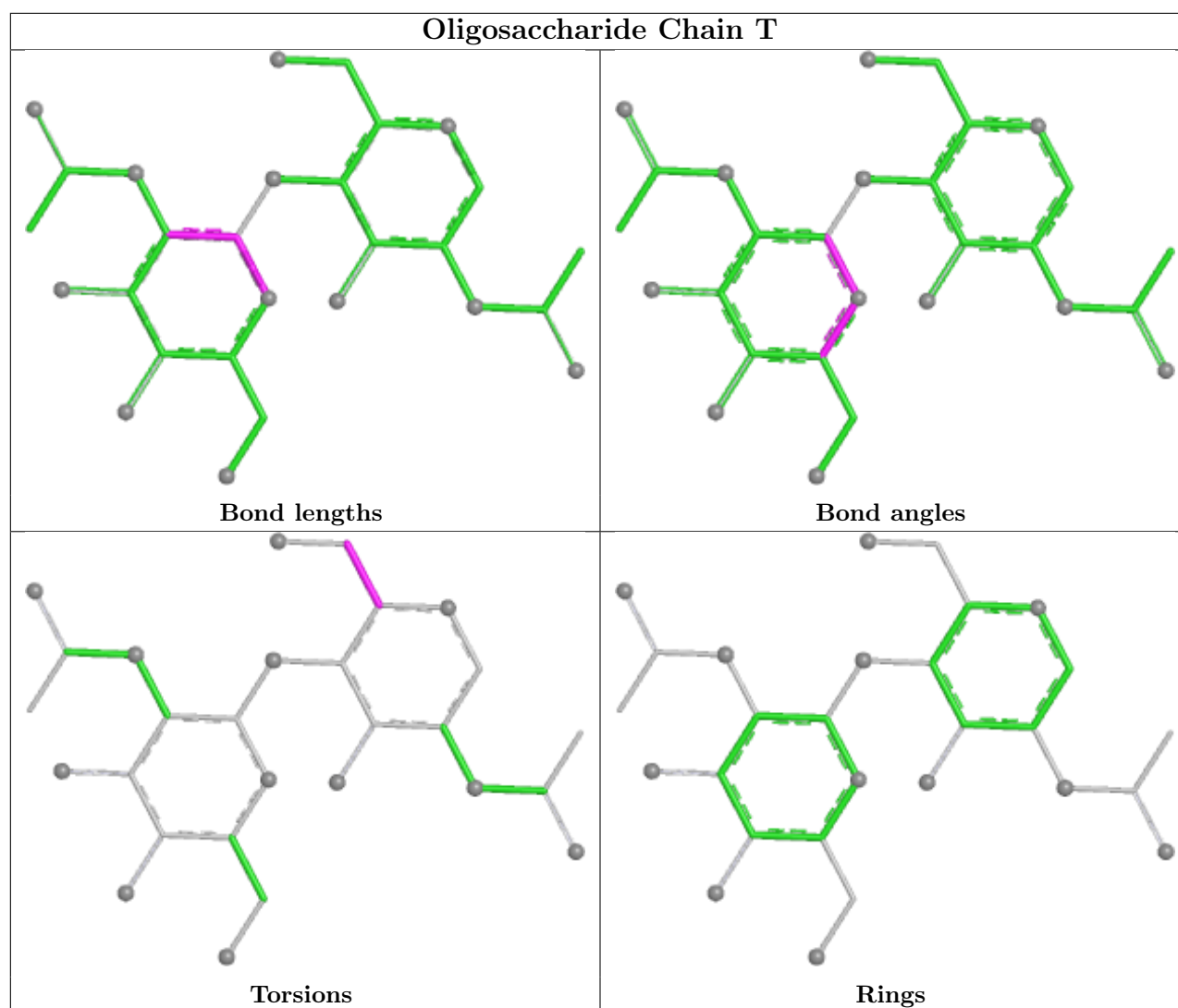


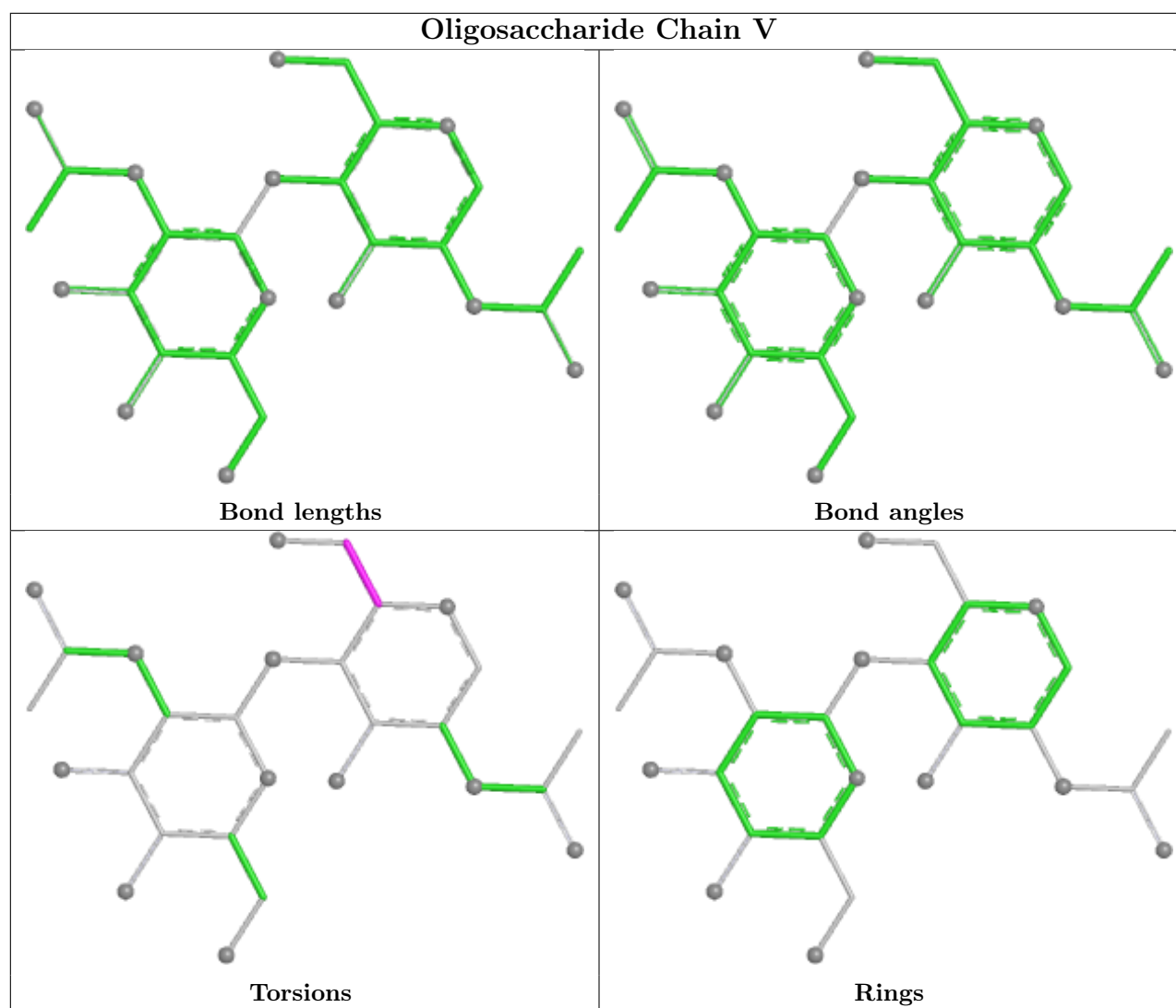


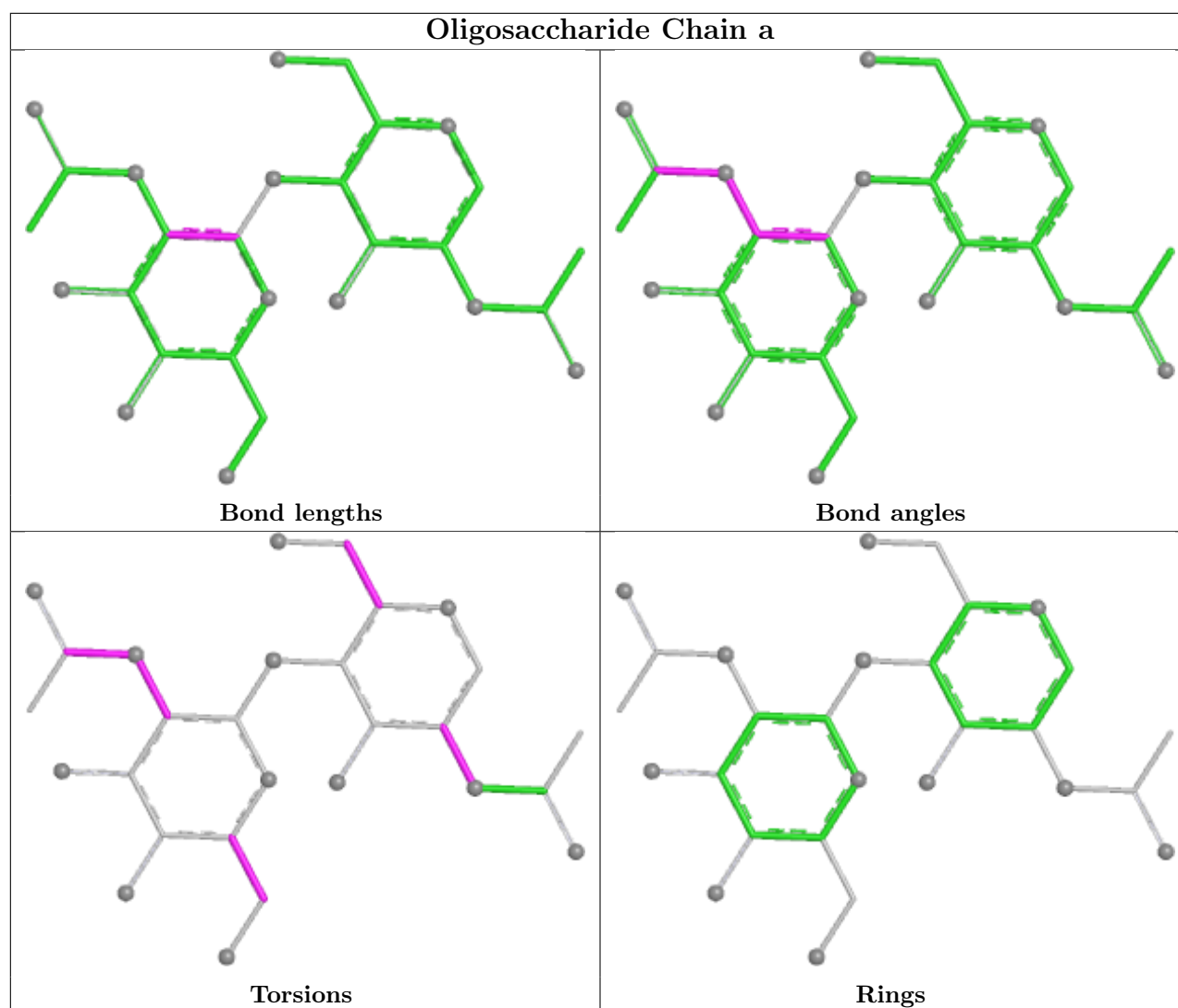












5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	B	601	1	14,14,15	0.47	0	17,19,21	0.39	0

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	601	NAG	C8-C7-N2-C2
6	B	601	NAG	O7-C7-N2-C2

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](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	494/505 (97%)	-0.18	4 (0%)	82 65	71, 121, 164, 252	1 (0%)
1	B	488/505 (96%)	-0.17	5 (1%)	79 61	82, 131, 177, 223	0
1	C	487/505 (96%)	-0.18	3 (0%)	85 71	87, 127, 181, 238	0
2	H	221/237 (93%)	0.09	4 (1%)	67 50	60, 159, 230, 292	0
2	M	221/237 (93%)	0.13	3 (1%)	73 55	85, 163, 219, 247	0
2	O	221/237 (93%)	0.03	6 (2%)	56 41	67, 131, 184, 233	0
3	L	214/215 (99%)	0.15	5 (2%)	61 45	95, 164, 271, 320	0
3	N	213/215 (99%)	0.09	3 (1%)	73 55	69, 157, 230, 294	1 (0%)
3	P	214/215 (99%)	-0.02	6 (2%)	55 40	77, 142, 180, 305	0
All	All	2773/2871 (96%)	-0.06	39 (1%)	73 55	60, 136, 213, 320	2 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	164	GLU	8.2
2	M	161	TYR	5.5
2	M	124	MET	4.3
3	P	2	SER	4.1
1	A	460	GLU	4.1
2	H	74	TRP	3.9
3	P	84	GLU	3.7
3	N	33	PHE	3.6
3	P	215	SER	3.4
1	B	457	GLU	3.2
3	L	2	SER	3.1
2	M	160	ASP	3.0
3	P	134	THR	2.6
1	A	383	ARG	2.6
3	L	66	SER	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	O	41	PRO	2.4
3	L	209	VAL	2.4
2	H	111	GLN	2.4
3	L	149	VAL	2.4
1	B	152	ASN	2.3
2	O	160	ASP	2.3
1	C	12	THR	2.3
2	O	101	ALA	2.3
2	O	159	LYS	2.3
3	N	3	VAL	2.2
3	P	98	TRP	2.2
1	B	256	GLY	2.2
2	H	46	GLU	2.2
1	B	8	ASN	2.2
1	A	173	GLN	2.2
3	P	174	LYS	2.2
1	C	8	ASN	2.2
3	N	173	ASN	2.2
2	H	165	PRO	2.1
3	L	52	ASN	2.1
2	O	163	PRO	2.1
1	A	124	SER	2.0
1	B	251	LEU	2.0
1	C	356	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	D	1	14/15	-	-	108,154,171,184	0
4	NAG	D	2	14/15	-	-	167,192,213,232	0
4	BMA	D	3	11/12	-	-	140,158,194,218	0
4	NAG	E	1	14/15	-	-	98,115,169,171	0

Continued on next page...

Continued from previous page...

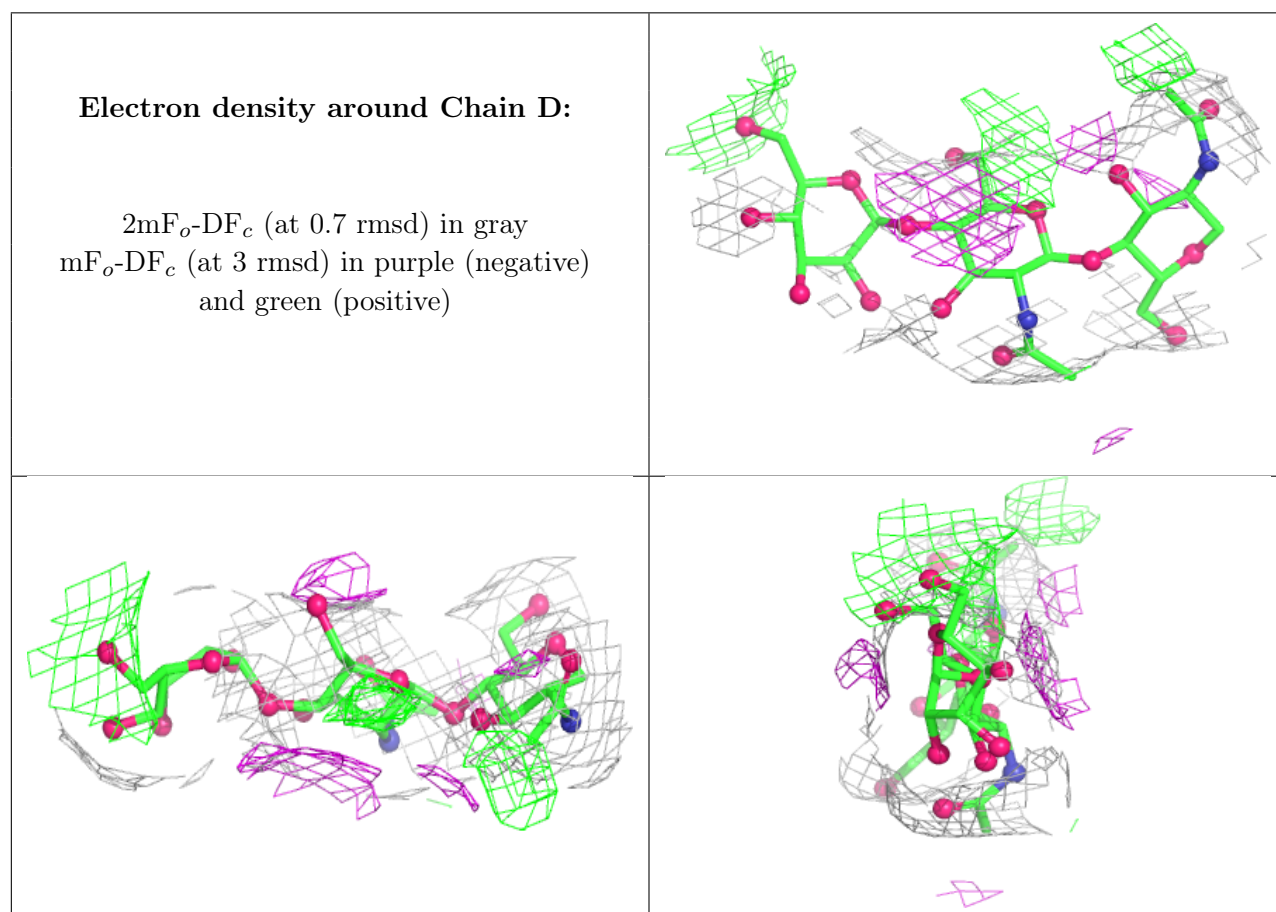
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	E	2	14/15	-	-	91,167,187,192	0
4	BMA	E	3	11/12	-	-	160,183,211,230	0
4	NAG	G	1	14/15	-	-	89,131,153,156	0
4	NAG	G	2	14/15	-	-	132,173,208,255	0
4	BMA	G	3	11/12	-	-	142,171,195,200	0
4	NAG	I	1	14/15	-	-	136,158,173,189	0
4	NAG	I	2	14/15	-	-	206,227,258,271	0
4	BMA	I	3	11/12	-	-	172,231,274,274	0
4	BMA	X	3	11/12	0.54	0.13	143,175,199,235	0
4	BMA	Z	3	11/12	0.55	0.12	216,264,275,279	0
5	NAG	T	1	14/15	0.59	0.15	124,195,217,221	0
4	BMA	J	3	11/12	0.61	0.13	208,226,276,297	0
4	BMA	Q	3	11/12	0.64	0.11	194,240,257,265	0
4	BMA	Y	3	11/12	0.64	0.12	188,228,236,238	0
5	NAG	T	2	14/15	0.64	0.14	142,213,244,252	0
4	BMA	W	3	11/12	0.67	0.11	132,165,192,207	0
4	BMA	K	3	11/12	0.68	0.12	174,236,242,246	0
5	NAG	S	2	14/15	0.70	0.13	197,211,220,221	0
4	NAG	U	2	14/15	0.71	0.14	146,178,228,235	0
4	NAG	Q	2	14/15	0.75	0.17	132,253,274,275	0
5	NAG	S	1	14/15	0.76	0.14	134,177,202,215	0
4	BMA	U	3	11/12	0.77	0.11	129,169,221,222	0
5	NAG	V	2	14/15	0.78	0.10	163,186,203,220	0
4	BMA	R	3	11/12	0.79	0.08	144,174,200,204	0
4	NAG	J	2	14/15	0.79	0.16	162,190,224,267	0
4	NAG	Z	2	14/15	0.81	0.10	168,234,244,264	0
4	NAG	J	1	14/15	0.86	0.11	134,169,199,218	0
4	NAG	Y	1	14/15	0.86	0.17	119,159,192,198	0
4	NAG	W	2	14/15	0.88	0.10	138,184,223,223	0
4	NAG	Q	1	14/15	0.88	0.18	105,184,244,280	0
4	NAG	R	2	14/15	0.89	0.12	115,195,237,244	0
4	NAG	U	1	14/15	0.89	0.09	79,128,170,172	0
5	NAG	V	1	14/15	0.90	0.09	129,162,195,198	0
4	NAG	W	1	14/15	0.90	0.11	93,141,165,188	0
4	NAG	X	2	14/15	0.91	0.12	109,186,219,238	0
5	NAG	F	1	14/15	-	-	145,189,229,247	0
5	NAG	F	2	14/15	-	-	145,221,245,260	0
4	NAG	Y	2	14/15	0.92	0.12	137,194,226,244	0
4	NAG	K	2	14/15	0.95	0.09	166,228,246,246	0
4	NAG	K	1	14/15	0.95	0.09	124,168,230,247	0
4	NAG	Z	1	14/15	0.96	0.07	128,186,219,223	0
4	NAG	R	1	14/15	0.97	0.08	120,131,161,170	0

Continued on next page...

Continued from previous page...

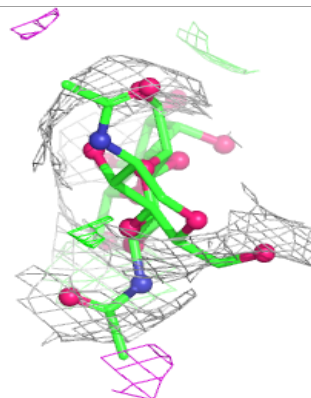
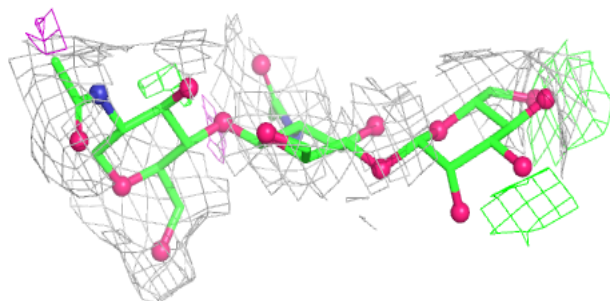
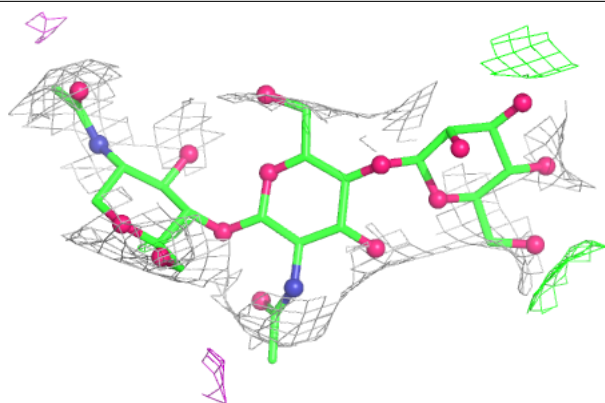
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	X	1	14/15	0.97	0.07	101,140,155,178	0
5	NAG	a	1	14/15	-	-	157,195,222,229	0
5	NAG	a	2	14/15	-	-	159,225,257,261	0

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

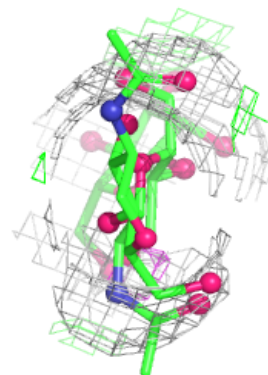
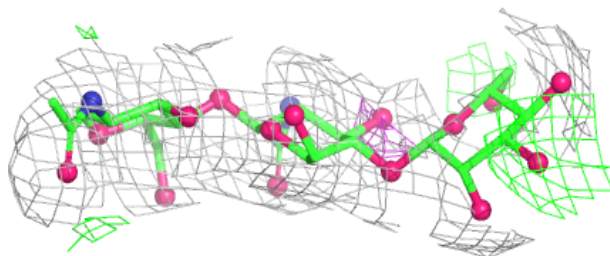
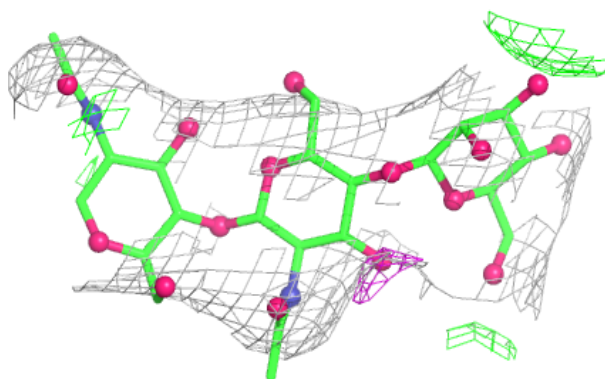


Electron density around Chain E:

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

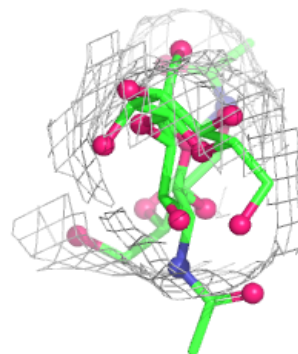
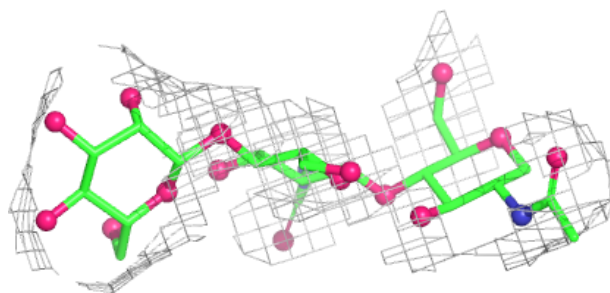
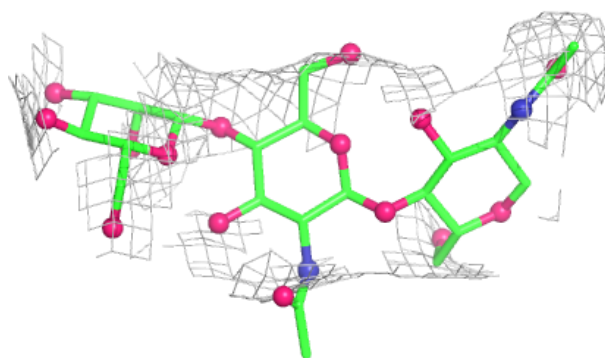
**Electron density around Chain G:**

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

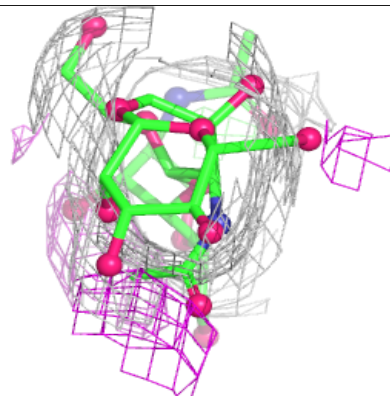
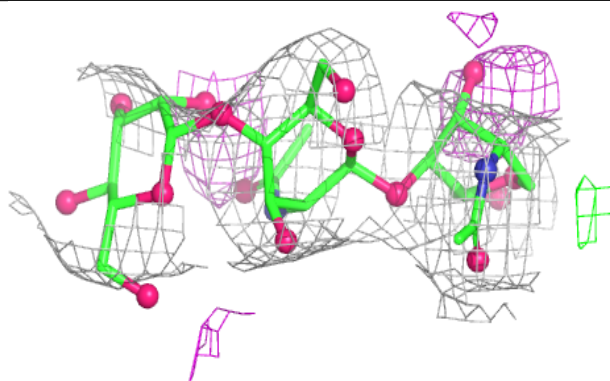
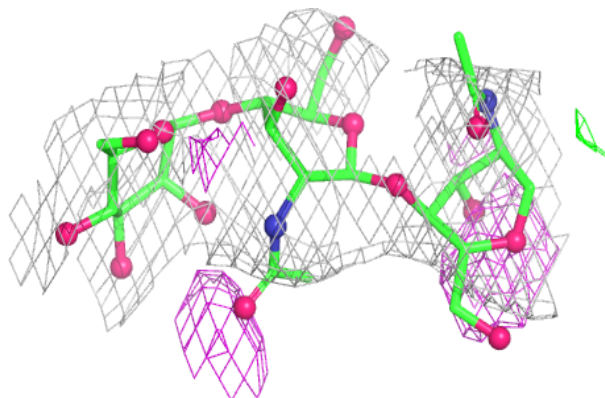


Electron density around Chain I:

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

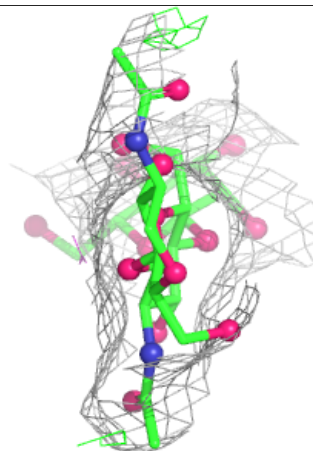
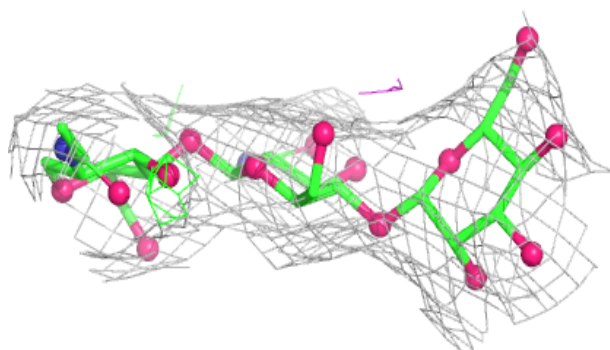
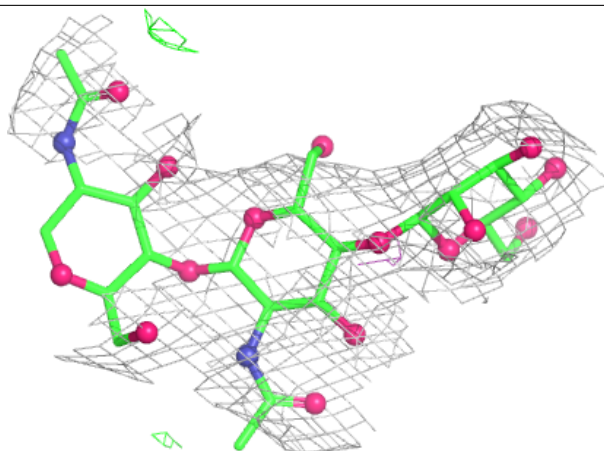
**Electron density around Chain J:**

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



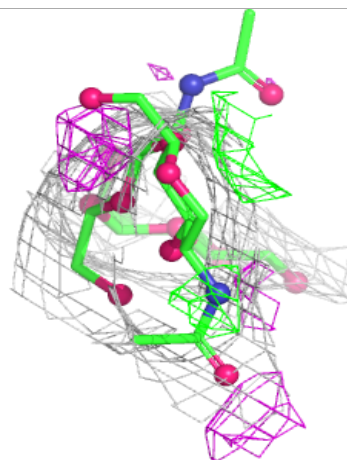
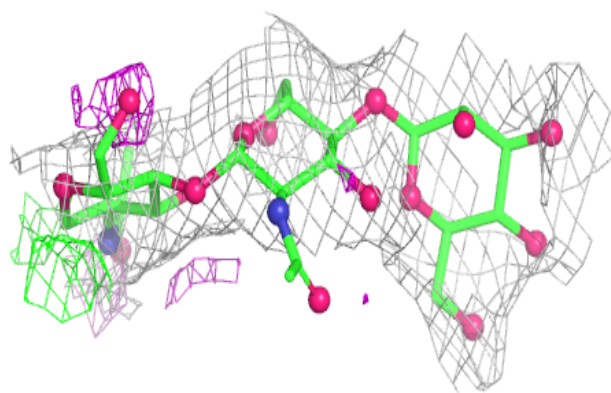
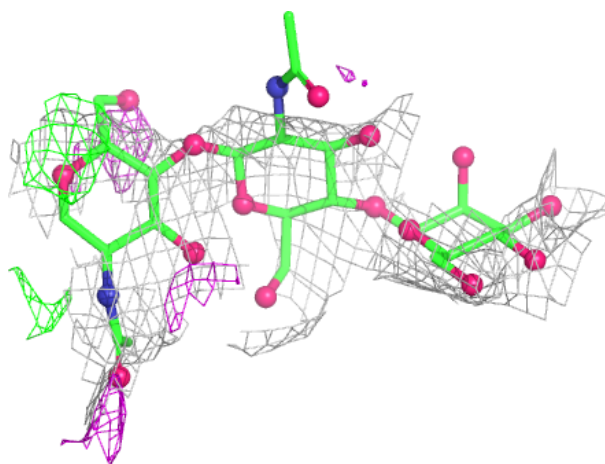
Electron density around Chain K:

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



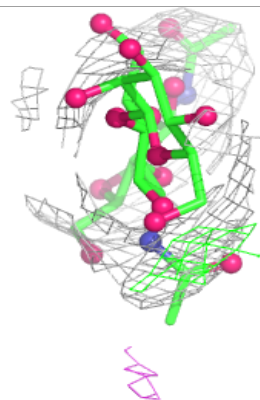
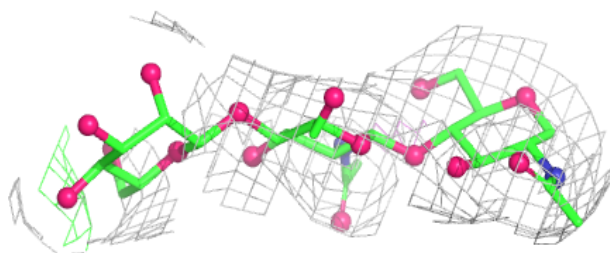
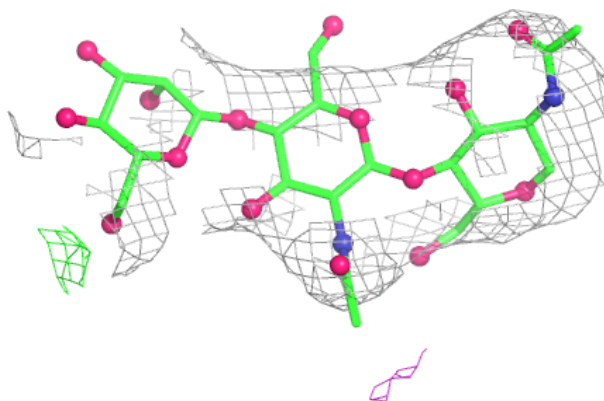
Electron density around Chain Q:

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



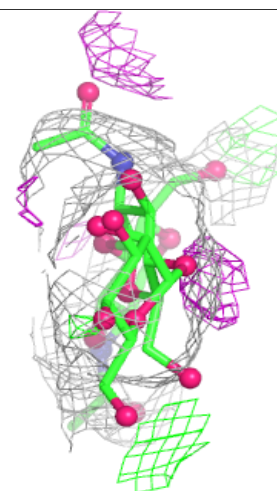
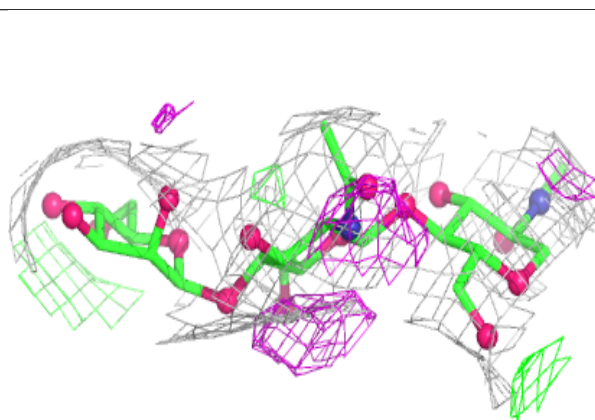
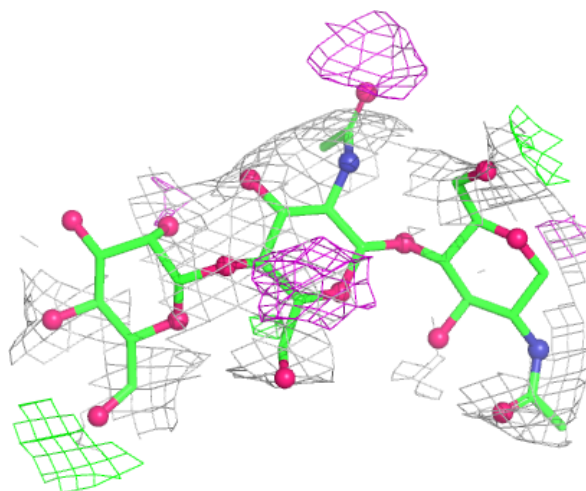
Electron density around Chain R:

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



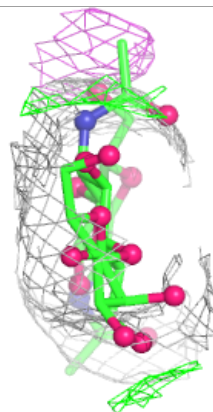
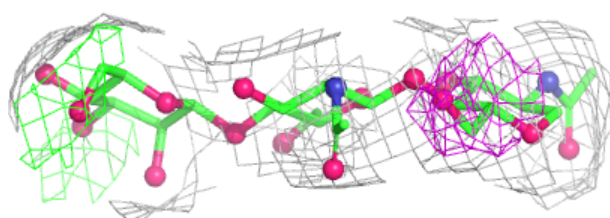
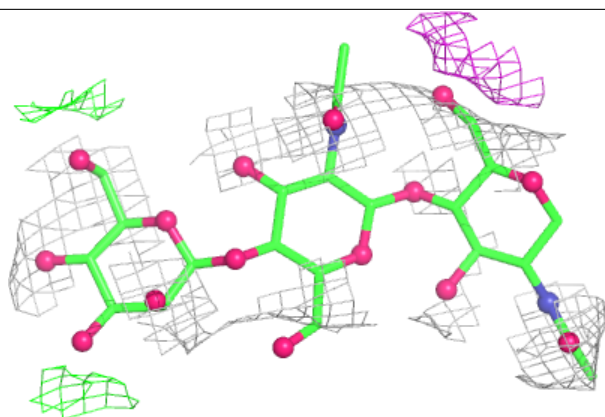
Electron density around Chain U:

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

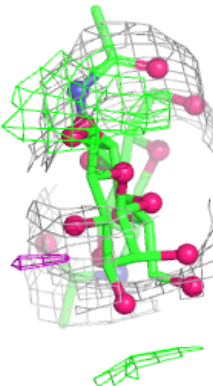
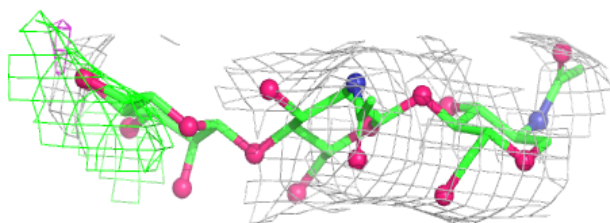
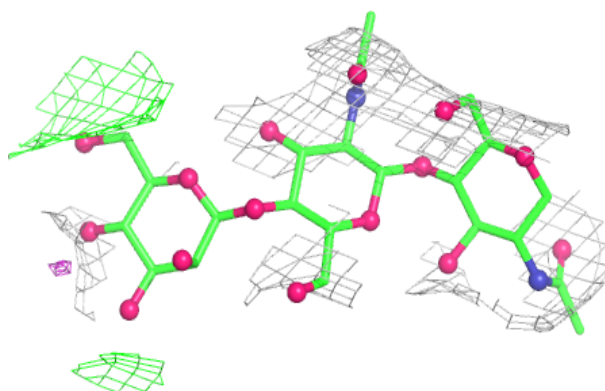


Electron density around Chain W:

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

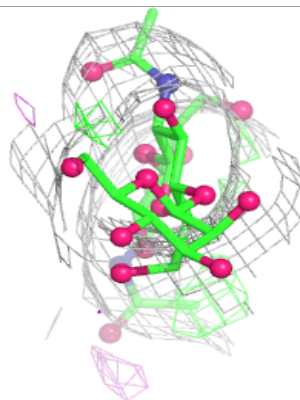
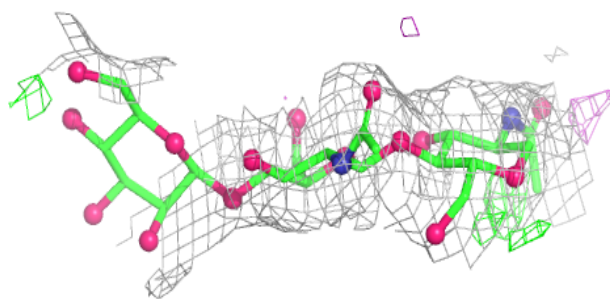
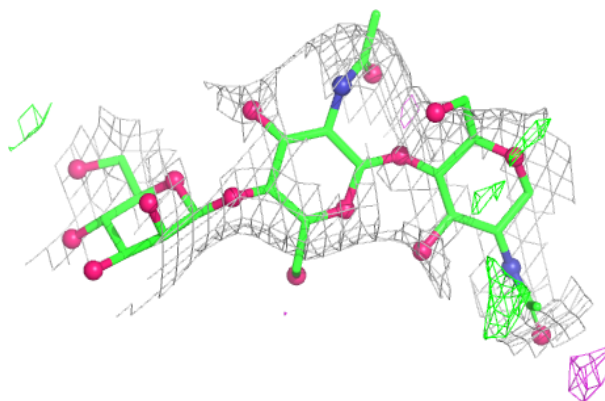
**Electron density around Chain X:**

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

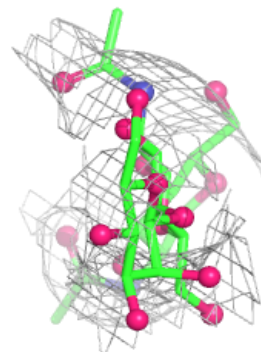
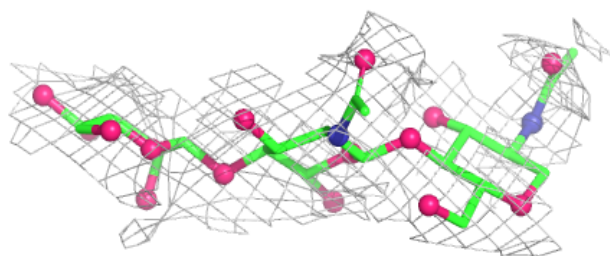
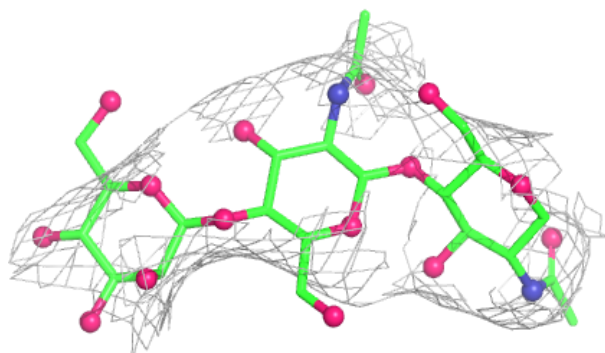


Electron density around Chain Y:

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

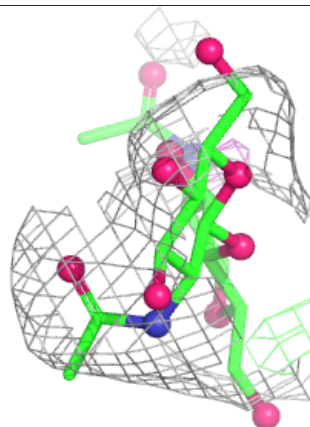
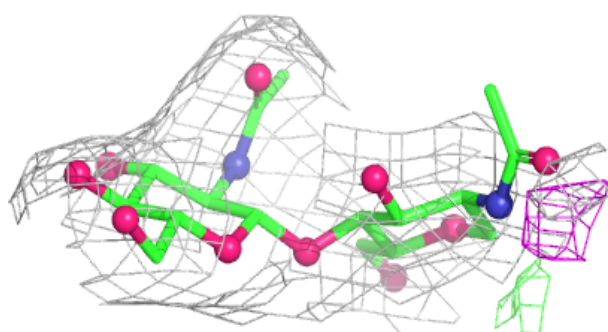
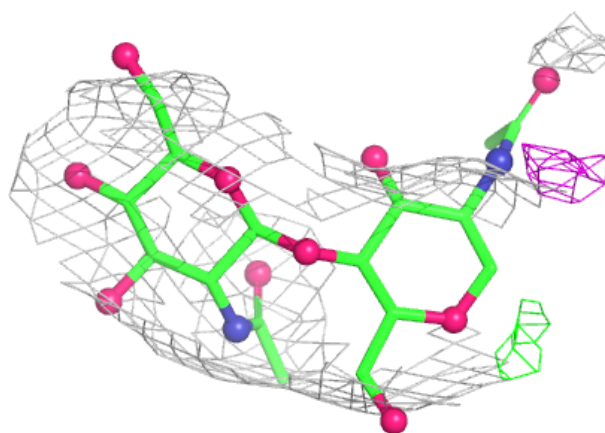
**Electron density around Chain Z:**

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

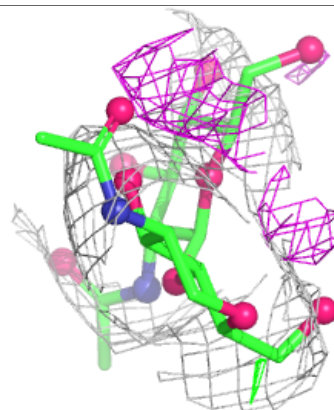
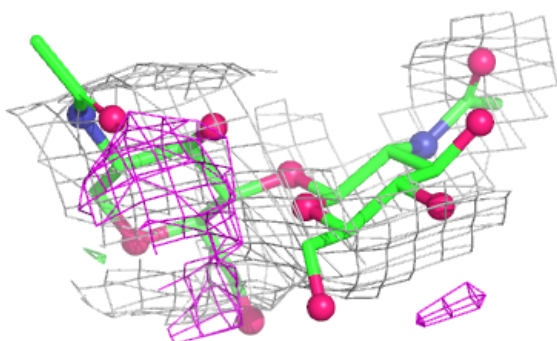
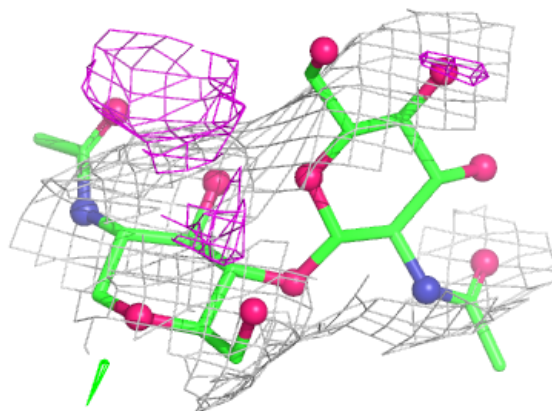


Electron density around Chain F:

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

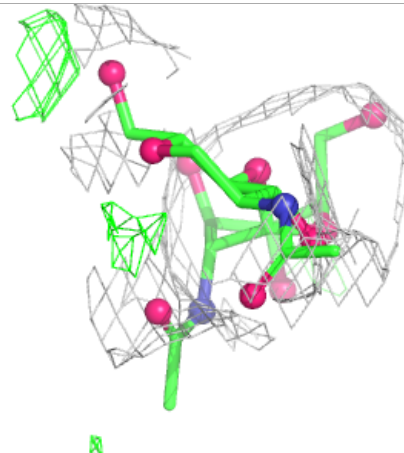
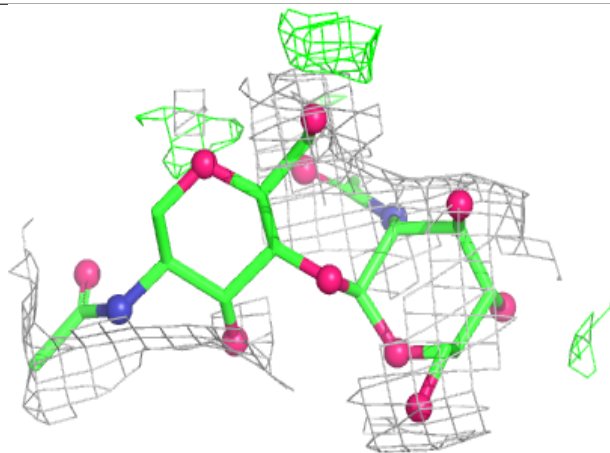
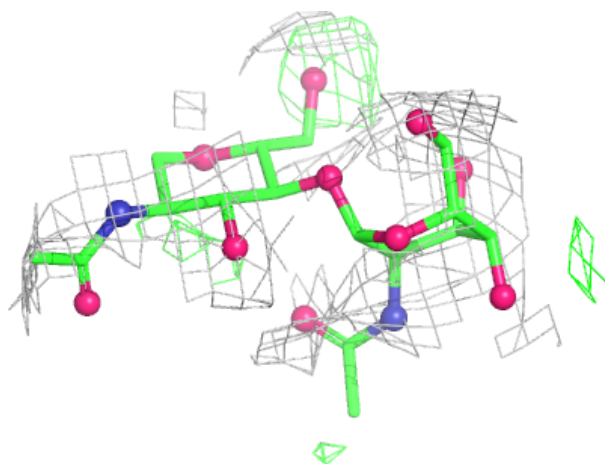
**Electron density around Chain S:**

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



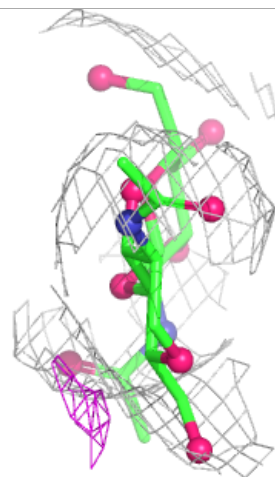
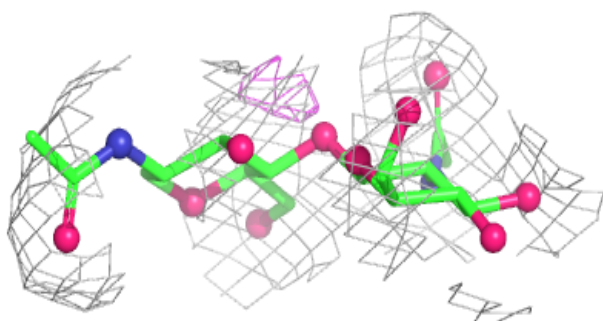
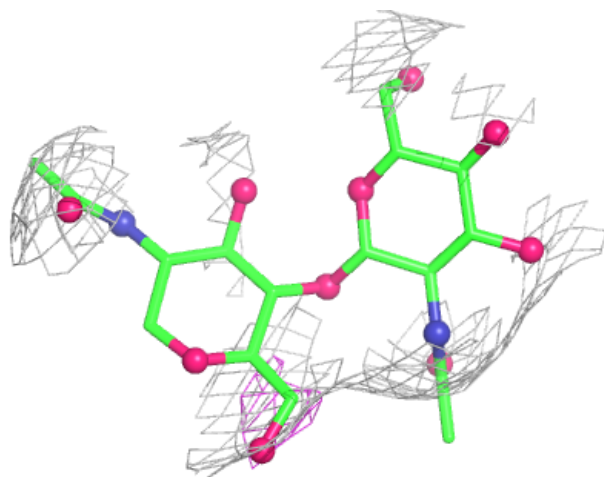
Electron density around Chain T:

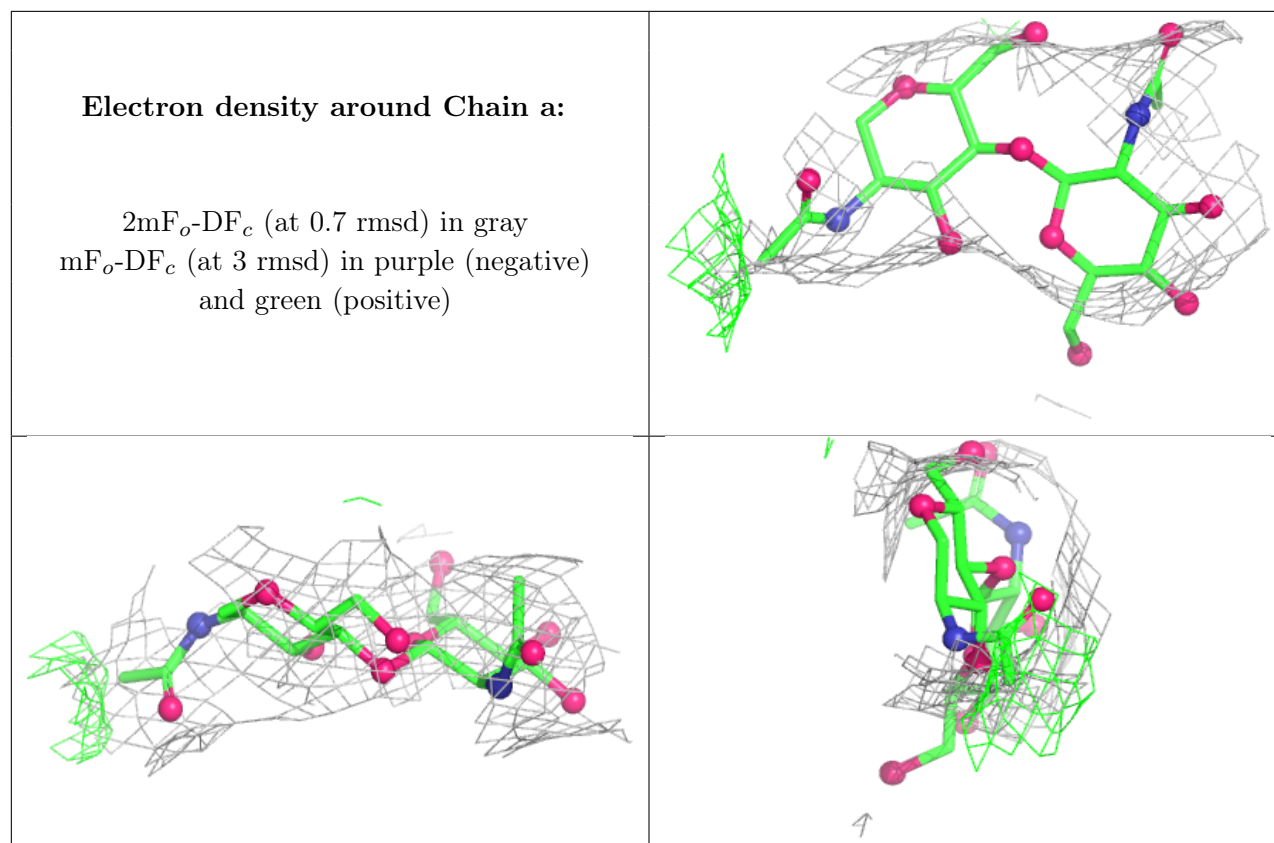
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain V:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	B	601	14/15	0.71	0.12	149,188,209,226	0

6.5 Other polymers [i](#)

There are no such residues in this entry.