



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 01:25 AM BST

PDB ID : 6FOF
Title : Crystal structure of a crystallized variant of h-Gal3: Gal-3[NTS/VII-IX]
Authors : Romero, A.; Flores-Ibarra, A.; Medrano, F.J.
Deposited on : 2018-02-07
Resolution : 2.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

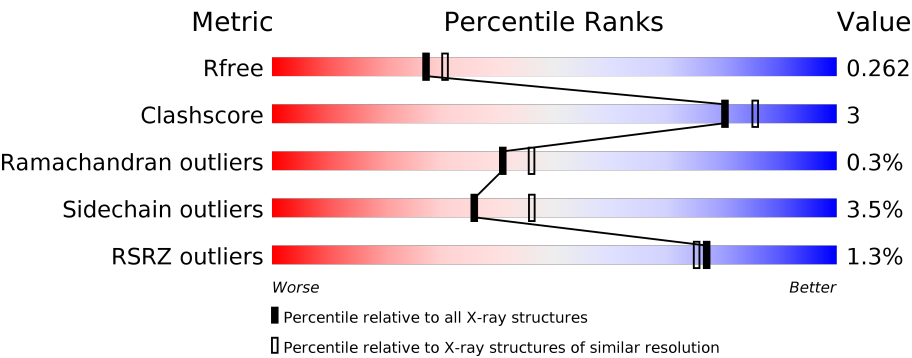
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	196	<div><div>%</div><div><div></div><div>67%</div><div>10%</div><div>•</div><div>22%</div></div></div>
1	B	196	<div><div>%</div><div><div></div><div>63%</div><div>6%</div><div>•</div><div>30%</div></div></div>
1	C	196	<div><div>%</div><div><div></div><div>64%</div><div>6%</div><div>•</div><div>30%</div></div></div>
1	D	196	<div><div></div><div><div></div><div>68%</div><div>8%</div><div>••</div><div>23%</div></div></div>
1	E	196	<div><div>%</div><div><div></div><div>63%</div><div>7%</div><div>•</div><div>30%</div></div></div>
1	F	196	<div><div>%</div><div><div></div><div>66%</div><div>10%</div><div>•</div><div>23%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	196	
1	H	196	
1	I	196	
1	J	196	
1	K	196	
1	L	196	
2	M	2	
2	N	2	
2	O	2	
2	P	2	
2	Q	2	
2	R	2	
2	S	2	
2	T	2	
2	U	2	
2	V	2	
2	W	2	
2	X	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
3	SO4	C	303	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14090 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 Galectin-3, Galectin-3.

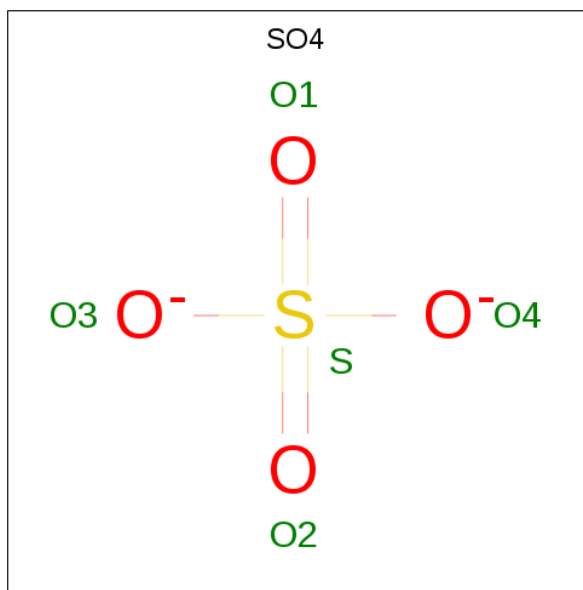
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	138	Total	C	N	O	S	0	0	0
			1108	708	200	197	3			
1	D	150	Total	C	N	O	S	0	0	0
			1180	754	212	211	3			
1	E	138	Total	C	N	O	S	0	0	0
			1108	708	200	197	3			
1	G	138	Total	C	N	O	S	0	0	0
			1108	708	200	197	3			
1	A	153	Total	C	N	O	S	0	0	0
			1212	771	219	219	3			
1	B	138	Total	C	N	O	S	0	0	0
			1108	708	200	197	3			
1	F	151	Total	C	N	O	S	0	0	0
			1200	763	217	217	3			
1	H	138	Total	C	N	O	S	0	1	0
			1110	709	200	198	3			
1	I	138	Total	C	N	O	S	0	0	0
			1108	708	200	197	3			
1	J	138	Total	C	N	O	S	0	0	0
			1108	708	200	197	3			
1	K	138	Total	C	N	O	S	0	0	0
			1108	708	200	197	3			
1	L	138	Total	C	N	O	S	0	0	0
			1108	708	200	197	3			

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	M	2	Total C O 23 12 11	0	0	0
2	N	2	Total C O 23 12 11	0	0	0
2	O	2	Total C O 23 12 11	0	0	0
2	P	2	Total C O 23 12 11	0	0	0
2	Q	2	Total C O 23 12 11	0	0	0
2	R	2	Total C O 23 12 11	0	0	0
2	S	2	Total C O 23 12 11	0	0	0
2	T	2	Total C O 23 12 11	0	0	0
2	U	2	Total C O 23 12 11	0	0	0
2	V	2	Total C O 23 12 11	0	0	0
2	W	2	Total C O 23 12 11	0	0	0
2	X	2	Total C O 23 12 11	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	K	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		

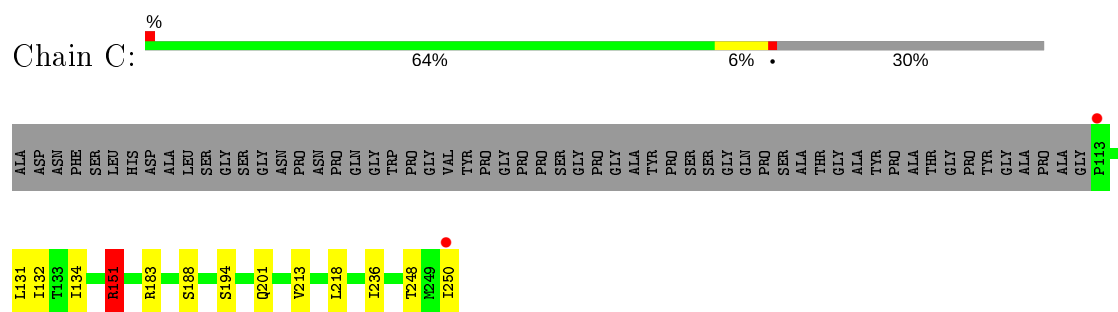
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	15	Total	O	0	0
			15	15		
4	D	9	Total	O	0	0
			9	9		
4	E	12	Total	O	0	0
			12	12		
4	G	10	Total	O	0	0
			10	10		
4	A	12	Total	O	0	0
			12	12		
4	B	16	Total	O	0	0
			16	16		
4	F	13	Total	O	0	0
			13	13		
4	H	10	Total	O	0	0
			10	10		
4	I	8	Total	O	0	0
			8	8		
4	J	9	Total	O	0	0
			9	9		
4	K	9	Total	O	0	0
			9	9		
4	L	5	Total	O	0	0
			5	5		

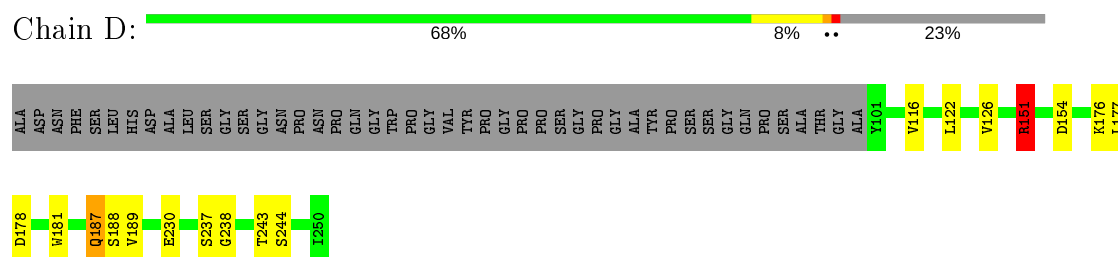
3 Residue-property plots [i](#)

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

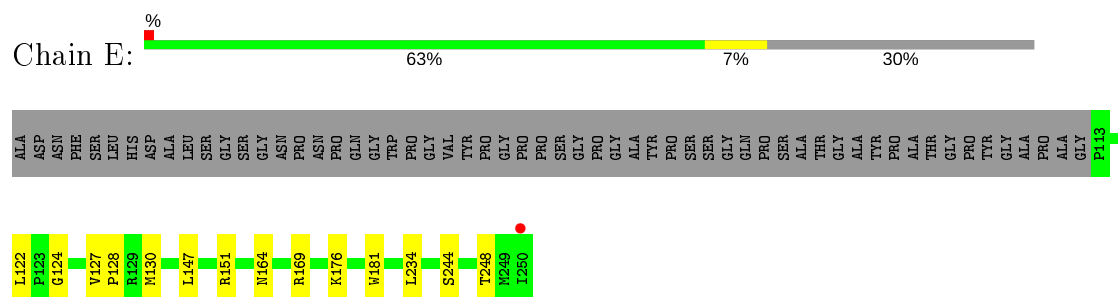
- Molecule 1: Galectin-3, Galectin-3



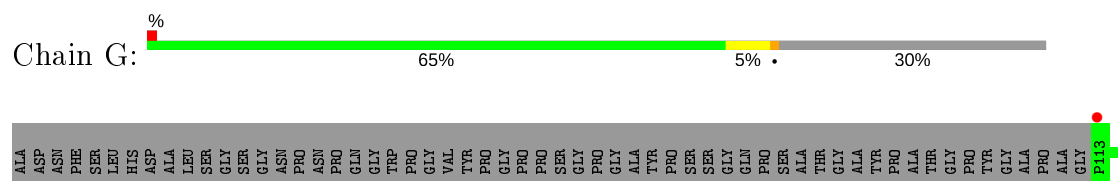
- Molecule 1: Galectin-3, Galectin-3



- Molecule 1: Galectin-3, Galectin-3

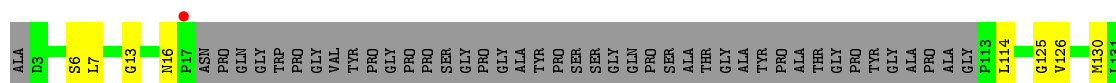


- Molecule 1: Galectin-3, Galectin-3

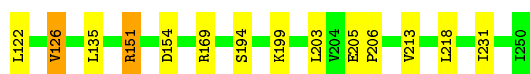
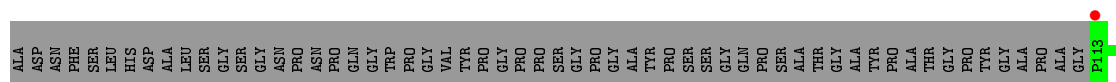




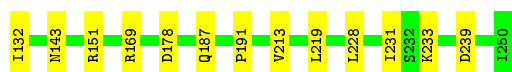
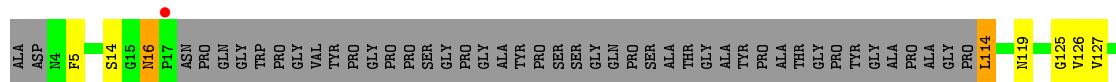
- Molecule 1: Galectin-3, Galectin-3



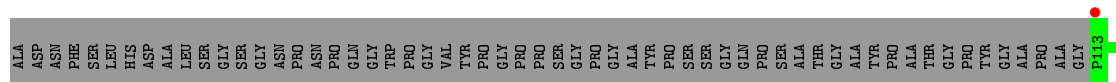
- Molecule 1: Galectin-3, Galectin-3



- Molecule 1: Galectin-3, Galectin-3

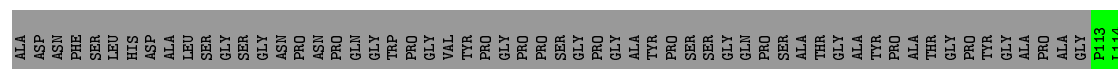


- Molecule 1: Galectin-3, Galectin-3

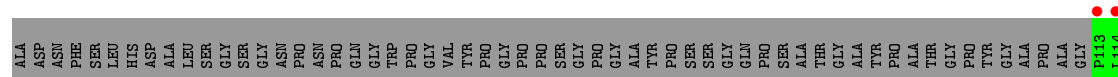


- Molecule 1: Galectin-3, Galectin-3

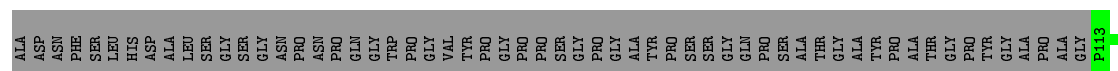




- Molecule 1: Galectin-3, Galectin-3



- Molecule 1: Galectin-3, Galectin-3



- Molecule 1: Galectin-3, Galectin-3



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose




- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



BGC1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain O:  100%BGC1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain P:  100%BGC1
GAL2


- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain Q:  100%BGC1
GAL2


- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain R:  50%  50%BGC1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain S:  100%BGC1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain T:  100%BGC1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain U:  100%BGC1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain V:  50% 50%

BGC1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain W:  50% 50%

BGC1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain X:  100%

BGC1
GAL2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.85Å 98.19Å 237.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.10 – 2.20 49.10 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.10-2.20) 100.0 (49.10-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.213 , 0.264 0.215 , 0.262	Depositor DCC
R_{free} test set	5607 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 17.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.060 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14090	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, GAL, SO4

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	0.79	1/1240 (0.1%)	0.95	5/1680 (0.3%)
1	B	0.73	0/1134	0.94	1/1537 (0.1%)
1	C	0.78	0/1134	0.98	3/1537 (0.2%)
1	D	0.74	0/1210	0.91	2/1645 (0.1%)
1	E	0.73	0/1134	0.88	2/1537 (0.1%)
1	F	0.75	0/1227	0.91	3/1662 (0.2%)
1	G	0.71	0/1134	0.88	0/1537
1	H	0.65	0/1140	0.88	3/1545 (0.2%)
1	I	0.65	0/1134	0.86	1/1537 (0.1%)
1	J	0.59	0/1134	0.83	2/1537 (0.1%)
1	K	0.62	0/1134	0.85	3/1537 (0.2%)
1	L	0.60	0/1134	0.85	2/1537 (0.1%)
All	All	0.70	1/13889 (0.0%)	0.89	27/18828 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	ARG	CZ-NH2	6.13	1.41	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	151	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	E	169	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	C	183	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	A	151	ARG	NE-CZ-NH2	7.07	123.83	120.30
1	H	169	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	H	169	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	I	151	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	L	169	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	H	178	ASP	CB-CA-C	6.26	122.93	110.40
1	C	151	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	K	183	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	E	169	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	A	169	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	F	169	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	207	ASP	CB-CA-C	-5.80	98.80	110.40
1	D	151	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	K	178	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	169	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	F	169	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	F	239	ASP	CB-CG-OD1	5.49	123.24	118.30
1	D	151	ARG	CG-CD-NE	5.43	123.21	111.80
1	A	6	SER	N-CA-CB	-5.38	102.43	110.50
1	J	162	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	J	129	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	151	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	K	151	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	L	162	ARG	NE-CZ-NH2	-5.15	117.73	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	177	LEU	Peptide
1	E	124	GLY	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	1212	0	1208	11	0
1	B	1108	0	1120	8	0
1	C	1108	0	1120	6	0
1	D	1180	0	1182	9	0
1	E	1108	0	1120	6	0
1	F	1200	0	1198	8	0
1	G	1108	0	1120	5	0
1	H	1110	0	1121	3	0
1	I	1108	0	1120	5	0
1	J	1108	0	1120	5	0
1	K	1108	0	1120	8	0
1	L	1108	0	1120	2	0
2	M	23	0	21	0	0
2	N	23	0	21	0	0
2	O	23	0	21	0	0
2	P	23	0	21	0	0
2	Q	23	0	21	0	0
2	R	23	0	21	0	0
2	S	23	0	21	0	0
2	T	23	0	21	0	0
2	U	23	0	21	0	0
2	V	23	0	21	0	0
2	W	23	0	21	1	0
2	X	23	0	21	0	0
3	B	10	0	0	0	0
3	C	20	0	0	4	0
3	D	10	0	0	1	0
3	E	5	0	0	1	0
3	F	5	0	0	0	0
3	G	15	0	0	1	0
3	H	20	0	0	1	0
3	I	10	0	0	0	0
3	J	5	0	0	1	0
3	K	15	0	0	1	0
3	L	5	0	0	1	0
4	A	12	0	0	0	0
4	B	16	0	0	0	0
4	C	15	0	0	0	0
4	D	9	0	0	0	0
4	E	12	0	0	1	0
4	F	13	0	0	0	0
4	G	10	0	0	0	0
4	H	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	8	0	0	0	0
4	J	9	0	0	0	0
4	K	9	0	0	1	0
4	L	5	0	0	0	0
All	All	14090	0	13921	76	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 3.

All (76) 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:E:151:ARG:NH1	3:E:302:SO4:O4	2.07	0.87
1:B:151:ARG:NH1	1:B:154:ASP:OD2	2.25	0.69
1:A:130:MET:HE2	1:A:132:ILE:HD11	1.74	0.68
1:G:151:ARG:NH2	3:G:304:SO4:O3	2.30	0.65
1:D:151:ARG:NH2	3:D:302:SO4:O1	2.32	0.62
1:C:188:SER:OG	3:C:305:SO4:O4	2.07	0.61
1:C:151:ARG:NH2	3:C:304:SO4:O1	2.34	0.60
3:H:302:SO4:O1	1:L:168:ARG:NH1	2.34	0.59
1:F:187:GLN:HE22	1:F:219:LEU:HB3	1.67	0.59
1:K:151:ARG:NH2	3:K:303:SO4:O1	2.35	0.59
1:L:151:ARG:NH2	3:L:302:SO4:O2	2.36	0.58
1:J:151:ARG:NH1	1:J:154:ASP:OD2	2.36	0.58
1:C:131:LEU:HB3	1:C:248:THR:HG22	1.85	0.56
1:H:178:ASP:CG	1:H:179:ASN:H	2.11	0.53
3:C:303:SO4:O1	1:A:168:ARG:NH1	2.42	0.53
1:K:147:LEU:HD11	1:K:200:ILE:HG21	1.91	0.53
1:G:191:PRO:HG2	1:G:213:VAL:HG11	1.91	0.52
1:E:176:LYS:HD3	1:E:181:TRP:CE2	2.45	0.52
1:I:210:LYS:HE2	1:I:220:GLN:HE21	1.76	0.51
1:H:158:HIS:O	1:H:173:CYS:HA	2.11	0.50
1:F:125:GLY:HA2	1:F:231:ILE:O	2.12	0.49
1:D:187:GLN:OE1	1:D:189:VAL:HB	2.12	0.49
1:E:122:LEU:HD22	1:E:130:MET:CE	2.42	0.49
1:A:130:MET:CE	1:A:132:ILE:HD11	2.42	0.49
1:D:116:VAL:HG11	1:D:238:GLY:O	2.13	0.49
1:D:122:LEU:HD13	1:D:126:VAL:HG12	1.95	0.48
1:B:203:LEU:HD21	1:B:205:GLU:OE1	2.14	0.47
1:D:151:ARG:NH1	1:D:154:ASP:OD2	2.47	0.47
1:G:116:VAL:HG13	1:G:237:SER:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:GLN:HE22	1:A:189:VAL:HB	1.79	0.47
1:A:162:ARG:CZ	1:A:172:VAL:HG21	2.46	0.46
1:D:116:VAL:HG13	1:D:237:SER:HA	1.96	0.46
1:I:171:ILE:HD12	1:I:218:LEU:HD21	1.97	0.46
1:C:132:ILE:O	1:C:201:GLN:HA	2.16	0.45
1:K:147:LEU:HD22	1:K:236:ILE:HG12	1.98	0.45
1:F:119:ASN:HD21	1:F:233:LYS:HG2	1.82	0.45
1:E:127:VAL:HG22	1:E:128:PRO:HD2	1.99	0.45
1:D:151:ARG:HD2	1:D:230:GLU:CB	2.47	0.45
1:D:176:LYS:HD2	1:D:181:TRP:CE2	2.52	0.44
1:J:126:VAL:HG23	1:J:228:LEU:HB3	2.00	0.44
1:I:132:ILE:O	1:I:201:GLN:HA	2.17	0.44
1:F:191:PRO:HG2	1:F:213:VAL:HG11	2.00	0.44
1:B:122:LEU:HD13	1:B:126:VAL:HG12	2.00	0.43
1:A:191:PRO:HG2	1:A:213:VAL:HB	1.99	0.43
1:D:151:ARG:HD2	1:D:230:GLU:HB2	2.00	0.43
1:J:151:ARG:NH2	3:J:302:SO4:O3	2.50	0.43
1:F:114:LEU:N	1:F:114:LEU:HD23	2.34	0.43
1:E:122:LEU:HD22	1:E:130:MET:HE1	2.00	0.43
1:C:213:VAL:HG23	1:C:218:LEU:HD22	2.02	0.42
1:I:134:ILE:HD12	1:I:134:ILE:N	2.34	0.42
1:K:168:ARG:HD2	4:K:408:HOH:O	2.19	0.42
1:J:205:GLU:HB3	1:J:206:PRO:CD	2.49	0.42
1:G:145:ILE:O	1:G:161:PRO:HD2	2.20	0.42
3:C:303:SO4:O3	1:A:168:ARG:NH1	2.53	0.42
1:A:126:VAL:HB	1:A:204:VAL:HG21	2.01	0.42
1:C:134:ILE:HD12	1:C:236:ILE:CD1	2.50	0.42
1:K:199:LYS:NZ	1:K:215:ASP:OD1	2.49	0.42
1:A:7:LEU:O	1:A:13:GLY:HA2	2.20	0.41
1:F:132:ILE:N	1:F:132:ILE:HD12	2.35	0.41
1:F:126:VAL:HG23	1:F:228:LEU:HB3	2.01	0.41
1:F:5:PHE:CE1	1:F:16:ASN:HB3	2.56	0.41
1:K:243:THR:O	1:K:244:SER:HB3	2.20	0.41
1:B:126:VAL:HG13	1:B:231:ILE:HB	2.03	0.41
1:B:213:VAL:HG23	1:B:218:LEU:HD22	2.03	0.41
1:E:147:LEU:HB3	1:E:234:LEU:HD11	2.01	0.41
1:A:125:GLY:HA2	1:A:231:ILE:O	2.21	0.41
1:B:135:LEU:CD2	1:B:199:LYS:HG3	2.51	0.41
1:B:199:LYS:O	1:B:213:VAL:HA	2.21	0.40
1:I:171:ILE:CD1	1:I:218:LEU:HD21	2.52	0.40
1:K:184:GLU:HG2	2:W:2:GAL:O6	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:176:LYS:HD2	1:G:181:TRP:CE2	2.56	0.40
1:H:187:GLN:OE1	1:H:189:VAL:HB	2.22	0.40
4:E:403:HOH:O	1:A:169:ARG:HD3	2.21	0.40
1:J:158:HIS:O	1:J:173:CYS:HA	2.21	0.40
1:K:122:LEU:O	1:K:125:GLY:N	2.54	0.40
1:B:205:GLU:HB3	1:B:206:PRO:CD	2.50	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	149/196 (76%)	145 (97%)	3 (2%)	1 (1%)	22	22
1	B	136/196 (69%)	131 (96%)	5 (4%)	0	100	100
1	C	136/196 (69%)	132 (97%)	4 (3%)	0	100	100
1	D	148/196 (76%)	142 (96%)	5 (3%)	1 (1%)	22	22
1	E	136/196 (69%)	133 (98%)	3 (2%)	0	100	100
1	F	147/196 (75%)	140 (95%)	6 (4%)	1 (1%)	22	22
1	G	136/196 (69%)	131 (96%)	5 (4%)	0	100	100
1	H	137/196 (70%)	132 (96%)	5 (4%)	0	100	100
1	I	136/196 (69%)	133 (98%)	2 (2%)	1 (1%)	22	22
1	J	136/196 (69%)	127 (93%)	9 (7%)	0	100	100
1	K	136/196 (69%)	129 (95%)	6 (4%)	1 (1%)	22	22
1	L	136/196 (69%)	126 (93%)	10 (7%)	0	100	100
All	All	1669/2352 (71%)	1601 (96%)	63 (4%)	5 (0%)	41	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	178	ASP
1	I	178	ASP
1	F	16	ASN
1	A	16	ASN
1	K	178	ASP

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	135/162 (83%)	132 (98%)	3 (2%)	52	65
1	B	124/162 (76%)	121 (98%)	3 (2%)	49	62
1	C	124/162 (76%)	121 (98%)	3 (2%)	49	62
1	D	129/162 (80%)	124 (96%)	5 (4%)	32	41
1	E	124/162 (76%)	121 (98%)	3 (2%)	49	62
1	F	134/162 (83%)	128 (96%)	6 (4%)	27	34
1	G	124/162 (76%)	121 (98%)	3 (2%)	49	62
1	H	125/162 (77%)	119 (95%)	6 (5%)	25	32
1	I	124/162 (76%)	118 (95%)	6 (5%)	25	32
1	J	124/162 (76%)	120 (97%)	4 (3%)	39	50
1	K	124/162 (76%)	118 (95%)	6 (5%)	25	32
1	L	124/162 (76%)	119 (96%)	5 (4%)	31	40
All	All	1515/1944 (78%)	1462 (96%)	53 (4%)	36	46

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	151	ARG
1	C	194	SER
1	C	250	ILE
1	D	151	ARG
1	D	187	GLN
1	D	188	SER

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Mol	Chain	Res	Type
1	D	243	THR
1	D	244	SER
1	E	164	ASN
1	E	244	SER
1	E	248	THR
1	G	151	ARG
1	G	187	GLN
1	G	210	LYS
1	A	114	LEU
1	A	151	ARG
1	A	210	LYS
1	B	126	VAL
1	B	151	ARG
1	B	194	SER
1	F	14	SER
1	F	114	LEU
1	F	127	VAL
1	F	143	ASN
1	F	151	ARG
1	F	178	ASP
1	H	122	LEU
1	H	178	ASP
1	H	187	GLN
1	H	210	LYS
1	H	233	LYS
1	H	243	THR
1	I	128	PRO
1	I	151	ARG
1	I	220	GLN
1	I	232	SER
1	I	241	ASP
1	I	248	THR
1	J	150	GLN
1	J	151	ARG
1	J	188	SER
1	J	248	THR
1	K	150	GLN
1	K	151	ARG
1	K	183	ARG
1	K	194	SER
1	K	196	LYS
1	K	230	GLU

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Mol	Chain	Res	Type
1	L	127	VAL
1	L	151	ARG
1	L	232	SER
1	L	248	THR
1	L	250	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	220	GLN
1	E	119	ASN
1	E	164	ASN
1	A	166	ASN
1	A	187	GLN
1	B	166	ASN
1	F	119	ASN
1	F	180	ASN
1	F	187	GLN
1	H	220	GLN
1	I	143	ASN
1	I	153	ASN
1	I	220	GLN
1	J	119	ASN
1	K	153	ASN
1	K	187	GLN
1	L	119	ASN
1	L	180	ASN
1	L	223	HIS

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 ⓘ

24 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	BGC	M	1	2	12,12,12	0.65	0	17,17,17	1.59	5 (29%)
2	GAL	M	2	2	11,11,12	0.62	0	15,15,17	1.21	2 (13%)
2	BGC	N	1	2	12,12,12	0.73	0	17,17,17	1.33	1 (5%)
2	GAL	N	2	2	11,11,12	0.46	0	15,15,17	1.08	1 (6%)
2	BGC	O	1	2	12,12,12	0.71	0	17,17,17	1.39	1 (5%)
2	GAL	O	2	2	11,11,12	0.96	0	15,15,17	1.33	2 (13%)
2	BGC	P	1	2	12,12,12	0.43	0	17,17,17	1.70	4 (23%)
2	GAL	P	2	2	11,11,12	0.66	0	15,15,17	1.15	1 (6%)
2	BGC	Q	1	2	12,12,12	0.77	0	17,17,17	2.30	7 (41%)
2	GAL	Q	2	2	11,11,12	1.23	1 (9%)	15,15,17	1.76	6 (40%)
2	BGC	R	1	2	12,12,12	0.65	0	17,17,17	1.54	4 (23%)
2	GAL	R	2	2	11,11,12	0.77	0	15,15,17	0.79	0
2	BGC	S	1	2	12,12,12	0.65	0	17,17,17	1.28	3 (17%)
2	GAL	S	2	2	11,11,12	0.79	0	15,15,17	1.36	1 (6%)
2	BGC	T	1	2	12,12,12	0.95	1 (8%)	17,17,17	1.94	6 (35%)
2	GAL	T	2	2	11,11,12	0.84	0	15,15,17	1.37	2 (13%)
2	BGC	U	1	2	12,12,12	0.68	0	17,17,17	1.60	2 (11%)
2	GAL	U	2	2	11,11,12	0.66	0	15,15,17	1.18	2 (13%)
2	BGC	V	1	2	12,12,12	0.46	0	17,17,17	0.80	0
2	GAL	V	2	2	11,11,12	0.54	0	15,15,17	1.08	2 (13%)
2	BGC	W	1	2	12,12,12	0.60	0	17,17,17	1.39	2 (11%)
2	GAL	W	2	2	11,11,12	0.78	0	15,15,17	0.93	1 (6%)
2	BGC	X	1	2	12,12,12	0.58	0	17,17,17	1.02	1 (5%)
2	GAL	X	2	2	11,11,12	0.84	0	15,15,17	1.66	3 (20%)

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	BGC	M	1	2	-	0/2/22/22	0/1/1/1
2	GAL	M	2	2	-	0/2/19/22	0/1/1/1
2	BGC	N	1	2	-	0/2/22/22	0/1/1/1
2	GAL	N	2	2	-	0/2/19/22	0/1/1/1
2	BGC	O	1	2	-	0/2/22/22	0/1/1/1
2	GAL	O	2	2	-	1/2/19/22	0/1/1/1
2	BGC	P	1	2	-	0/2/22/22	0/1/1/1
2	GAL	P	2	2	-	0/2/19/22	0/1/1/1
2	BGC	Q	1	2	-	2/2/22/22	0/1/1/1
2	GAL	Q	2	2	-	1/2/19/22	0/1/1/1
2	BGC	R	1	2	-	1/2/22/22	0/1/1/1
2	GAL	R	2	2	-	0/2/19/22	0/1/1/1
2	BGC	S	1	2	-	1/2/22/22	0/1/1/1
2	GAL	S	2	2	-	0/2/19/22	0/1/1/1
2	BGC	T	1	2	-	0/2/22/22	0/1/1/1
2	GAL	T	2	2	-	0/2/19/22	0/1/1/1
2	BGC	U	1	2	-	0/2/22/22	0/1/1/1
2	GAL	U	2	2	-	0/2/19/22	0/1/1/1
2	BGC	V	1	2	-	0/2/22/22	0/1/1/1
2	GAL	V	2	2	-	0/2/19/22	0/1/1/1
2	BGC	W	1	2	-	0/2/22/22	0/1/1/1
2	GAL	W	2	2	-	0/2/19/22	0/1/1/1
2	BGC	X	1	2	-	0/2/22/22	0/1/1/1
2	GAL	X	2	2	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	2	GAL	O5-C1	-3.16	1.38	1.43
2	T	1	BGC	O3-C3	2.05	1.47	1.43

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	2	GAL	C1-O5-C5	4.89	118.81	112.19
2	Q	1	BGC	C6-C5-C4	3.98	122.31	113.00
2	T	1	BGC	O3-C3-C4	3.86	119.26	110.35
2	Q	1	BGC	O4-C4-C3	-3.82	101.53	110.35
2	T	1	BGC	C1-O5-C5	-3.80	106.50	113.66
2	Q	1	BGC	C1-O5-C5	-3.76	106.57	113.66
2	U	1	BGC	O5-C1-C2	-3.43	104.16	110.28
2	Q	1	BGC	O5-C1-C2	-3.38	104.25	110.28
2	P	1	BGC	C1-O5-C5	-3.11	107.80	113.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	1	BGC	O4-C4-C3	-3.06	103.27	110.35
2	T	2	GAL	O5-C1-C2	-3.01	106.12	110.77
2	O	2	GAL	O3-C3-C2	-2.99	104.26	109.99
2	Q	2	GAL	C3-C4-C5	-2.87	105.12	110.24
2	M	1	BGC	O5-C1-C2	-2.87	105.16	110.28
2	N	1	BGC	C1-O5-C5	-2.87	108.25	113.66
2	P	1	BGC	O2-C2-C3	-2.81	103.85	110.35
2	Q	2	GAL	O4-C4-C5	2.78	116.19	109.30
2	O	1	BGC	O5-C1-C2	-2.77	105.35	110.28
2	N	2	GAL	O5-C5-C6	-2.76	102.88	107.20
2	Q	2	GAL	O5-C5-C6	2.68	111.41	107.20
2	V	2	GAL	O3-C3-C2	-2.68	104.87	109.99
2	Q	1	BGC	O1-C1-O5	-2.65	102.43	110.38
2	R	1	BGC	O1-C1-O5	-2.65	102.43	110.38
2	R	1	BGC	C6-C5-C4	2.65	119.20	113.00
2	Q	1	BGC	O1-C1-C2	2.64	116.46	109.03
2	P	1	BGC	C3-C4-C5	2.63	114.93	110.24
2	R	1	BGC	C1-O5-C5	-2.60	108.76	113.66
2	S	2	GAL	O3-C3-C2	-2.58	105.04	109.99
2	M	1	BGC	C1-O5-C5	-2.58	108.80	113.66
2	X	2	GAL	O3-C3-C4	2.53	116.20	110.35
2	M	1	BGC	O5-C5-C6	2.50	112.64	106.44
2	P	1	BGC	O5-C1-C2	-2.46	105.89	110.28
2	S	1	BGC	O5-C5-C4	-2.46	105.22	109.69
2	O	2	GAL	C1-O5-C5	-2.44	108.88	112.19
2	W	1	BGC	O1-C1-O5	-2.43	103.08	110.38
2	M	2	GAL	O5-C5-C6	2.41	110.98	107.20
2	U	2	GAL	O3-C3-C2	-2.41	105.39	109.99
2	T	1	BGC	O5-C1-C2	-2.38	106.04	110.28
2	Q	2	GAL	O3-C3-C4	-2.37	104.88	110.35
2	M	2	GAL	C3-C4-C5	-2.36	106.03	110.24
2	W	1	BGC	O2-C2-C1	2.35	114.61	109.16
2	T	1	BGC	O4-C4-C5	-2.34	103.49	109.30
2	Q	2	GAL	O2-C2-C3	-2.29	105.56	110.14
2	M	1	BGC	C1-C2-C3	-2.27	105.61	110.31
2	V	2	GAL	O5-C5-C6	-2.25	103.67	107.20
2	W	2	GAL	O3-C3-C2	-2.25	105.69	109.99
2	X	2	GAL	O2-C2-C1	-2.25	104.56	109.15
2	T	1	BGC	C4-C3-C2	-2.24	106.92	110.82
2	U	1	BGC	O1-C1-O5	-2.23	103.68	110.38
2	X	1	BGC	O1-C1-O5	-2.19	103.80	110.38
2	S	1	BGC	O4-C4-C3	-2.14	105.41	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	2	GAL	O5-C5-C4	-2.12	105.68	110.83
2	U	2	GAL	C1-C2-C3	-2.10	107.08	109.67
2	S	1	BGC	C1-O5-C5	-2.09	109.72	113.66
2	P	2	GAL	O5-C1-C2	2.06	113.95	110.77
2	M	1	BGC	C3-C4-C5	2.05	113.90	110.24
2	T	1	BGC	C6-C5-C4	2.03	117.77	113.00
2	Q	2	GAL	C6-C5-C4	-2.03	108.25	113.00
2	Q	1	BGC	C4-C3-C2	-2.01	107.32	110.82

There are no chirality outliers.

All (6) torsion outliers are listed below:

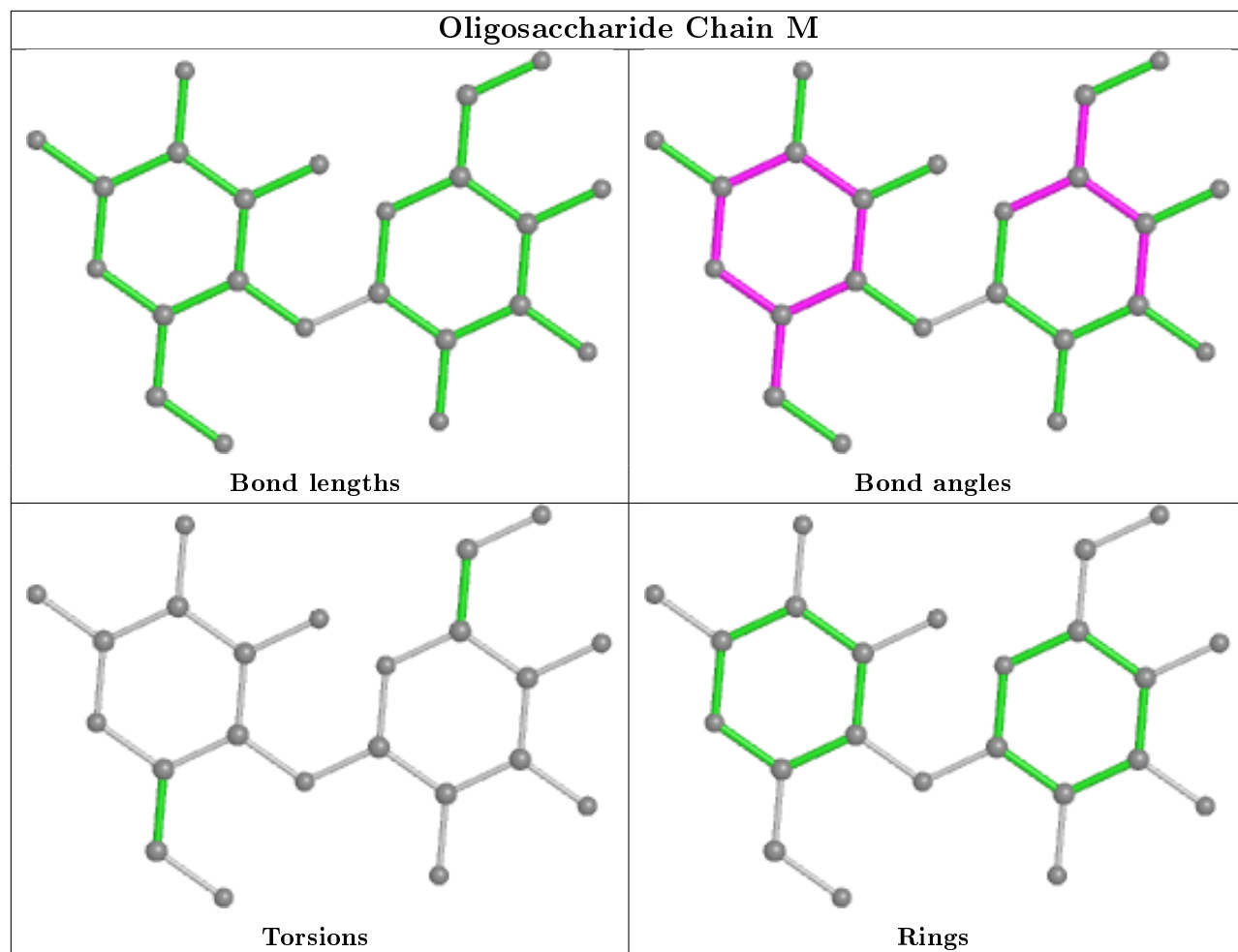
Mol	Chain	Res	Type	Atoms
2	Q	1	BGC	C4-C5-C6-O6
2	Q	1	BGC	O5-C5-C6-O6
2	Q	2	GAL	O5-C5-C6-O6
2	S	1	BGC	C4-C5-C6-O6
2	O	2	GAL	O5-C5-C6-O6
2	R	1	BGC	C4-C5-C6-O6

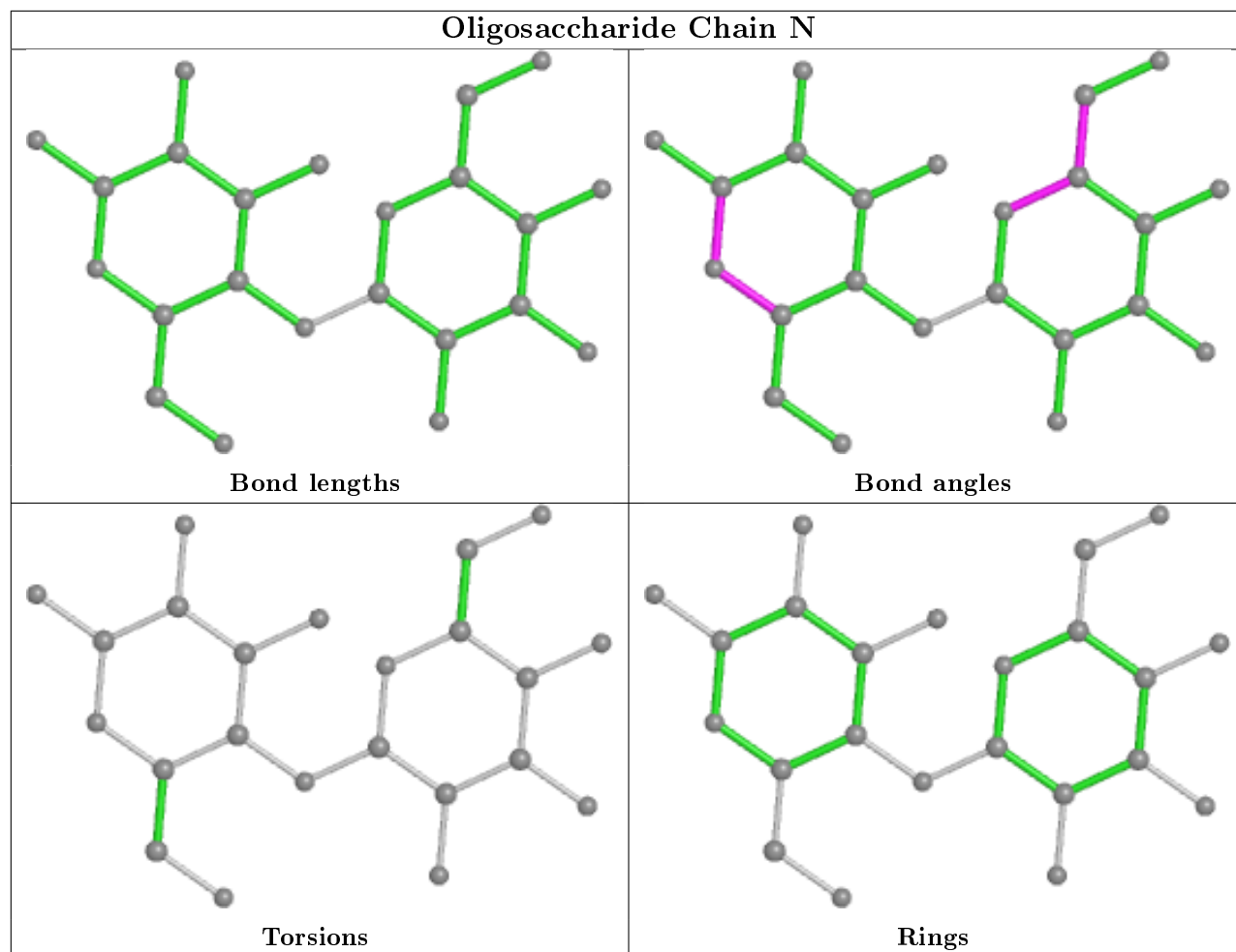
There are no ring outliers.

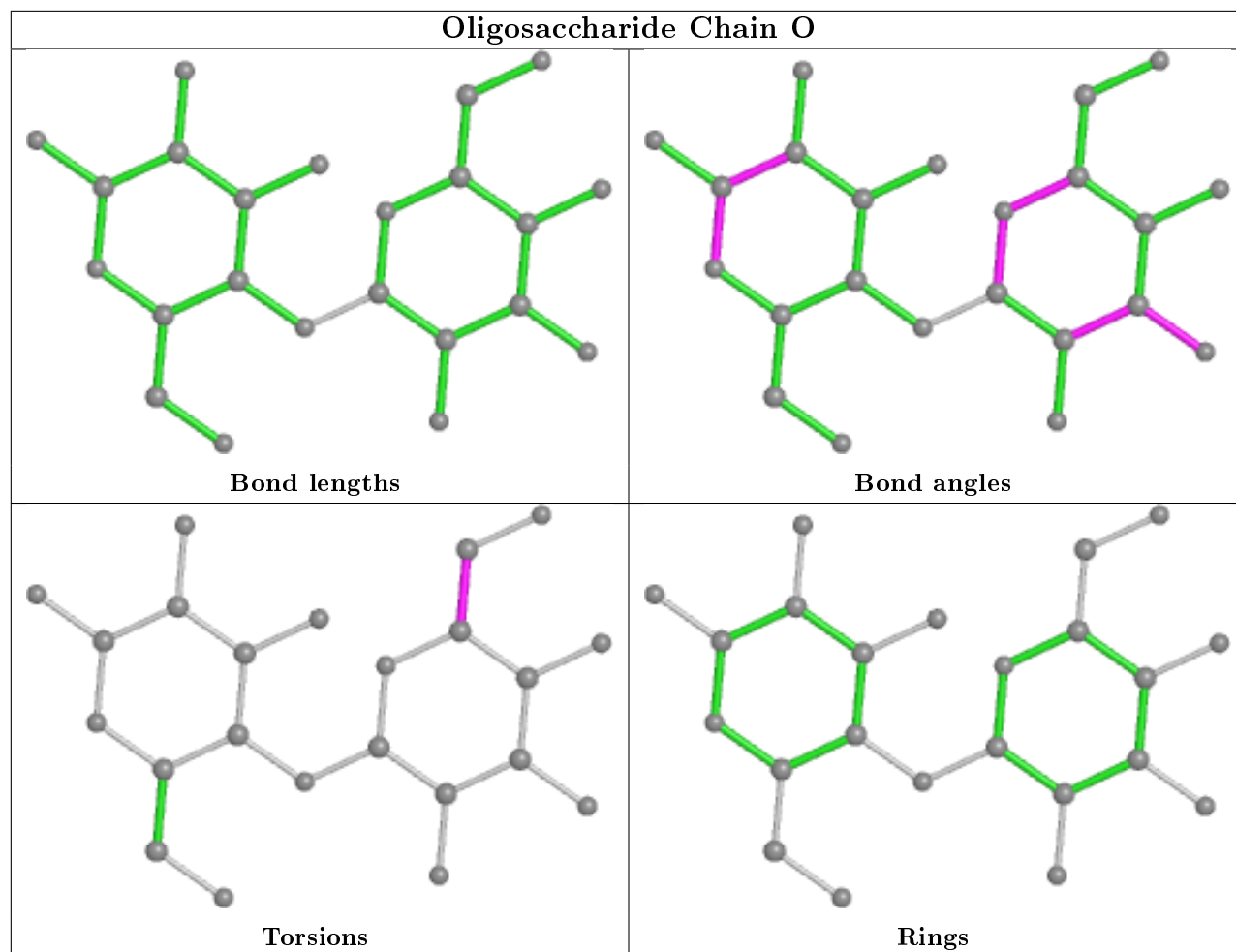
1 monomer is involved in 1 short contact:

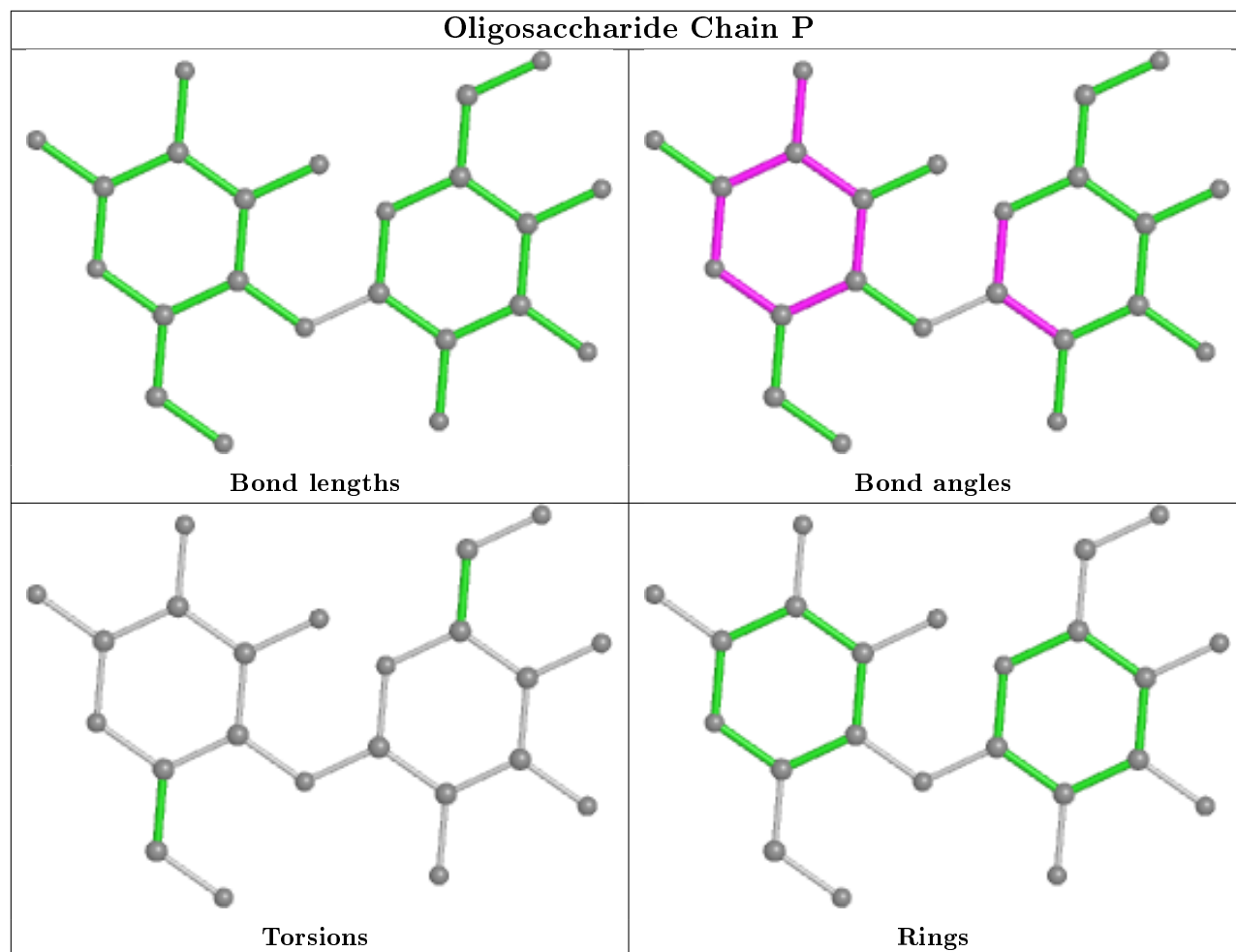
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	W	2	GAL	1	0

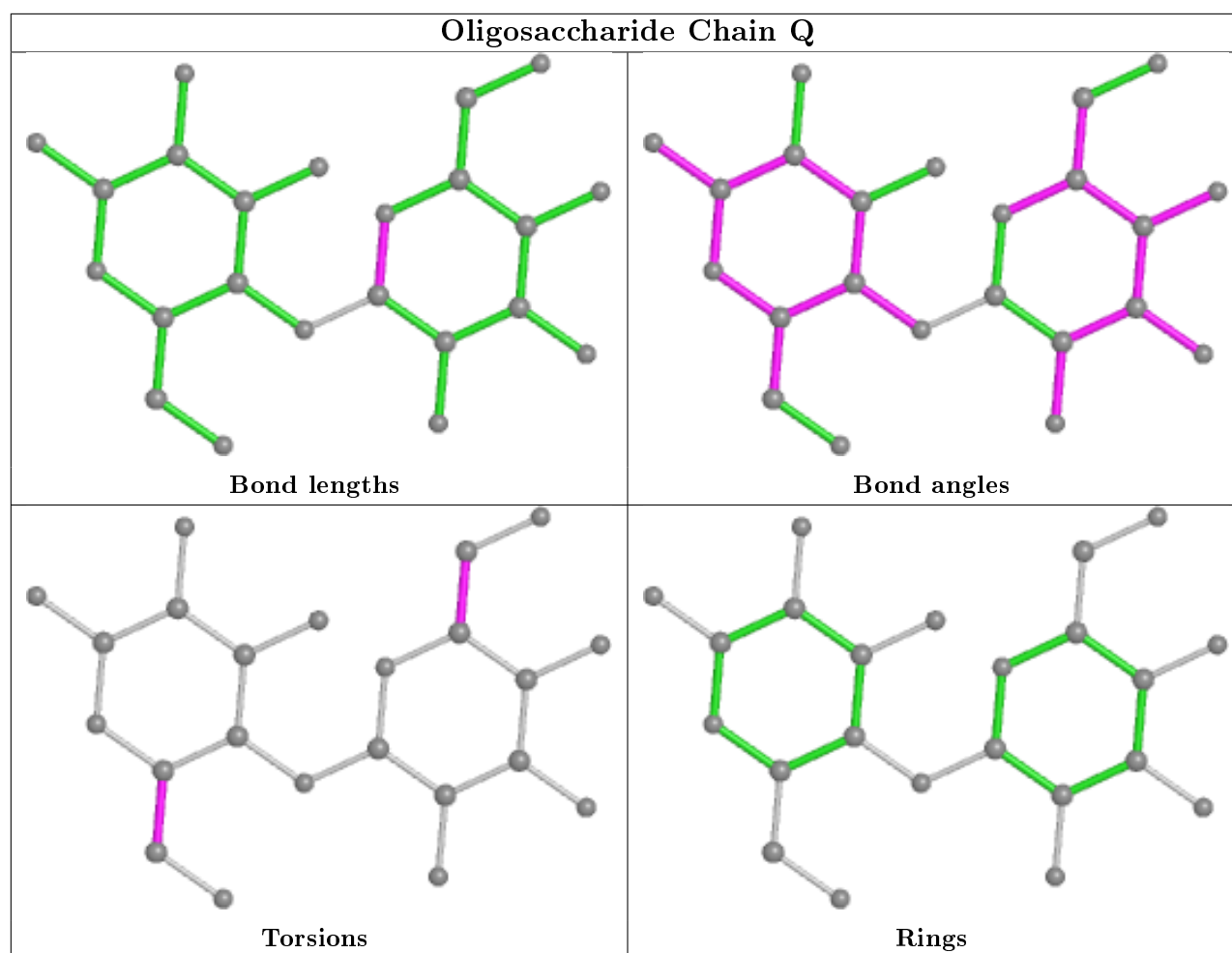
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

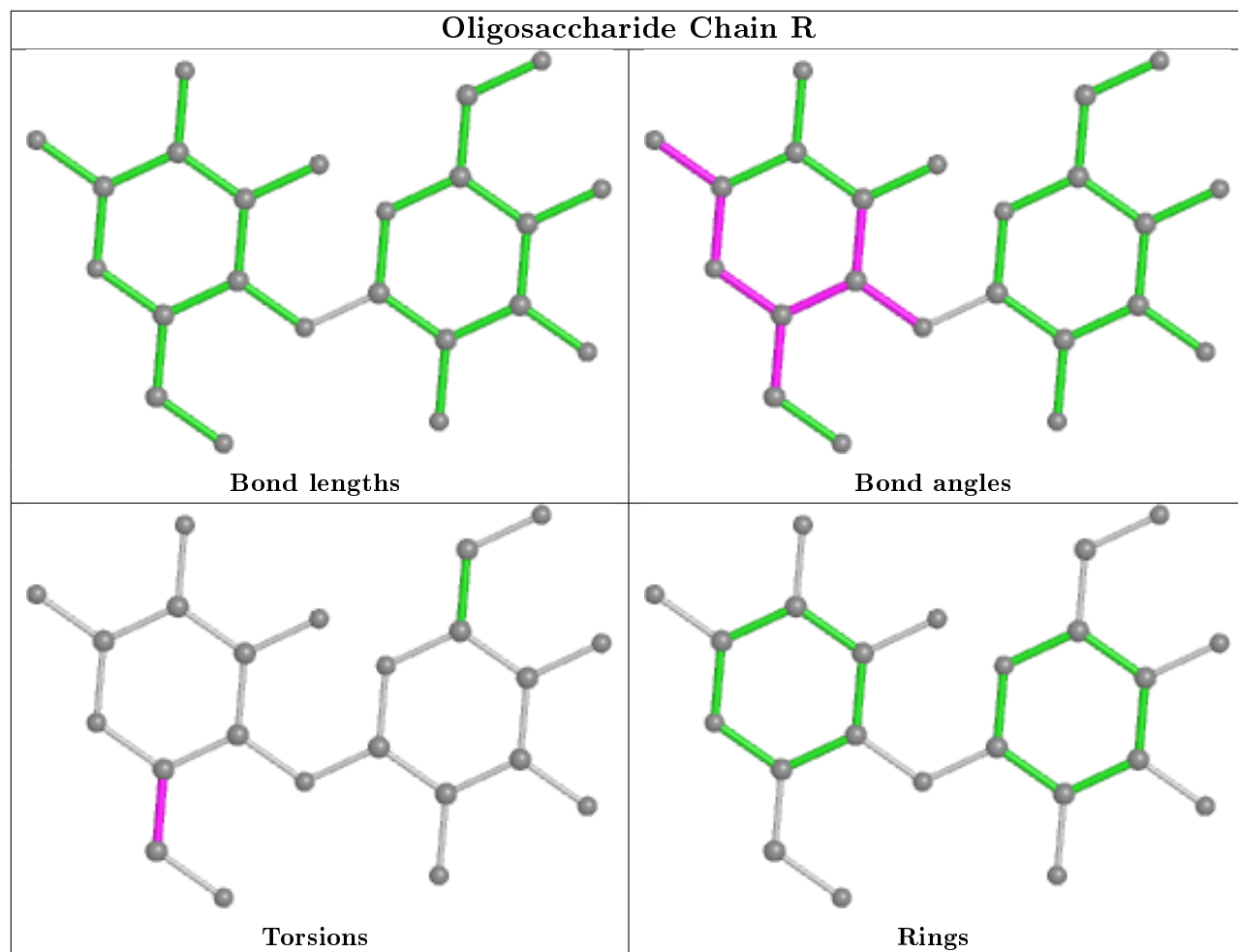


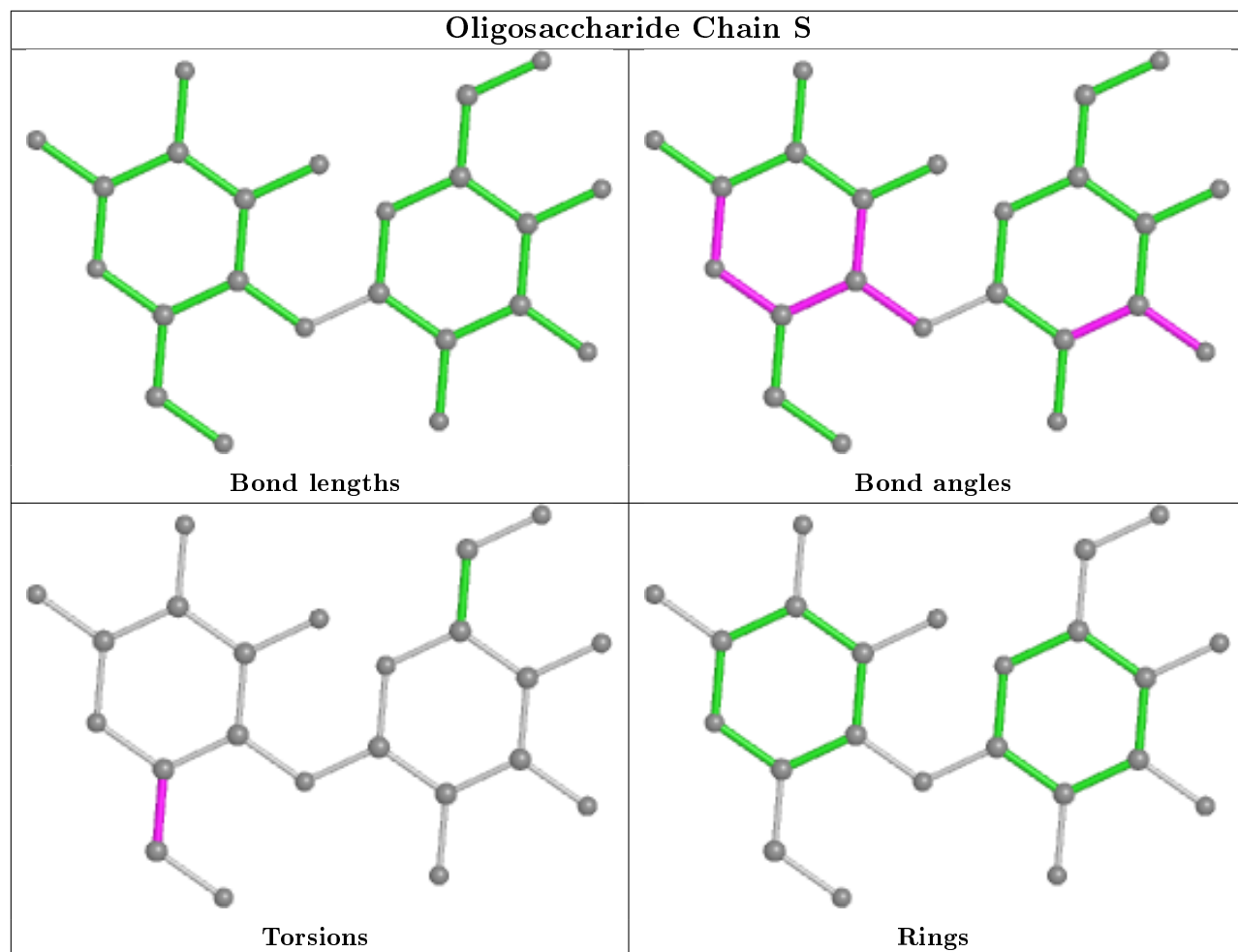


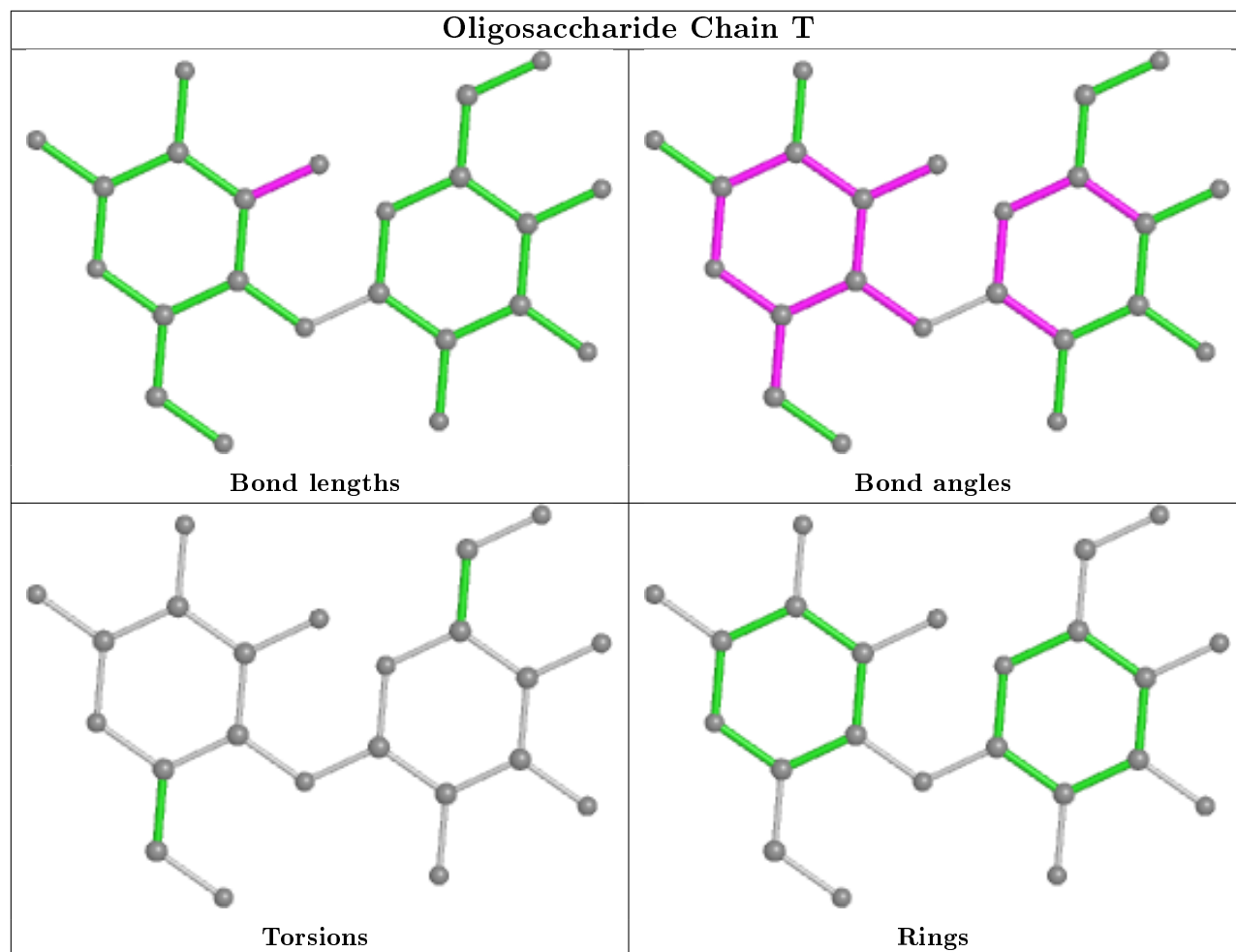


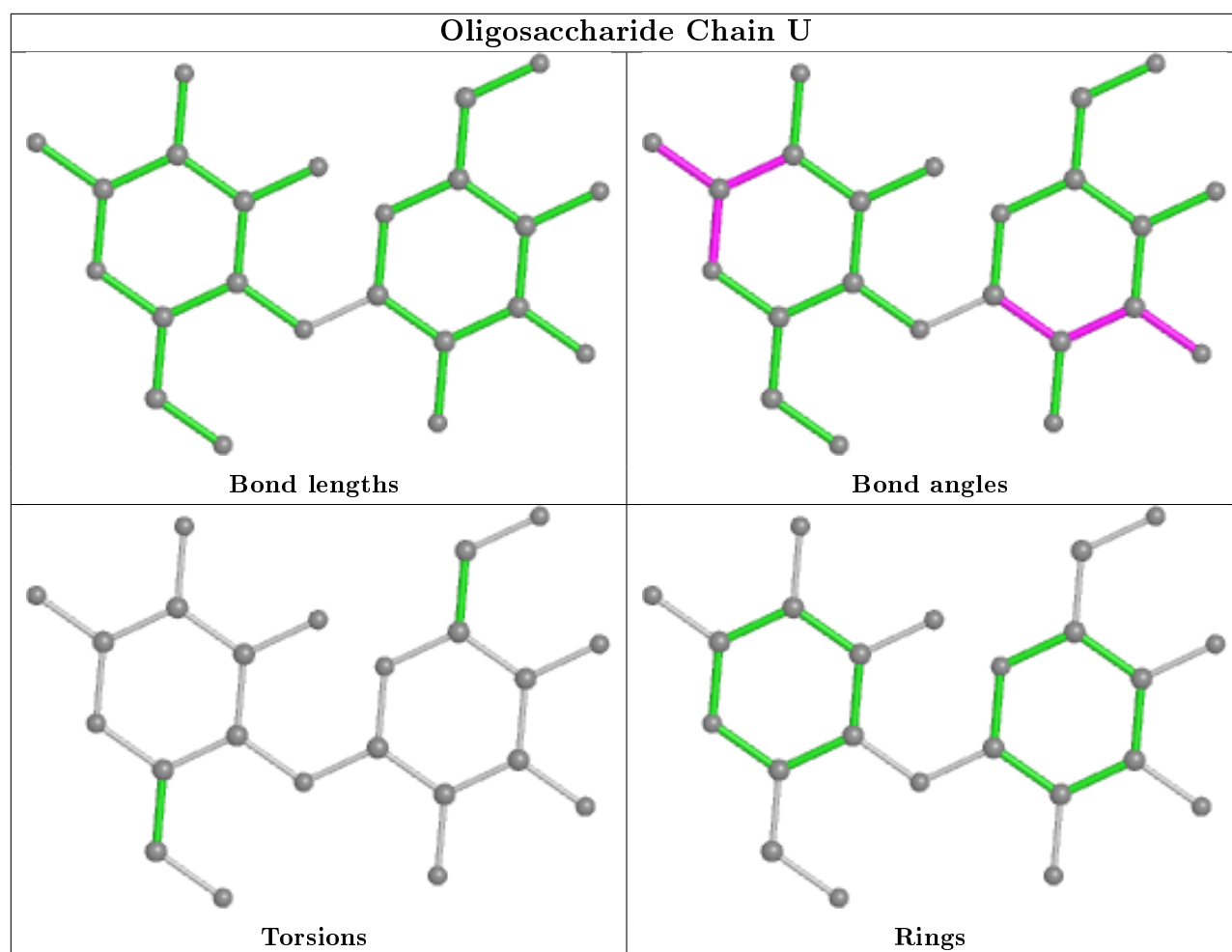


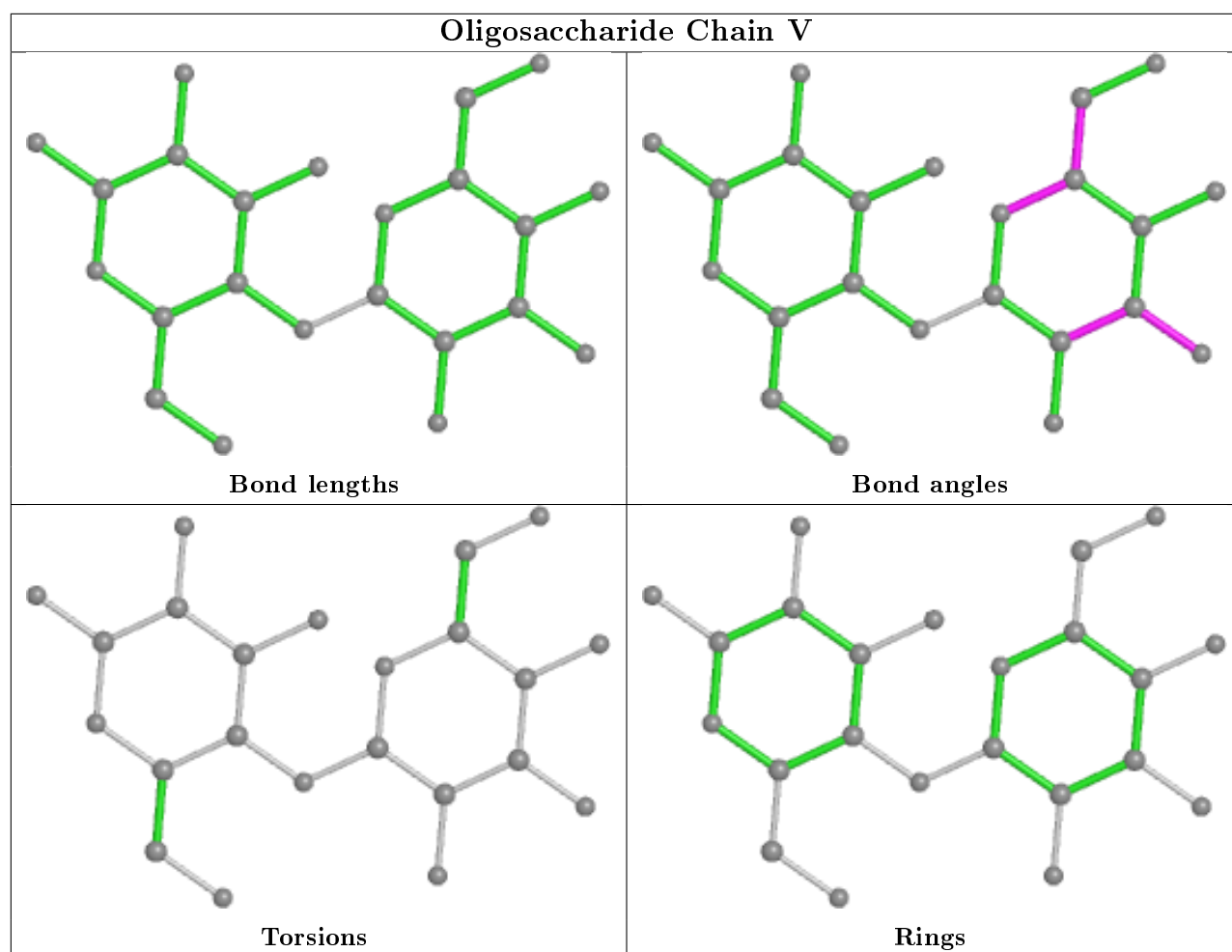


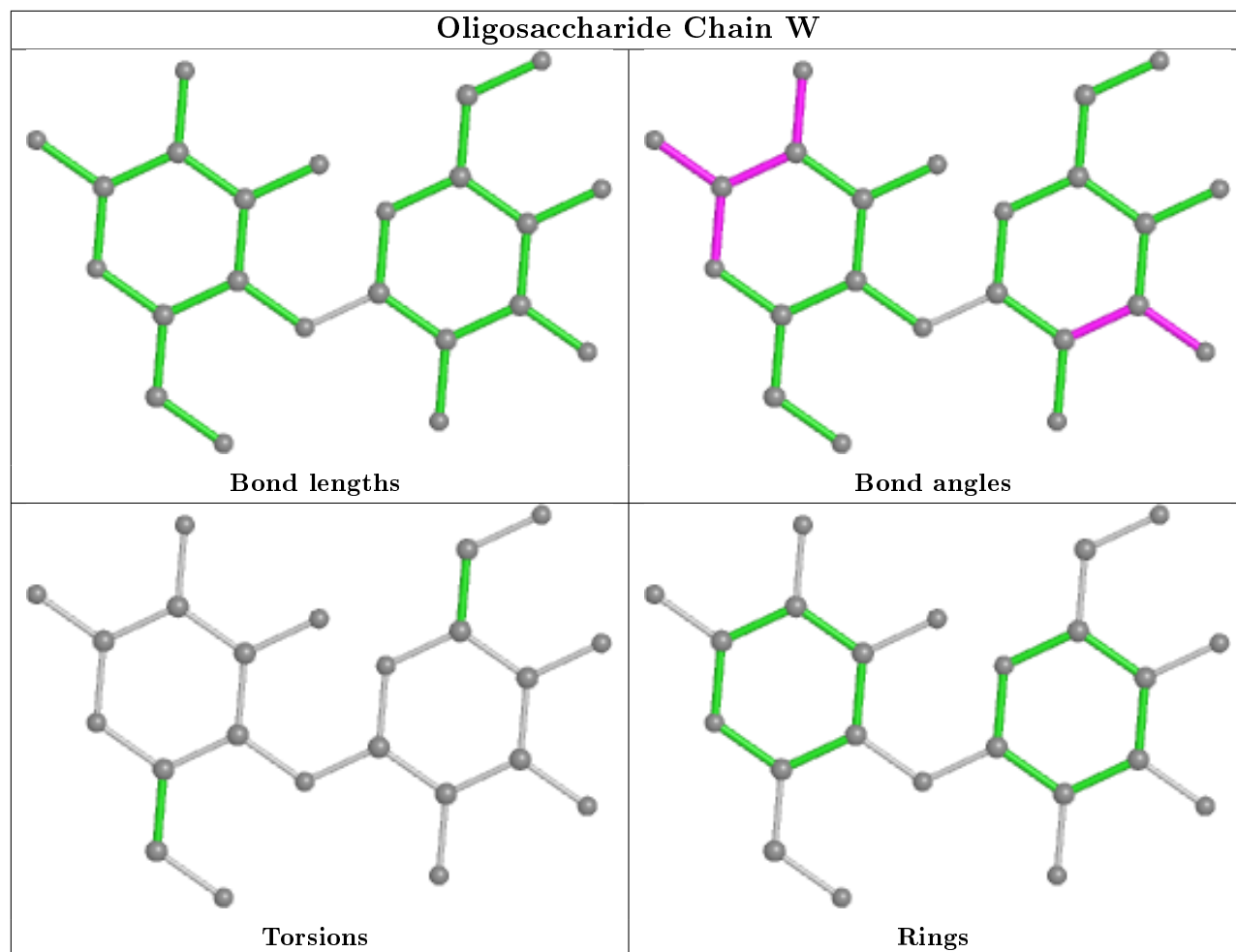


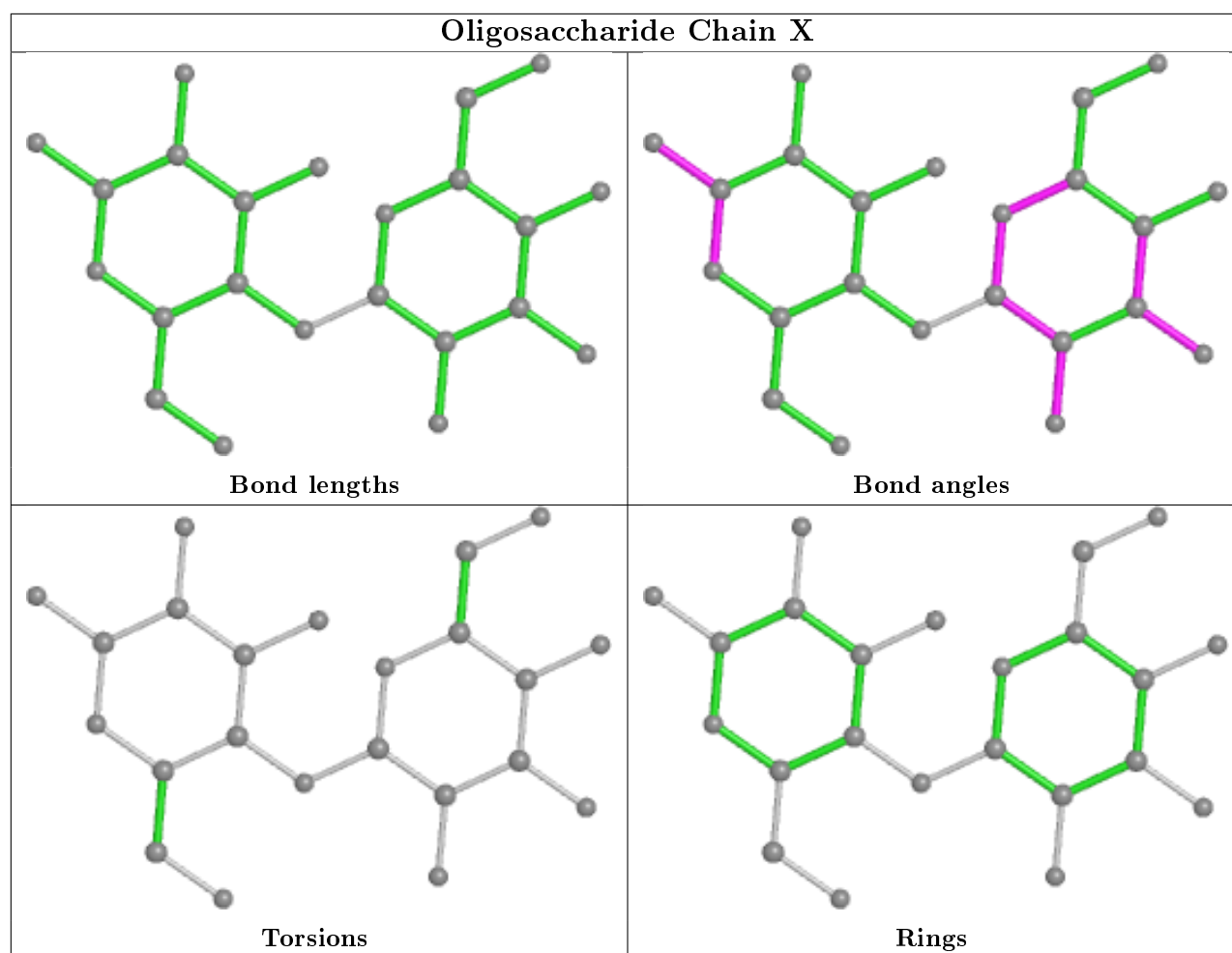












5.6 Ligand geometry [i](#)

24 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	$\# Z > 2$
3	SO4	B	303	-	4,4,4	0.50	0	6,6,6	0.74	0
3	SO4	I	303	-	4,4,4	0.32	0	6,6,6	0.43	0
3	SO4	K	303	-	4,4,4	0.46	0	6,6,6	0.25	0
3	SO4	J	302	-	4,4,4	0.45	0	6,6,6	0.43	0
3	SO4	G	302	-	4,4,4	0.31	0	6,6,6	0.92	0
3	SO4	H	303	-	4,4,4	0.44	0	6,6,6	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	C	304	-	4,4,4	0.44	0	6,6,6	0.84	0
3	SO4	C	303	-	4,4,4	0.30	0	6,6,6	0.54	0
3	SO4	C	305	-	4,4,4	0.15	0	6,6,6	0.35	0
3	SO4	K	302	-	4,4,4	0.23	0	6,6,6	0.55	0
3	SO4	D	303	-	4,4,4	0.28	0	6,6,6	0.49	0
3	SO4	G	304	-	4,4,4	0.27	0	6,6,6	0.46	0
3	SO4	F	302	-	4,4,4	0.08	0	6,6,6	0.83	0
3	SO4	H	302	-	4,4,4	0.30	0	6,6,6	0.37	0
3	SO4	K	304	-	4,4,4	0.41	0	6,6,6	0.25	0
3	SO4	B	302	-	4,4,4	0.59	0	6,6,6	0.69	0
3	SO4	L	302	-	4,4,4	0.41	0	6,6,6	0.19	0
3	SO4	E	302	-	4,4,4	0.98	0	6,6,6	0.85	0
3	SO4	H	304	-	4,4,4	0.43	0	6,6,6	0.44	0
3	SO4	D	302	-	4,4,4	0.27	0	6,6,6	0.45	0
3	SO4	C	302	-	4,4,4	0.36	0	6,6,6	0.46	0
3	SO4	H	305	-	4,4,4	0.42	0	6,6,6	0.30	0
3	SO4	I	302	-	4,4,4	0.30	0	6,6,6	0.69	0
3	SO4	G	303	-	4,4,4	0.36	0	6,6,6	0.39	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	303	SO4	1	0
3	J	302	SO4	1	0
3	C	304	SO4	1	0
3	C	303	SO4	2	0
3	C	305	SO4	1	0
3	G	304	SO4	1	0
3	H	302	SO4	1	0
3	L	302	SO4	1	0
3	E	302	SO4	1	0
3	D	302	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	153/196 (78%)	-0.43	1 (0%) 87 86	24, 37, 55, 85	0
1	B	138/196 (70%)	-0.44	1 (0%) 87 86	25, 41, 57, 106	0
1	C	138/196 (70%)	-0.41	2 (1%) 75 73	26, 36, 52, 88	0
1	D	150/196 (76%)	-0.33	0 100 100	26, 44, 65, 69	0
1	E	138/196 (70%)	-0.39	1 (0%) 87 86	26, 40, 59, 102	0
1	F	151/196 (77%)	-0.31	1 (0%) 87 86	26, 41, 59, 100	0
1	G	138/196 (70%)	-0.27	2 (1%) 75 73	28, 47, 69, 120	0
1	H	138/196 (70%)	-0.33	1 (0%) 87 86	29, 49, 69, 110	0
1	I	138/196 (70%)	-0.20	1 (0%) 87 86	36, 51, 73, 100	0
1	J	138/196 (70%)	-0.25	2 (1%) 75 73	34, 53, 79, 118	0
1	K	138/196 (70%)	-0.13	3 (2%) 62 59	34, 57, 88, 97	0
1	L	138/196 (70%)	-0.07	7 (5%) 28 26	30, 56, 84, 122	0
All	All	1696/2352 (72%)	-0.30	22 (1%) 77 75	24, 44, 73, 122	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	113	PRO	6.4
1	G	113	PRO	5.6
1	E	250	ILE	5.2
1	C	250	ILE	3.5
1	G	250	ILE	3.5
1	F	17	PRO	3.3
1	L	115	ILE	3.2
1	J	113	PRO	3.1
1	L	114	LEU	2.9
1	B	113	PRO	2.8
1	I	115	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	250	ILE	2.7
1	C	113	PRO	2.6
1	L	247	TYR	2.5
1	K	129	ARG	2.3
1	H	113	PRO	2.3
1	L	129	ARG	2.2
1	L	122	LEU	2.2
1	J	114	LEU	2.1
1	K	124	GLY	2.0
1	A	17	PRO	2.0
1	K	250	ILE	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.

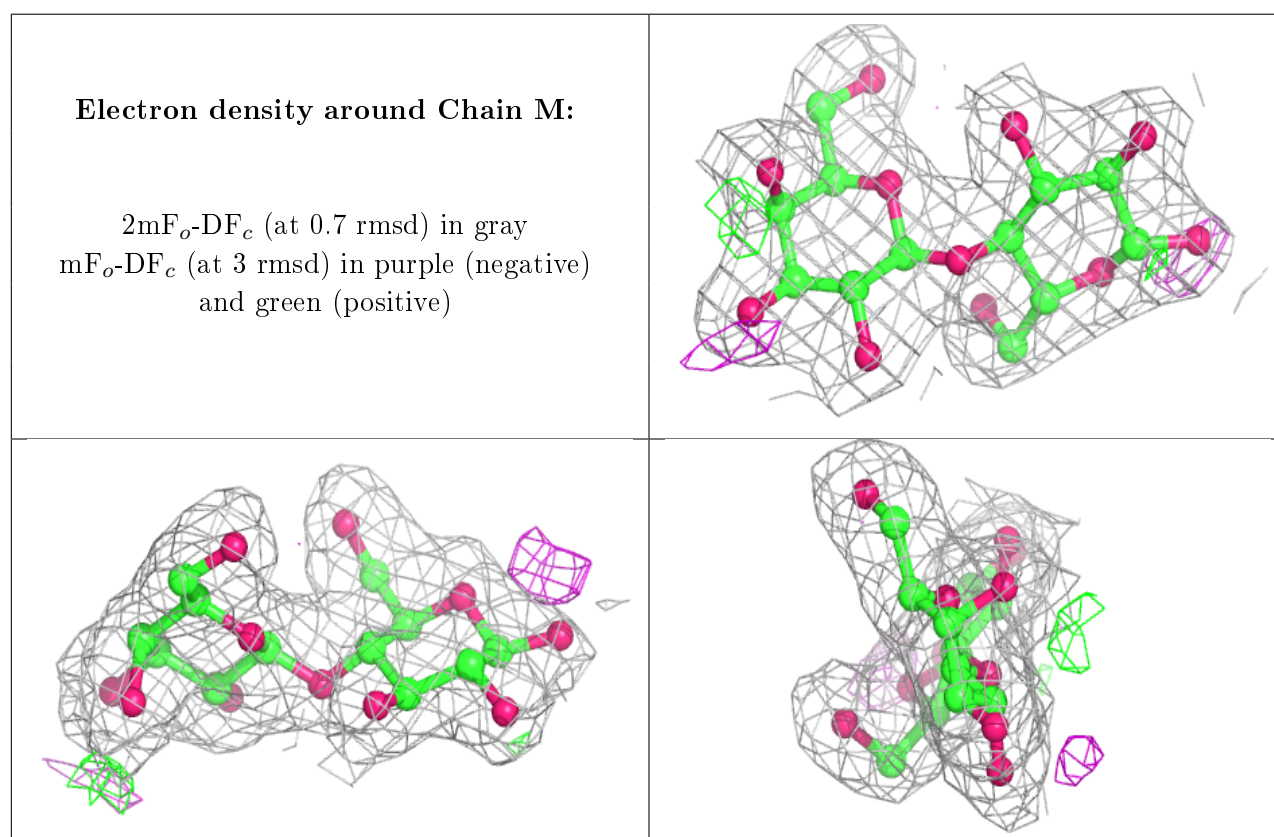
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BGC	O	1	12/12	0.95	0.13	27,31,36,52	0
2	BGC	M	1	12/12	0.96	0.10	29,31,34,47	0
2	BGC	R	1	12/12	0.96	0.11	24,28,35,36	0
2	GAL	W	2	11/12	0.96	0.11	32,34,36,39	0
2	BGC	X	1	12/12	0.96	0.12	31,37,41,47	0
2	BGC	T	1	12/12	0.97	0.10	25,29,31,37	0
2	BGC	N	1	12/12	0.97	0.10	26,29,37,37	0
2	GAL	T	2	11/12	0.97	0.10	25,26,29,30	0
2	BGC	V	1	12/12	0.97	0.11	33,36,44,44	0
2	BGC	S	1	12/12	0.97	0.11	28,31,36,51	0
2	BGC	W	1	12/12	0.97	0.11	30,34,49,55	0
2	BGC	P	1	12/12	0.97	0.10	28,33,36,49	0
2	GAL	X	2	11/12	0.97	0.12	29,31,34,36	0
2	BGC	U	1	12/12	0.97	0.10	29,34,42,45	0
2	GAL	V	2	11/12	0.98	0.10	30,33,35,39	0
2	GAL	P	2	11/12	0.98	0.09	24,28,29,29	0
2	GAL	N	2	11/12	0.98	0.11	26,27,29,31	0

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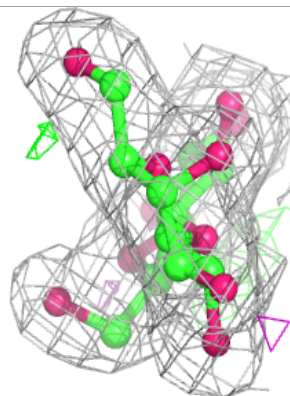
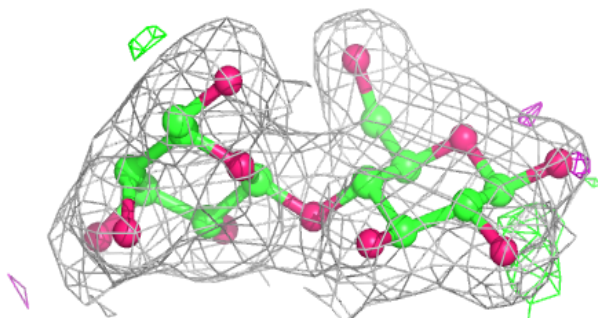
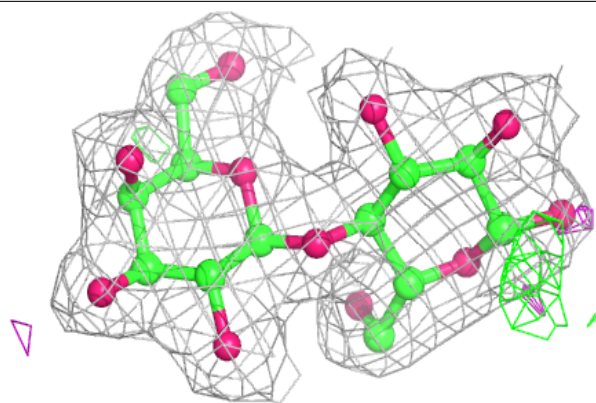
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GAL	M	2	11/12	0.98	0.09	25,26,30,30	0
2	BGC	Q	1	12/12	0.98	0.12	25,28,35,44	0
2	GAL	Q	2	11/12	0.98	0.10	21,22,24,26	0
2	GAL	S	2	11/12	0.98	0.10	19,24,25,27	0
2	GAL	U	2	11/12	0.98	0.10	27,30,31,33	0
2	GAL	O	2	11/12	0.98	0.11	24,24,25,26	0
2	GAL	R	2	11/12	0.99	0.10	21,24,25,29	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.

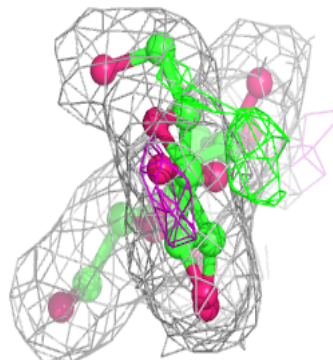
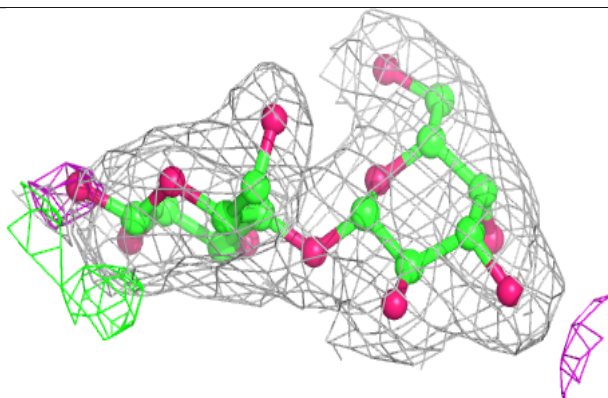
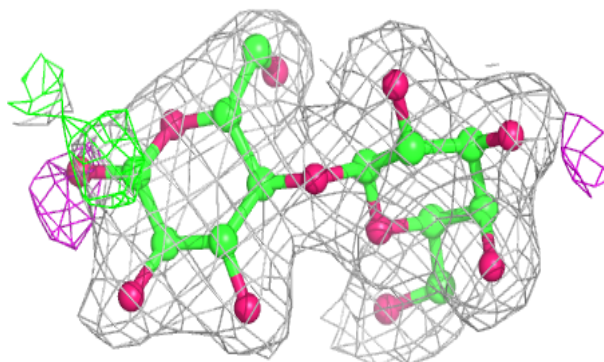


Electron density around Chain N:

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

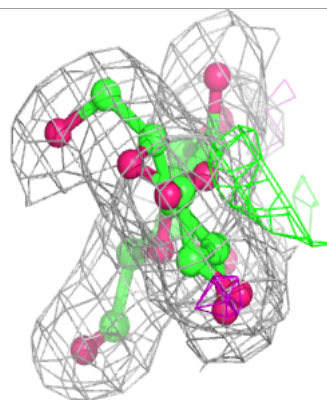
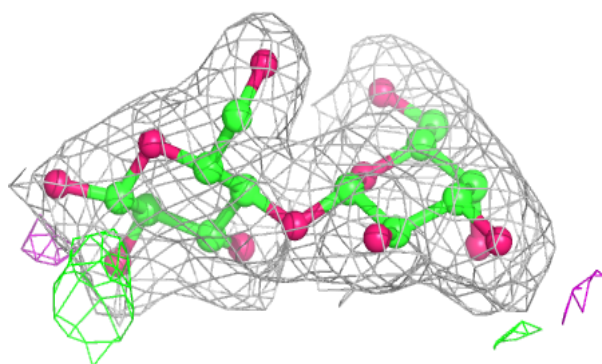
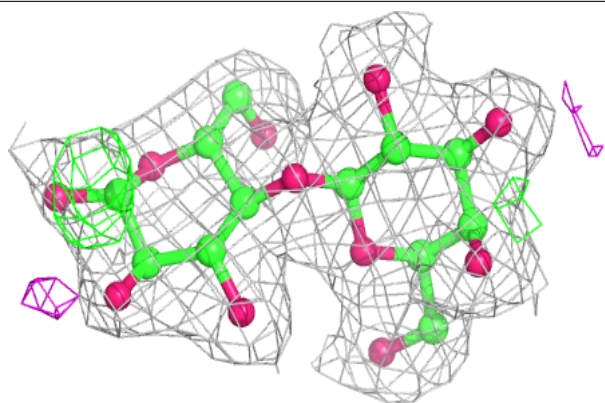
**Electron density around Chain O:**

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

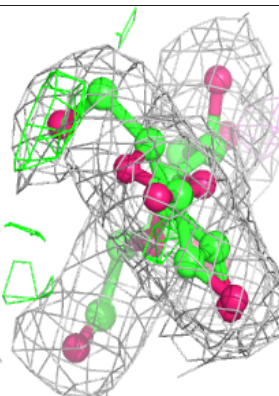
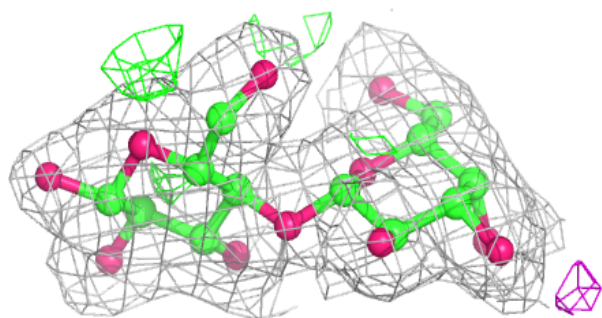
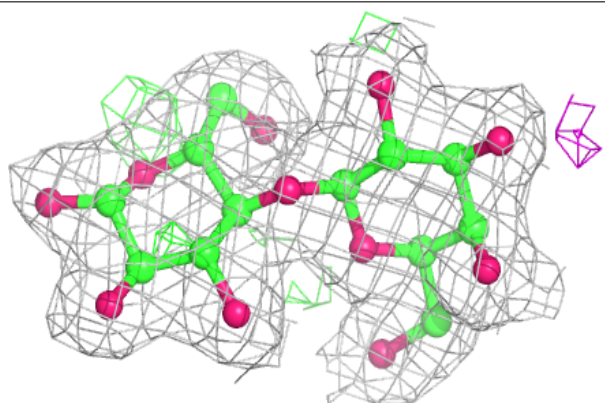


Electron density around Chain P:

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

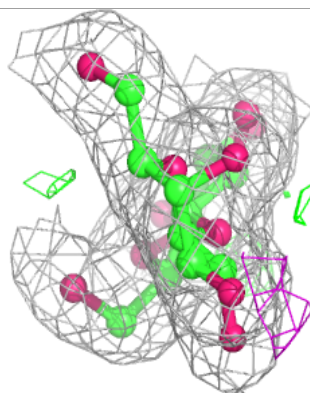
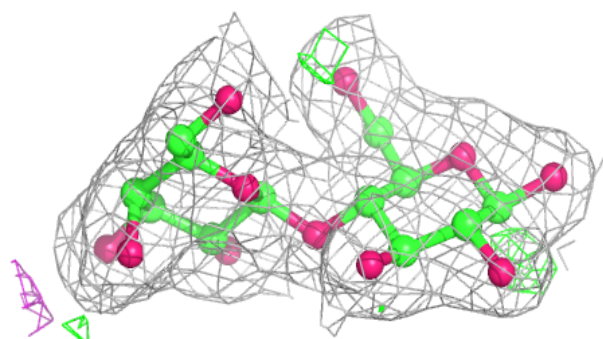
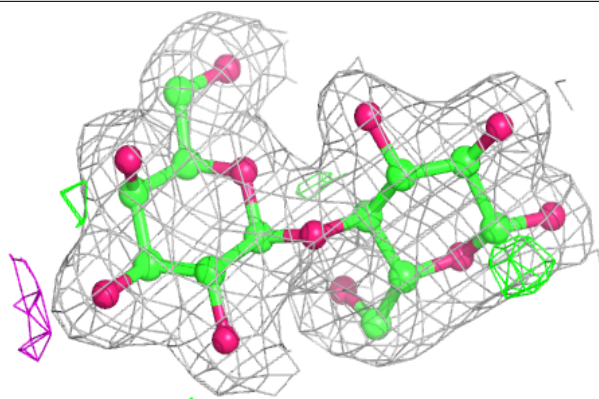
**Electron density around Chain Q:**

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

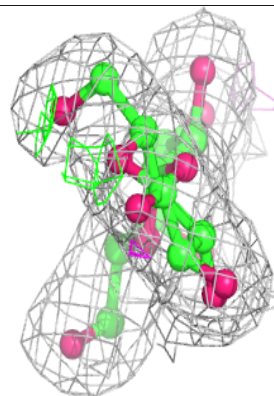
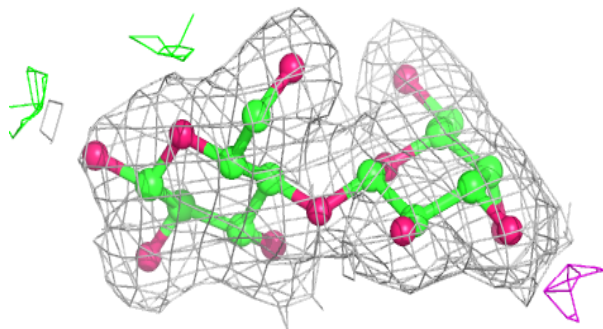
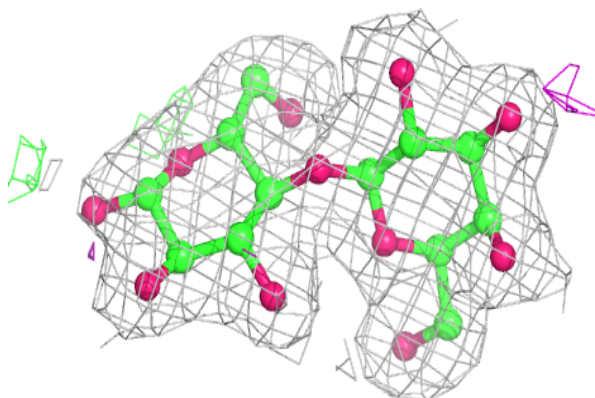


Electron density around Chain R:

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

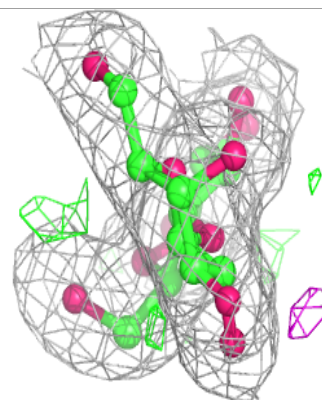
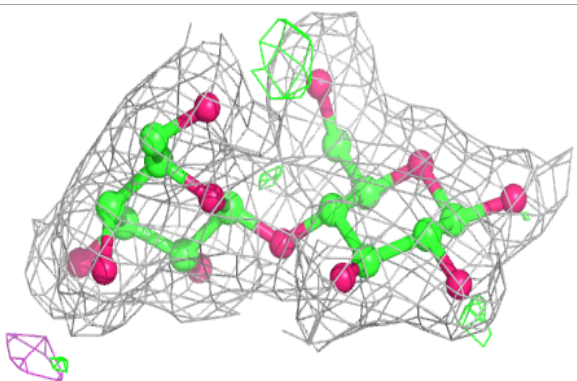
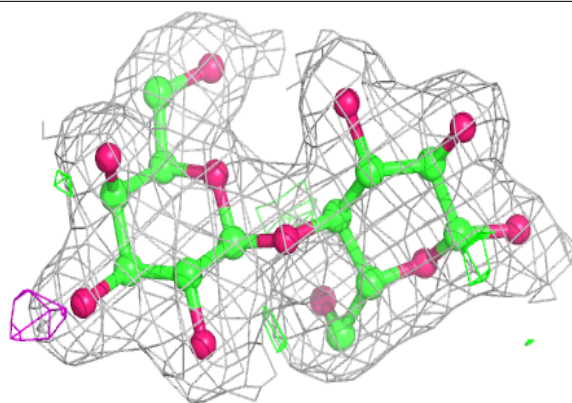
**Electron density around Chain S:**

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

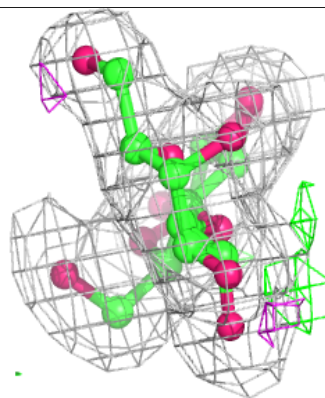
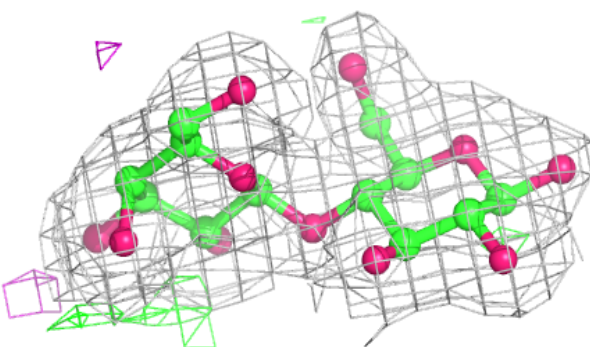
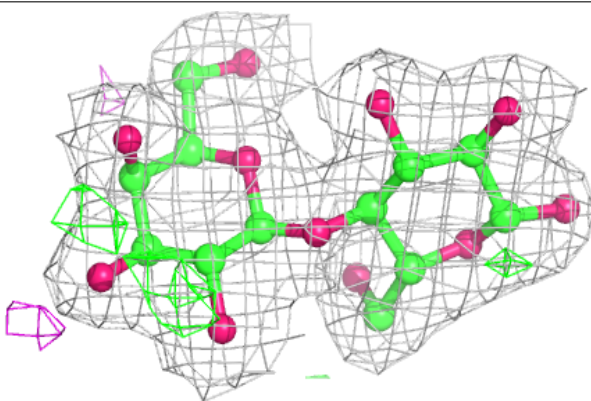


Electron density around Chain T:

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

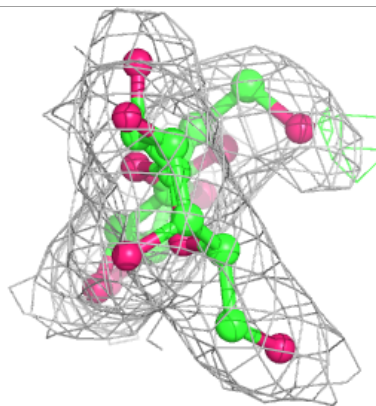
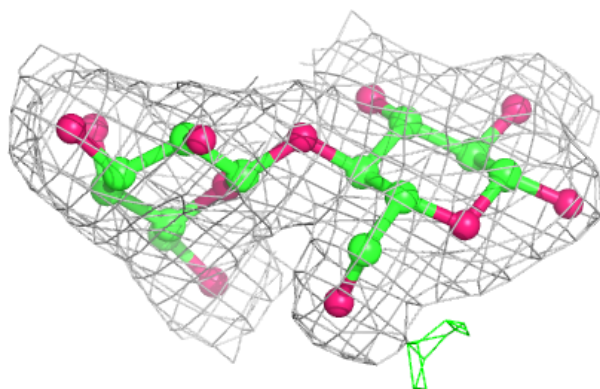
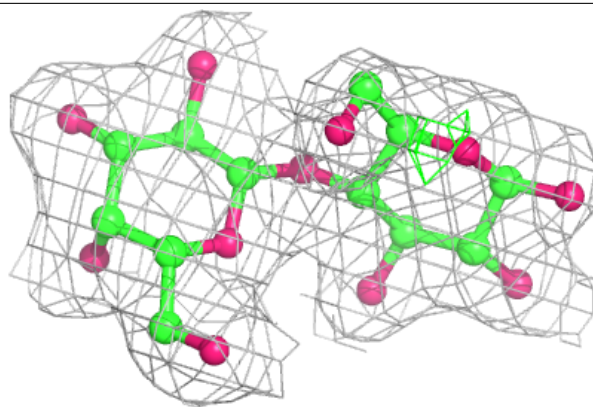
**Electron density around Chain U:**

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

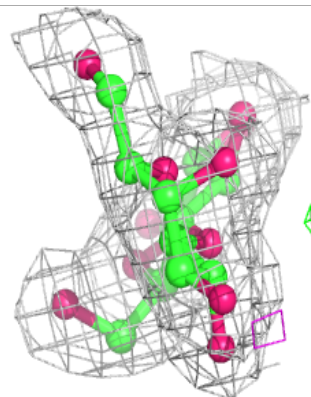
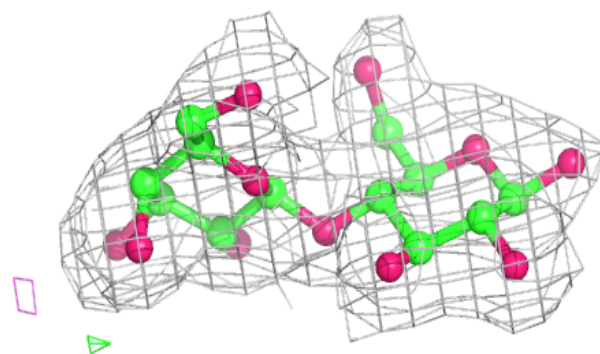
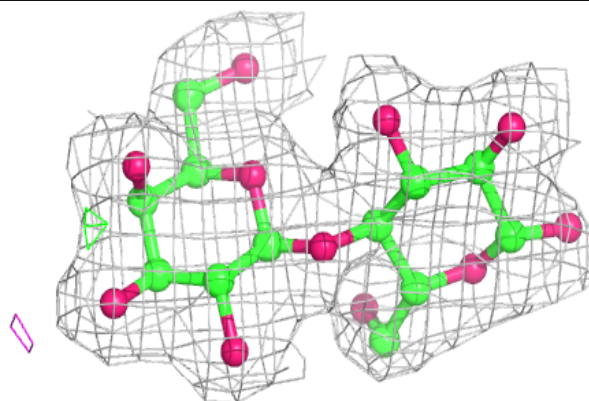


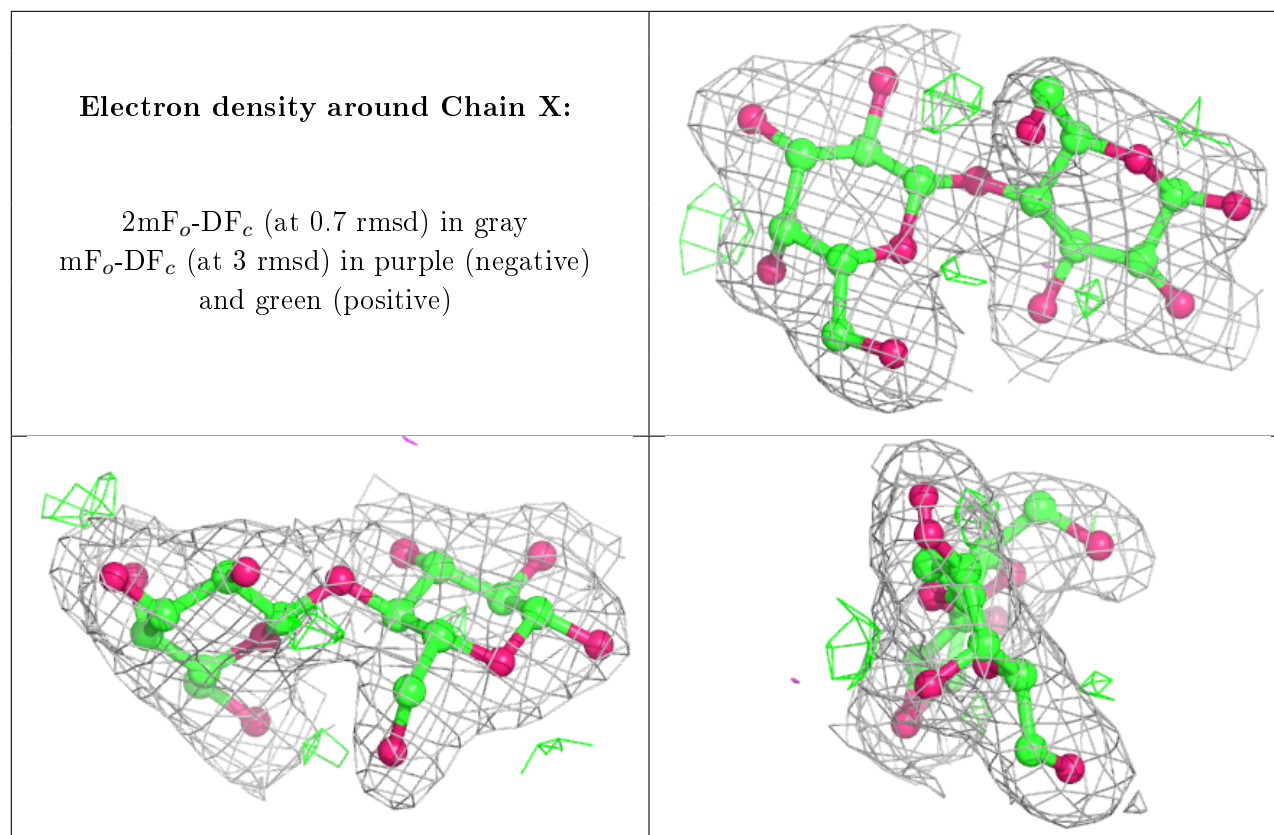
Electron density around Chain V:

$2mF_o-DF_c$ (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)





6.4 Ligands ⓘ

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
3	SO4	H	304	5/5	0.86	0.20	83,100,110,111	0
3	SO4	K	304	5/5	0.96	0.18	86,92,97,109	0
3	SO4	D	303	5/5	0.97	0.09	57,61,66,75	0
3	SO4	H	302	5/5	0.97	0.10	74,74,78,79	0
3	SO4	I	303	5/5	0.97	0.10	45,55,60,62	0
3	SO4	J	302	5/5	0.97	0.09	47,52,59,64	0
3	SO4	H	303	5/5	0.98	0.07	50,53,56,61	0
3	SO4	K	302	5/5	0.98	0.11	49,50,54,56	0
3	SO4	L	302	5/5	0.98	0.09	58,59,64,65	0
3	SO4	K	303	5/5	0.98	0.08	49,51,61,64	0
3	SO4	G	303	5/5	0.98	0.09	59,61,68,71	0
3	SO4	G	304	5/5	0.99	0.10	45,47,51,55	0
3	SO4	F	302	5/5	0.99	0.12	35,35,40,40	0
3	SO4	C	304	5/5	0.99	0.10	34,35,40,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	C	303	5/5	0.99	0.10	52,55,60,61	0
3	SO4	B	302	5/5	0.99	0.14	32,36,39,40	0
3	SO4	C	305	5/5	0.99	0.10	58,60,68,69	0
3	SO4	E	302	5/5	0.99	0.07	39,40,42,47	0
3	SO4	G	302	5/5	0.99	0.11	38,38,43,43	0
3	SO4	D	302	5/5	0.99	0.08	39,43,48,51	0
3	SO4	C	302	5/5	0.99	0.13	34,38,38,48	0
3	SO4	H	305	5/5	0.99	0.07	57,65,66,71	0
3	SO4	I	302	5/5	0.99	0.13	41,42,43,47	0
3	SO4	B	303	5/5	0.99	0.10	37,38,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.