



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:59 PM UTC

PDB ID : 6SKE / pdb_00006ske
Title : Teneurin 2 in complex with Latrophilin 2 Lec domain
Authors : Shahin, M.; Jackson, V.A.; Carrasquero, M.; Lowe, E.; Seiradake, E.
Deposited on : 2019-08-15
Resolution : 3.62 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

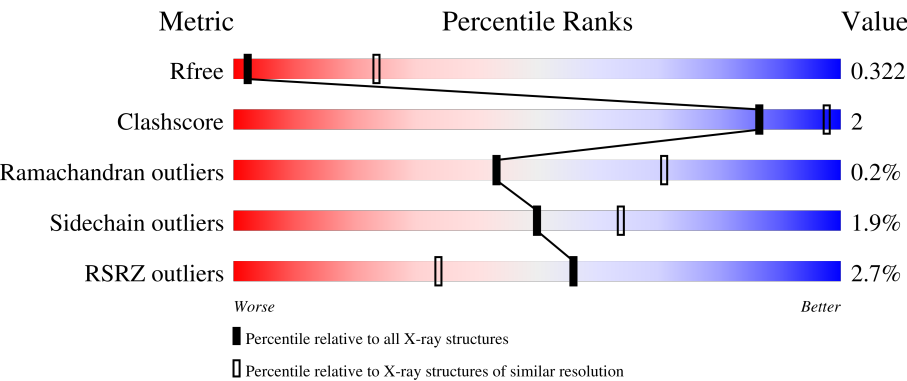
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.62 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.



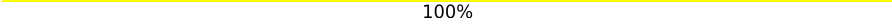
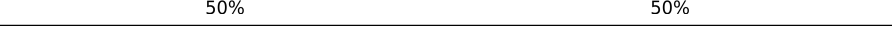
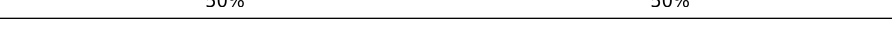
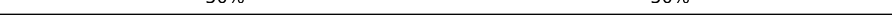
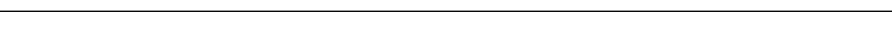
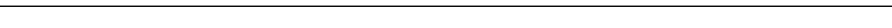
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1062 (3.72-3.52)
Clashscore	190562	1092 (3.72-3.52)
Ramachandran outliers	187476	1057 (3.72-3.52)
Sidechain outliers	187428	1055 (3.72-3.52)
RSRZ outliers	180081	1060 (3.72-3.52)

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	1756	3% 90% 9%
1	C	1756	3% 91% 9%
2	B	108	2% 87% 11%
2	D	108	2% 85% 11%
3	E	8	12% 88%

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Mol	Chain	Length	Quality of chain
3	K	8	 12%88%
4	F	2	 50%50%
4	G	2	 50%50%
4	H	2	 100%
4	I	2	 50%50%
4	J	2	 50%50%
4	L	2	 50%50%
4	M	2	 50%50%
4	N	2	 100%
4	O	2	 100%
4	P	2	 50%50%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 30006 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.

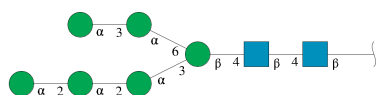
- Molecule 1 is a protein called Teneurin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1752	Total	C	N	O	S	0	1	0
			13851	8739	2400	2653	59			
1	C	1752	Total	C	N	O	S	0	1	0
			13851	8739	2400	2653	59			

- Molecule 2 is a protein called Adhesion G protein-coupled receptor L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	96	Total	C	N	O	S	0	0	0
			757	468	125	153	11			
2	D	96	Total	C	N	O	S	0	0	0
			757	468	125	153	11			

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



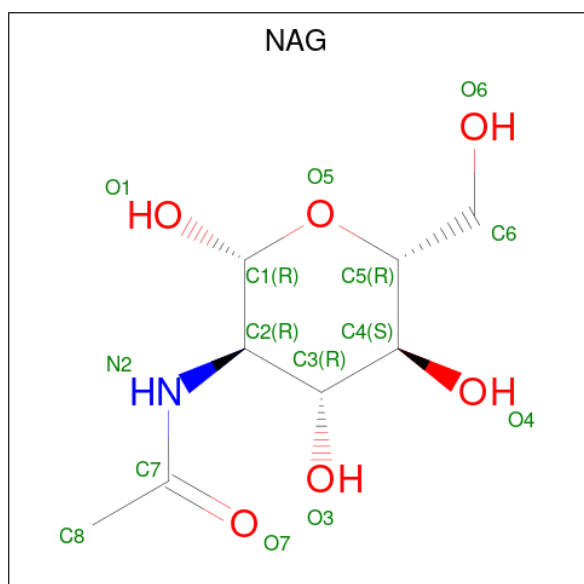
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	8	Total	C	N	O	0	0	0
			94	52	2	40			
3	K	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 4 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
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	105	Total	O	0	0
			105	105		
6	C	105	Total	O	0	0
			105	105		

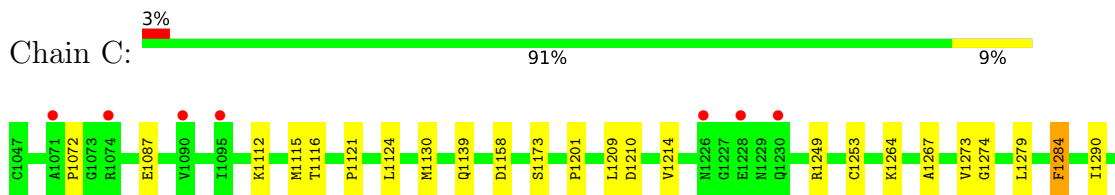
3 Residue-property plots

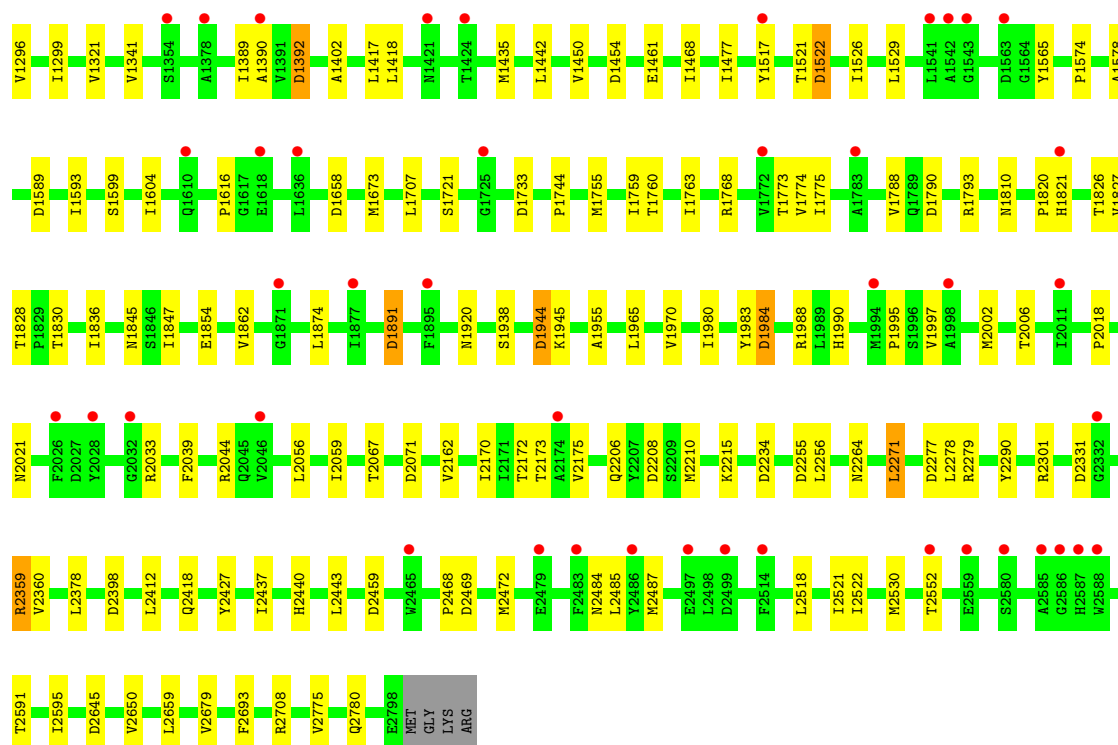
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Teneurin-2

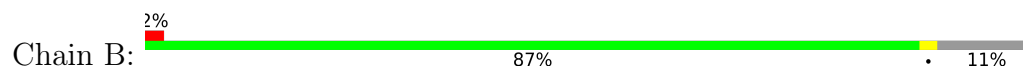


• Molecule 1: Teneurin-2

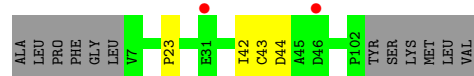
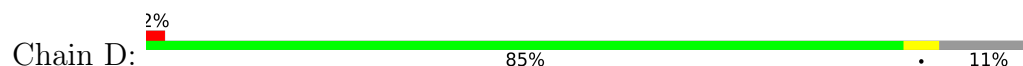




• Molecule 2: Adhesion G protein-coupled receptor L2



• Molecule 2: Adhesion G protein-coupled receptor L2



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



• Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1

-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  12% 88%



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

Chain F:  50% 50%



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

Chain G:  50% 50%



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

Chain H:  100%



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

Chain I:  50% 50%



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

Chain J:  50% 50%



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

Chain L:  50% 50%



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

Chain M:  50%  50%



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

Chain N:  100%



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

Chain O:  100%



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

Chain P:  50%  50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.87Å 109.92Å 152.21Å 90.19° 93.99° 111.93°	Depositor
Resolution (Å)	84.00 – 3.62 84.00 – 3.62	Depositor EDS
% Data completeness (in resolution range)	96.0 (84.00-3.62) 96.0 (84.00-3.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.58Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.270 , 0.269 0.319 , 0.322	Depositor DCC
R_{free} test set	2997 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	92.6	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 95.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	30006	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.01% 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, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.71	0/14147	1.15	32/19182 (0.2%)
1	C	0.71	0/14147	1.14	31/19182 (0.2%)
2	B	0.67	0/772	1.07	0/1048
2	D	0.66	0/772	1.07	0/1048
All	All	0.71	0/29838	1.14	63/40460 (0.2%)

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1984	ASP	CA-CB-CG	7.04	119.64	112.60
1	C	1984	ASP	CA-CB-CG	7.02	119.62	112.60
1	C	1658	ASP	CA-CB-CG	6.75	119.35	112.60
1	A	1658	ASP	CA-CB-CG	6.71	119.31	112.60
1	A	2331	ASP	CA-CB-CG	6.41	119.01	112.60
1	C	2331	ASP	CA-CB-CG	6.39	118.99	112.60
1	A	2234	ASP	CA-CB-CG	5.96	118.56	112.60
1	C	2234	ASP	CA-CB-CG	5.96	118.56	112.60
1	C	2645	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	2208	ASP	CA-CB-CG	5.86	118.46	112.60
1	C	2255	ASP	CA-CB-CG	5.86	118.45	112.60
1	A	2255	ASP	CA-CB-CG	5.85	118.45	112.60
1	C	2208	ASP	CA-CB-CG	5.85	118.45	112.60
1	A	1522	ASP	N-CA-C	-5.82	106.35	113.50
1	A	2645	ASP	CA-CB-CG	5.82	118.42	112.60
1	C	1920	ASN	CA-CB-CG	5.79	118.39	112.60
1	C	1522	ASP	N-CA-C	-5.77	106.40	113.50
1	A	2775	VAL	N-CA-C	-5.74	105.52	110.74
1	A	1920	ASN	CA-CB-CG	5.72	118.33	112.60
1	C	2775	VAL	N-CA-C	-5.69	105.56	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2459	ASP	CA-CB-CG	5.65	118.25	112.60
1	C	1589	ASP	CA-C-N	5.64	128.16	120.54
1	C	1589	ASP	C-N-CA	5.64	128.16	120.54
1	C	2459	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	1589	ASP	CA-C-N	5.61	128.12	120.54
1	A	1589	ASP	C-N-CA	5.61	128.12	120.54
1	C	1158	ASP	CA-CB-CG	5.52	118.12	112.60
1	A	1210	ASP	CA-CB-CG	5.49	118.09	112.60
1	C	2595	ILE	N-CA-C	-5.49	105.50	110.82
1	A	2595	ILE	N-CA-C	-5.49	105.50	110.82
1	C	1210	ASP	CA-CB-CG	5.46	118.06	112.60
1	C	1209	LEU	CA-C-N	5.44	128.98	120.82
1	C	1209	LEU	C-N-CA	5.44	128.98	120.82
1	A	1209	LEU	CA-C-N	5.41	128.94	120.82
1	A	1209	LEU	C-N-CA	5.41	128.94	120.82
1	A	2021	ASN	CA-CB-CG	5.39	117.99	112.60
1	C	1945	LYS	N-CA-C	-5.34	106.27	112.89
1	C	2021	ASN	CA-CB-CG	5.33	117.93	112.60
1	A	1945	LYS	N-CA-C	-5.33	106.28	112.89
1	A	2398	ASP	CA-CB-CG	5.30	117.90	112.60
1	C	2398	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	1392	ASP	CA-C-N	5.27	127.34	120.28
1	A	1392	ASP	C-N-CA	5.27	127.34	120.28
1	C	1392	ASP	CA-C-N	5.23	127.29	120.28
1	C	1392	ASP	C-N-CA	5.23	127.29	120.28
1	C	1565	TYR	CA-C-N	5.18	127.22	120.28
1	C	1565	TYR	C-N-CA	5.18	127.22	120.28
1	A	1565	TYR	CA-C-N	5.18	127.22	120.28
1	A	1565	TYR	C-N-CA	5.18	127.22	120.28
1	A	1944	ASP	CA-CB-CG	5.17	117.78	112.60
1	C	1944	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	1322	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	1810	ASN	CA-CB-CG	5.08	117.68	112.60
1	A	1158	ASP	CA-CB-CG	5.07	117.67	112.60
1	C	2277	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	2277	ASP	CA-CB-CG	5.04	117.64	112.60
1	C	1810	ASN	CA-CB-CG	5.03	117.63	112.60
1	C	1733	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	1733	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	1983	TYR	CA-C-N	5.02	131.31	121.66
1	A	1983	TYR	C-N-CA	5.02	131.31	121.66
1	C	1983	TYR	CA-C-N	5.00	131.27	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1983	TYR	C-N-CA	5.00	131.27	121.66

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	13851	0	13600	64	0
1	C	13851	0	13600	62	0
2	B	757	0	707	3	0
2	D	757	0	707	4	0
3	E	94	0	79	0	0
3	K	94	0	79	0	0
4	F	28	0	25	0	0
4	G	28	0	25	0	0
4	H	28	0	25	0	0
4	I	28	0	25	0	0
4	J	28	0	25	0	0
4	L	28	0	25	0	0
4	M	28	0	25	0	0
4	N	28	0	25	0	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
5	A	56	0	52	0	0
5	C	56	0	52	0	0
6	A	105	0	0	0	0
6	C	105	0	0	0	0
All	All	30006	0	29126	123	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 2.

All (123) 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:B:23:PRO:HB3	1:C:2172:THR:HG21	1.61	0.82
1:C:1821:HIS:HD2	1:C:1830:THR:HG21	1.47	0.79
1:A:1821:HIS:HD2	1:A:1830:THR:HG21	1.47	0.78
1:A:2172:THR:HG21	2:D:23:PRO:HB3	1.73	0.69
1:C:2468:PRO:HB3	1:C:2485:LEU:HB3	1.75	0.69
1:A:2468:PRO:HB3	1:A:2485:LEU:HB3	1.75	0.68
1:A:1130:MET:HB2	1:A:1173:SER:HB2	1.78	0.65
1:A:1821:HIS:CD2	1:A:1830:THR:HG21	2.31	0.65
1:C:1821:HIS:CD2	1:C:1830:THR:HG21	2.31	0.65
1:C:1130:MET:HB2	1:C:1173:SER:HB2	1.79	0.65
1:A:1424:THR:HG21	1:C:2067:THR:HG22	1.79	0.64
1:C:1201:PRO:HB3	1:C:1214:VAL:HB	1.80	0.64
1:A:1201:PRO:HB3	1:A:1214:VAL:HB	1.80	0.62
1:A:2264:ASN:HD21	1:A:2271:LEU:HD22	1.65	0.62
1:C:2264:ASN:HD21	1:C:2271:LEU:HD22	1.65	0.62
1:A:1521:THR:HB	1:A:1574:PRO:HD2	1.84	0.60
1:C:1521:THR:HB	1:C:1574:PRO:HD2	1.84	0.59
1:A:1891:ASP:OD2	2:D:43:CYS:HA	2.03	0.58
1:C:2173:THR:HG22	1:C:2175:VAL:H	1.69	0.58
1:A:2173:THR:HG22	1:A:2175:VAL:H	1.69	0.57
1:A:1873:ASN:ND2	2:D:44:ASP:HB3	2.20	0.56
1:A:2290:TYR:CZ	1:A:2301:ARG:HG3	2.42	0.55
1:A:1773:THR:HG23	1:A:1788:VAL:HB	1.88	0.55
1:C:2418:GLN:HB2	1:C:2427:TYR:HB3	1.89	0.55
1:C:1955:ALA:HB3	1:C:2210:MET:HE3	1.89	0.55
1:C:2290:TYR:CZ	1:C:2301:ARG:HG3	2.41	0.55
1:C:1274:GLY:HA2	1:C:1321:VAL:HG11	1.89	0.54
1:A:1367:PHE:HB2	1:C:2071:ASP:HA	1.89	0.54
1:A:2418:GLN:HB2	1:A:2427:TYR:HB3	1.89	0.54
1:C:1854:GLU:HB2	1:C:1862:VAL:HB	1.91	0.53
1:A:1955:ALA:HB3	1:A:2210:MET:HE3	1.89	0.53
1:A:1854:GLU:HB2	1:A:1862:VAL:HB	1.90	0.53
1:A:1390:ALA:HB1	1:A:1450:VAL:HG23	1.89	0.53
1:A:1970:VAL:HG22	1:A:1980:ILE:HG12	1.91	0.52
1:C:1773:THR:HG23	1:C:1788:VAL:HB	1.90	0.52
1:C:1390:ALA:HB1	1:C:1450:VAL:HG23	1.91	0.52
2:B:43:CYS:HA	1:C:1891:ASP:OD2	2.10	0.52
1:C:2359:ARG:HH12	1:C:2530:MET:HE3	1.74	0.52
1:A:1274:GLY:HA2	1:A:1321:VAL:HG11	1.92	0.52
1:C:1970:VAL:HG22	1:C:1980:ILE:HG12	1.91	0.51
1:A:2359:ARG:HH12	1:A:2530:MET:HE3	1.74	0.51
1:C:1299:ILE:HD12	1:C:1341:VAL:HG11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2469:ASP:HB3	1:C:2472:MET:HE3	1.94	0.50
1:C:1827:VAL:HG13	1:C:1828:THR:HG23	1.94	0.50
1:A:1299:ILE:HD12	1:A:1341:VAL:HG11	1.94	0.50
1:A:2071:ASP:HB2	1:A:2078:LYS:HG3	1.94	0.50
1:A:2469:ASP:HB3	1:A:2472:MET:HE3	1.94	0.50
1:C:1130:MET:HG2	1:C:1139:GLN:HG2	1.93	0.50
1:A:1130:MET:HG2	1:A:1139:GLN:HG2	1.93	0.50
1:A:1827:VAL:HG13	1:A:1828:THR:HG23	1.94	0.49
1:A:2039:PHE:HB2	1:A:2044:ARG:HB2	1.95	0.49
1:C:1744:PRO:HB2	1:C:2006:THR:HG21	1.94	0.49
1:A:1744:PRO:HB2	1:A:2006:THR:HG21	1.94	0.49
1:A:1820:PRO:HB3	1:A:1826:THR:HA	1.94	0.49
1:A:1442:LEU:HG	1:A:1461:GLU:HG3	1.95	0.49
1:C:2039:PHE:HB2	1:C:2044:ARG:HB2	1.94	0.48
1:C:1273:VAL:HG23	1:C:1578:ALA:HB1	1.95	0.48
1:C:1442:LEU:HG	1:C:1461:GLU:HG3	1.95	0.48
1:C:1820:PRO:HB3	1:C:1826:THR:HA	1.95	0.48
1:C:2659:LEU:HD21	1:C:2679:VAL:HG11	1.96	0.48
1:A:1273:VAL:HG23	1:A:1578:ALA:HB1	1.95	0.47
1:A:1788:VAL:HG22	1:A:1793:ARG:HG2	1.97	0.47
1:C:1995:PRO:HB2	1:C:2256:LEU:HB3	1.96	0.47
1:A:1995:PRO:HB2	1:A:2256:LEU:HB3	1.96	0.47
1:A:1290:ILE:HG12	1:A:1296:VAL:HG22	1.96	0.46
1:A:2056:LEU:HD21	1:A:2059:ILE:HD11	1.98	0.46
1:A:1517:TYR:HB3	1:A:1529:LEU:HD11	1.97	0.46
1:C:2056:LEU:HD21	1:C:2059:ILE:HD11	1.97	0.46
1:C:1290:ILE:HG12	1:C:1296:VAL:HG22	1.96	0.46
1:C:1517:TYR:HB3	1:C:1529:LEU:HD11	1.96	0.46
1:A:2659:LEU:HD21	1:A:2679:VAL:HG11	1.96	0.46
1:C:1755:MET:HG3	1:C:1759:ILE:HG12	1.98	0.46
1:C:1788:VAL:HG22	1:C:1793:ARG:HG2	1.98	0.46
1:A:1522:ASP:HB2	1:A:1526:ILE:HB	1.98	0.45
1:A:1755:MET:HG3	1:A:1759:ILE:HG12	1.98	0.45
1:A:2206:GLN:HB2	1:A:2215:LYS:HB3	1.99	0.45
1:C:2518:LEU:HB3	1:C:2522:ILE:HD12	1.99	0.45
1:C:2206:GLN:HB2	1:C:2215:LYS:HB3	1.99	0.44
1:C:1249:ARG:HB3	1:C:1264:LYS:HB3	1.99	0.44
1:C:1522:ASP:HB2	1:C:1526:ILE:HB	1.98	0.44
1:C:1121:PRO:HG2	1:C:1124:LEU:HB2	2.00	0.44
1:A:2518:LEU:HB3	1:A:2522:ILE:HD12	1.99	0.44
1:A:1121:PRO:HG2	1:A:1124:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1417:LEU:HD21	1:C:1468:ILE:HG21	2.00	0.43
2:B:23:PRO:HB3	1:C:2172:THR:CG2	2.41	0.43
1:C:1267:ALA:HB3	1:C:1284:PHE:HB2	2.00	0.43
1:A:1427:ARG:HB2	1:C:2780:GLN:OE1	2.19	0.43
1:C:1279:LEU:HD23	1:C:1290:ILE:HD12	2.01	0.43
1:C:2650:VAL:HG12	1:C:2708:ARG:HB3	2.01	0.43
1:A:1836:ILE:HB	1:A:1845:ASN:HB2	2.01	0.43
1:A:1938:SER:H	1:A:2210:MET:HE1	1.84	0.43
1:A:1267:ALA:HB3	1:A:1284:PHE:HB2	2.00	0.42
1:A:1249:ARG:HB3	1:A:1264:LYS:HB3	2.00	0.42
1:A:1279:LEU:HD23	1:A:1290:ILE:HD12	2.01	0.42
1:C:2484:ASN:HB3	1:C:2487:MET:HG2	2.01	0.42
1:A:1072:PRO:HB2	1:A:1087:GLU:HG2	2.02	0.42
1:A:1417:LEU:HD21	1:A:1468:ILE:HG21	2.01	0.42
1:A:2650:VAL:HG12	1:A:2708:ARG:HB3	2.01	0.42
1:C:1874:LEU:HD13	1:C:2521:ILE:HD12	2.01	0.42
1:C:1707:LEU:HB3	1:C:1721:SER:HB2	2.02	0.42
1:C:1836:ILE:HB	1:C:1845:ASN:HB2	2.01	0.42
1:C:2018:PRO:HD2	1:C:2279:ARG:HG2	2.02	0.42
1:A:2360:VAL:HG21	1:A:2443:LEU:HD21	2.01	0.42
1:A:2693:PHE:CD2	1:A:2708:ARG:HG3	2.55	0.42
1:A:1874:LEU:HD13	1:A:2521:ILE:HD12	2.01	0.42
1:C:1938:SER:H	1:C:2210:MET:HE1	1.84	0.42
1:C:1072:PRO:HB2	1:C:1087:GLU:HG2	2.02	0.42
1:A:1707:LEU:HB3	1:A:1721:SER:HB2	2.02	0.41
1:A:2484:ASN:HB3	1:A:2487:MET:HG2	2.01	0.41
1:C:1768:ARG:HH22	1:C:2033:ARG:HD2	1.85	0.41
1:C:1616:PRO:HG2	1:C:1830:THR:HG22	2.02	0.41
1:C:2162:VAL:HG11	1:C:2378:LEU:HD11	2.03	0.41
1:C:2693:PHE:CD2	1:C:2708:ARG:HG3	2.55	0.41
1:A:1616:PRO:HG2	1:A:1830:THR:HG22	2.02	0.41
1:A:1893:ARG:HG3	2:D:42:ILE:HD11	2.03	0.41
1:A:2018:PRO:HD2	1:A:2279:ARG:HG2	2.02	0.41
1:C:1760:THR:HG22	1:C:1775:ILE:HG23	2.03	0.41
1:C:2360:VAL:HG21	1:C:2443:LEU:HD21	2.02	0.41
1:A:2436:VAL:HG12	1:A:2437:ILE:HD12	2.03	0.40
1:A:1768:ARG:HH22	1:A:2033:ARG:HD2	1.85	0.40
1:A:1944:ASP:HB3	1:A:1946:GLN:H	1.87	0.40
1:A:2162:VAL:HG11	1:A:2378:LEU:HD11	2.03	0.40
1:C:1984:ASP:HB2	1:C:1988:ARG:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1751/1756 (100%)	1688 (96%)	58 (3%)	5 (0%)	36	64
1	C	1751/1756 (100%)	1689 (96%)	58 (3%)	4 (0%)	43	71
2	B	94/108 (87%)	92 (98%)	2 (2%)	0	100	100
2	D	94/108 (87%)	92 (98%)	2 (2%)	0	100	100
All	All	3690/3728 (99%)	3561 (96%)	120 (3%)	9 (0%)	43	71

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1284	PHE
1	A	1997	VAL
1	C	1284	PHE
1	C	1997	VAL
1	A	1402	ALA
1	A	1790	ASP
1	C	1402	ALA
1	C	1790	ASP
1	A	1326	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1527/1529 (100%)	1495 (98%)	32 (2%)	47	62
1	C	1527/1529 (100%)	1495 (98%)	32 (2%)	47	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	88/98 (90%)	88 (100%)	0	100	100
2	D	88/98 (90%)	88 (100%)	0	100	100
All	All	3230/3254 (99%)	3166 (98%)	64 (2%)	50	63

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1112	LYS
1	A	1115	MET
1	A	1116	THR
1	A	1253	CYS
1	A	1389	ILE
1	A	1392	ASP
1	A	1418	LEU
1	A	1435	MET
1	A	1454	ASP
1	A	1477	ILE
1	A	1593	ILE
1	A	1599	SER
1	A	1604	ILE
1	A	1673	MET
1	A	1763	ILE
1	A	1774	VAL
1	A	1847	ILE
1	A	1891	ASP
1	A	1944	ASP
1	A	1965	LEU
1	A	1990[A]	HIS
1	A	1990[B]	HIS
1	A	2002	MET
1	A	2170	ILE
1	A	2271	LEU
1	A	2278	LEU
1	A	2359	ARG
1	A	2412	LEU
1	A	2437	ILE
1	A	2440	HIS
1	A	2552	THR
1	A	2591	THR
1	C	1112	LYS
1	C	1115	MET

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Mol	Chain	Res	Type
1	C	1116	THR
1	C	1253	CYS
1	C	1389	ILE
1	C	1392	ASP
1	C	1418	LEU
1	C	1435	MET
1	C	1454	ASP
1	C	1477	ILE
1	C	1593	ILE
1	C	1599	SER
1	C	1604	ILE
1	C	1673	MET
1	C	1763	ILE
1	C	1774	VAL
1	C	1847	ILE
1	C	1891	ASP
1	C	1944	ASP
1	C	1965	LEU
1	C	1990[A]	HIS
1	C	1990[B]	HIS
1	C	2002	MET
1	C	2170	ILE
1	C	2271	LEU
1	C	2278	LEU
1	C	2359	ARG
1	C	2412	LEU
1	C	2437	ILE
1	C	2440	HIS
1	C	2552	THR
1	C	2591	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1203	ASN
1	A	1285	ASN
1	A	1311	ASN
1	A	1353	ASN
1	A	1439	GLN
1	A	1473	GLN
1	A	1483	HIS
1	A	1631	GLN

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Mol	Chain	Res	Type
1	A	1683	GLN
1	A	1701	GLN
1	A	1797	GLN
1	A	1892	HIS
1	A	2124	ASN
1	A	2156	HIS
1	A	2206	GLN
1	A	2238	GLN
1	A	2418	GLN
1	A	2491	ASN
1	A	2502	ASN
1	A	2549	GLN
1	A	2587	HIS
1	A	2681	GLN
1	A	2741	GLN
1	A	2763	ASN
2	B	73	GLN
1	C	1285	ASN
1	C	1311	ASN
1	C	1473	GLN
1	C	1483	HIS
1	C	1631	GLN
1	C	1683	GLN
1	C	1701	GLN
1	C	1892	HIS
1	C	2156	HIS
1	C	2206	GLN
1	C	2238	GLN
1	C	2418	GLN
1	C	2491	ASN
1	C	2502	ASN
1	C	2549	GLN
1	C	2587	HIS
1	C	2681	GLN
1	C	2741	GLN
1	C	2763	ASN
2	D	73	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 ⓘ

36 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	E	1	1,3	14,14,15	0.40	0	17,19,21	0.81	1 (5%)
3	NAG	E	2	3	14,14,15	0.41	0	17,19,21	1.24	3 (17%)
3	BMA	E	3	3	11,11,12	0.64	0	15,15,17	0.67	0
3	MAN	E	4	3	11,11,12	0.75	0	15,15,17	0.99	1 (6%)
3	MAN	E	5	3	11,11,12	0.68	0	15,15,17	0.78	1 (6%)
3	MAN	E	6	3	11,11,12	0.65	0	15,15,17	0.73	1 (6%)
3	MAN	E	7	3	11,11,12	0.76	0	15,15,17	1.32	1 (6%)
3	MAN	E	8	3	11,11,12	0.59	0	15,15,17	0.91	1 (6%)
4	NAG	F	1	1,4	14,14,15	0.45	0	17,19,21	0.80	0
4	NAG	F	2	4	14,14,15	0.43	0	17,19,21	0.84	1 (5%)
4	NAG	G	1	1,4	14,14,15	0.47	0	17,19,21	0.56	0
4	NAG	G	2	4	14,14,15	0.42	0	17,19,21	0.94	1 (5%)
4	NAG	H	1	1,4	14,14,15	0.43	0	17,19,21	0.86	1 (5%)
4	NAG	H	2	4	14,14,15	0.42	0	17,19,21	0.95	1 (5%)
4	NAG	I	1	1,4	14,14,15	0.46	0	17,19,21	0.80	0
4	NAG	I	2	4	14,14,15	0.44	0	17,19,21	0.71	1 (5%)
4	NAG	J	1	1,4	14,14,15	0.46	0	17,19,21	0.83	0
4	NAG	J	2	4	14,14,15	0.41	0	17,19,21	1.11	1 (5%)
3	NAG	K	1	1,3	14,14,15	0.40	0	17,19,21	0.82	1 (5%)
3	NAG	K	2	3	14,14,15	0.40	0	17,19,21	1.24	3 (17%)
3	BMA	K	3	3	11,11,12	0.64	0	15,15,17	0.67	0
3	MAN	K	4	3	11,11,12	0.75	0	15,15,17	0.99	1 (6%)
3	MAN	K	5	3	11,11,12	0.66	0	15,15,17	0.79	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	K	6	3	11,11,12	0.66	0	15,15,17	0.73	1 (6%)
3	MAN	K	7	3	11,11,12	0.75	0	15,15,17	1.32	1 (6%)
3	MAN	K	8	3	11,11,12	0.58	0	15,15,17	0.91	1 (6%)
4	NAG	L	1	1,4	14,14,15	0.45	0	17,19,21	0.80	0
4	NAG	L	2	4	14,14,15	0.42	0	17,19,21	0.84	1 (5%)
4	NAG	M	1	1,4	14,14,15	0.46	0	17,19,21	0.57	0
4	NAG	M	2	4	14,14,15	0.40	0	17,19,21	0.93	1 (5%)
4	NAG	N	1	1,4	14,14,15	0.44	0	17,19,21	0.87	1 (5%)
4	NAG	N	2	4	14,14,15	0.43	0	17,19,21	0.95	1 (5%)
4	NAG	O	1	1,4	14,14,15	0.47	0	17,19,21	0.80	0
4	NAG	O	2	4	14,14,15	0.45	0	17,19,21	0.70	0
4	NAG	P	1	1,4	14,14,15	0.45	0	17,19,21	0.84	0
4	NAG	P	2	4	14,14,15	0.40	0	17,19,21	1.11	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	2/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	MAN	E	5	3	-	0/2/19/22	0/1/1/1
3	MAN	E	6	3	-	0/2/19/22	0/1/1/1
3	MAN	E	7	3	-	0/2/19/22	0/1/1/1
3	MAN	E	8	3	-	2/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	4/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	BMA	K	3	3	-	2/2/19/22	0/1/1/1
3	MAN	K	4	3	-	0/2/19/22	0/1/1/1
3	MAN	K	5	3	-	0/2/19/22	0/1/1/1
3	MAN	K	6	3	-	0/2/19/22	0/1/1/1
3	MAN	K	7	3	-	0/2/19/22	0/1/1/1
3	MAN	K	8	3	-	2/2/19/22	0/1/1/1
4	NAG	L	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
4	NAG	M	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	4/6/23/26	0/1/1/1
4	NAG	N	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	7	MAN	C1-O5-C5	4.33	117.99	112.19
3	K	7	MAN	C1-O5-C5	4.32	117.98	112.19
3	K	2	NAG	C2-N2-C7	2.98	126.89	122.90
3	E	2	NAG	C2-N2-C7	2.97	126.88	122.90
3	E	4	MAN	C1-O5-C5	2.84	115.99	112.19
4	P	2	NAG	C2-N2-C7	2.82	126.68	122.90
3	K	4	MAN	C1-O5-C5	2.81	115.95	112.19
4	J	2	NAG	C2-N2-C7	2.79	126.64	122.90
3	K	5	MAN	C1-O5-C5	2.70	115.80	112.19
4	G	2	NAG	C2-N2-C7	2.65	126.45	122.90
3	E	5	MAN	C1-O5-C5	2.65	115.73	112.19
4	M	2	NAG	C2-N2-C7	2.62	126.42	122.90
3	K	2	NAG	O5-C1-C2	2.52	115.19	111.29
3	E	2	NAG	O5-C1-C2	2.50	115.16	111.29
3	K	1	NAG	C1-O5-C5	2.36	115.35	112.19
4	N	2	NAG	C1-C2-N2	-2.35	106.73	110.43
3	K	6	MAN	C1-O5-C5	2.34	115.32	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	C1-O5-C5	2.34	115.32	112.19
4	F	2	NAG	C2-N2-C7	2.32	126.01	122.90
3	E	6	MAN	C1-O5-C5	2.32	115.30	112.19
4	H	2	NAG	C1-C2-N2	-2.32	106.77	110.43
4	L	2	NAG	C2-N2-C7	2.25	125.92	122.90
3	K	2	NAG	C1-C2-N2	-2.20	106.96	110.43
3	E	2	NAG	C1-C2-N2	-2.19	106.98	110.43
4	N	1	NAG	C2-N2-C7	2.18	125.83	122.90
4	H	1	NAG	C2-N2-C7	2.14	125.77	122.90
3	E	8	MAN	C1-O5-C5	2.07	114.95	112.19
3	K	8	MAN	C1-O5-C5	2.04	114.91	112.19
4	I	2	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
4	M	1	NAG	C8-C7-N2-C2
4	M	1	NAG	O7-C7-N2-C2
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
4	O	2	NAG	C8-C7-N2-C2
4	O	2	NAG	O7-C7-N2-C2
3	E	3	BMA	C4-C5-C6-O6
3	K	3	BMA	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
3	K	3	BMA	O5-C5-C6-O6
3	E	8	MAN	C4-C5-C6-O6
3	K	8	MAN	C4-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
4	G	2	NAG	C8-C7-N2-C2
4	M	2	NAG	C8-C7-N2-C2
3	E	8	MAN	O5-C5-C6-O6

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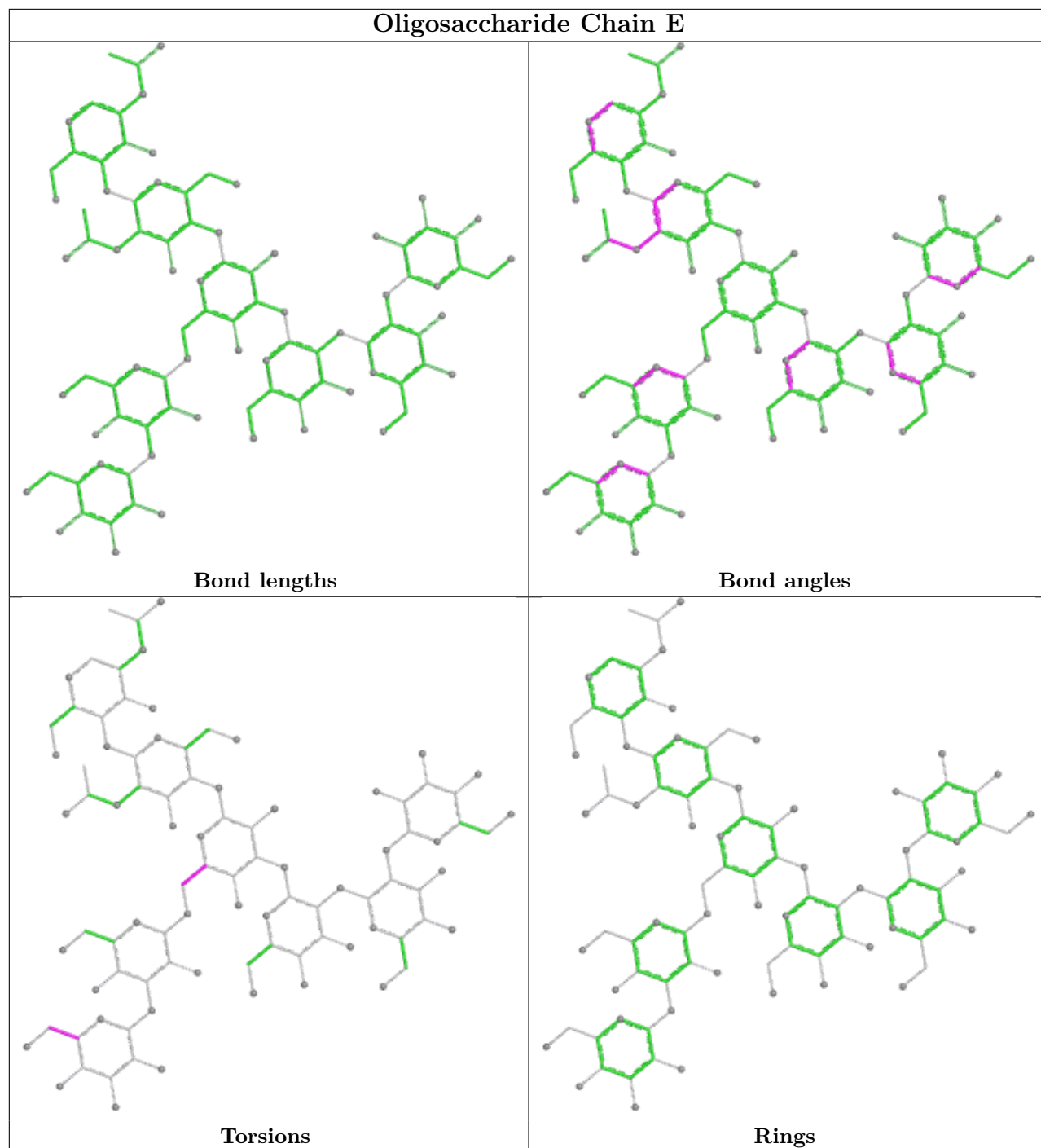
Mol	Chain	Res	Type	Atoms
3	K	8	MAN	O5-C5-C6-O6
4	G	2	NAG	O7-C7-N2-C2
4	M	2	NAG	O7-C7-N2-C2
4	F	1	NAG	C8-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	L	1	NAG	C8-C7-N2-C2
4	N	1	NAG	C8-C7-N2-C2
4	I	1	NAG	C8-C7-N2-C2
4	O	1	NAG	C8-C7-N2-C2
4	L	1	NAG	O7-C7-N2-C2
4	M	2	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	F	1	NAG	O7-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
4	N	1	NAG	O7-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
4	O	1	NAG	O7-C7-N2-C2
4	M	2	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6

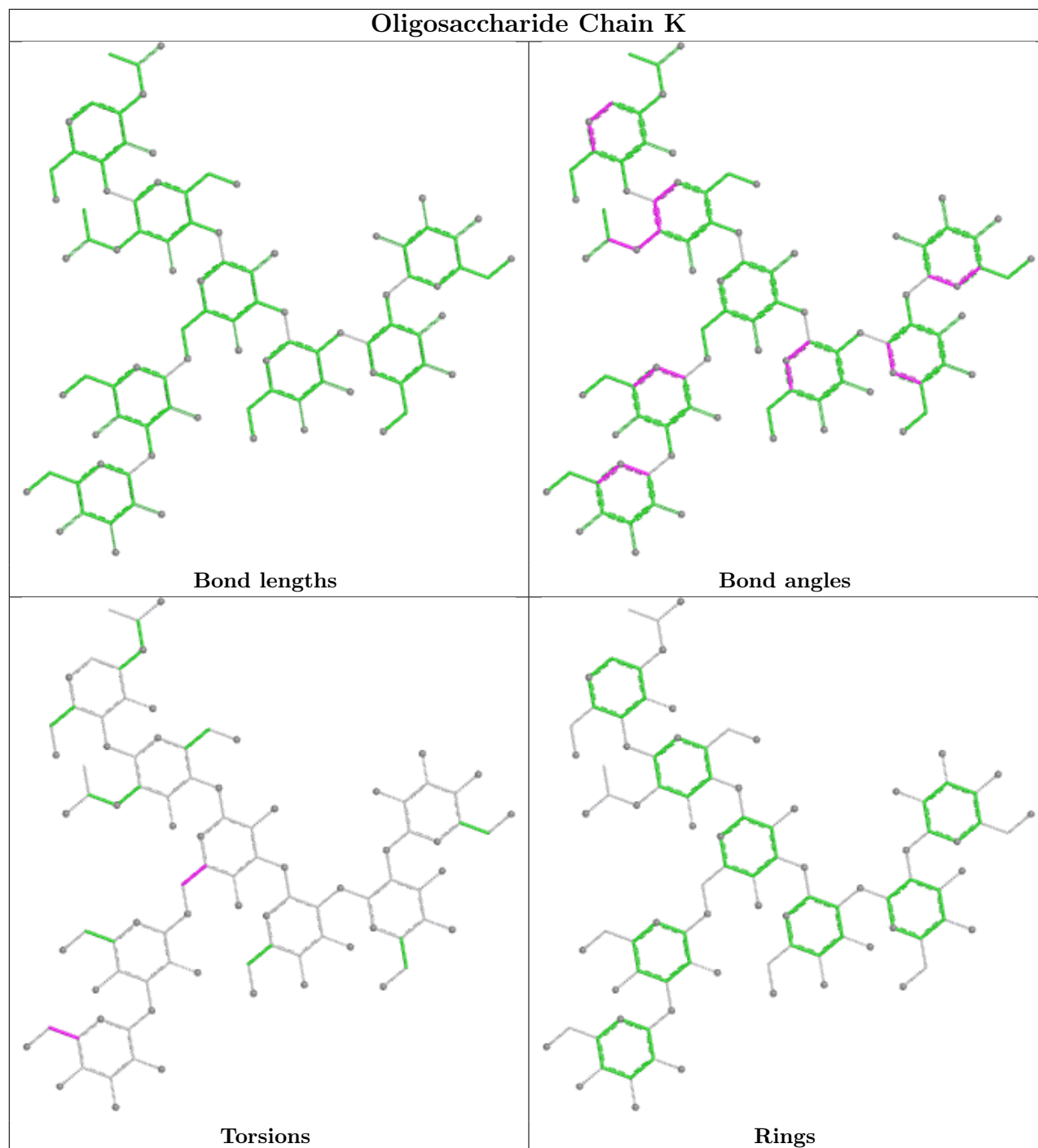
There are no ring outliers.

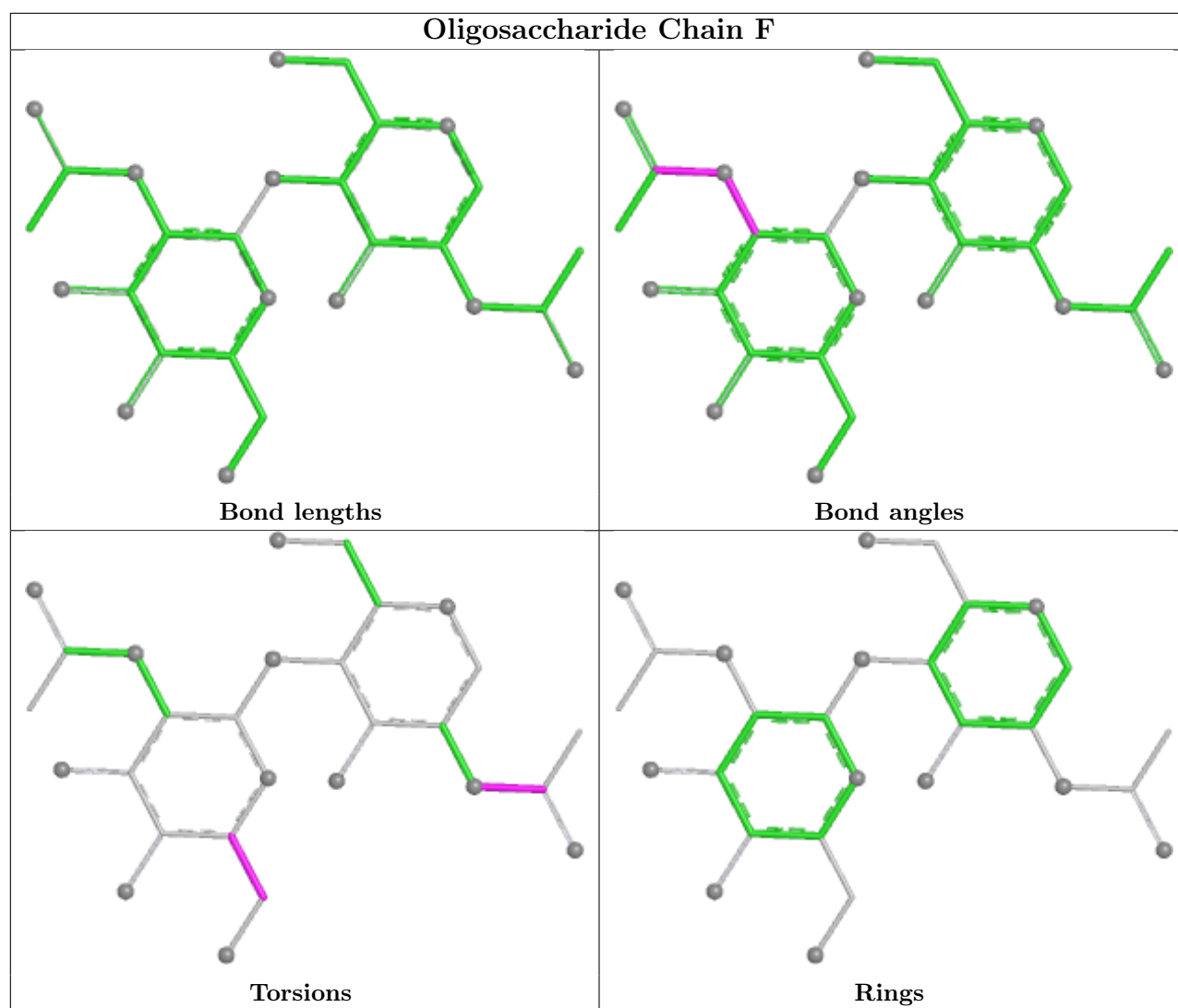
No monomer is involved in short contacts.

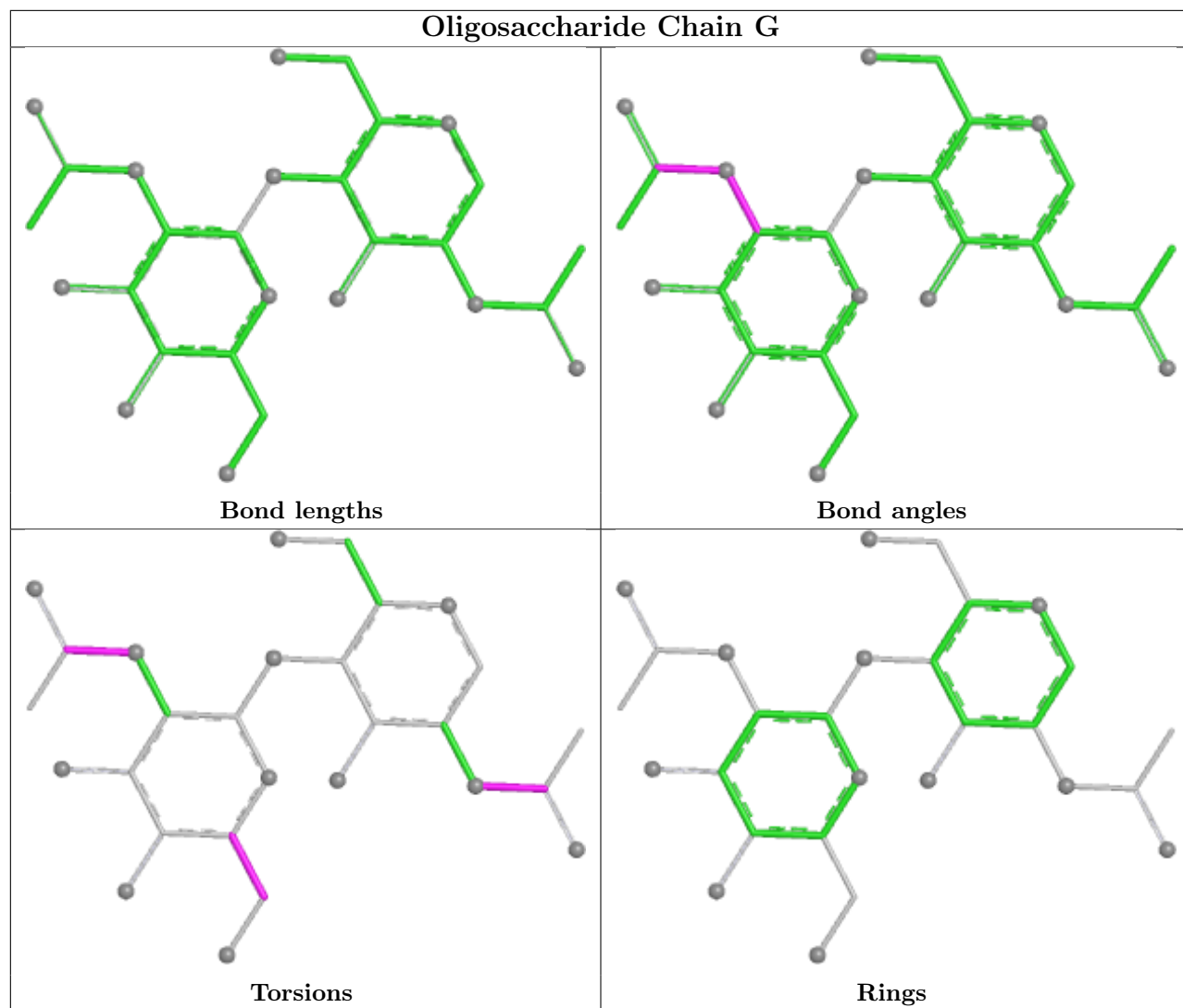
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

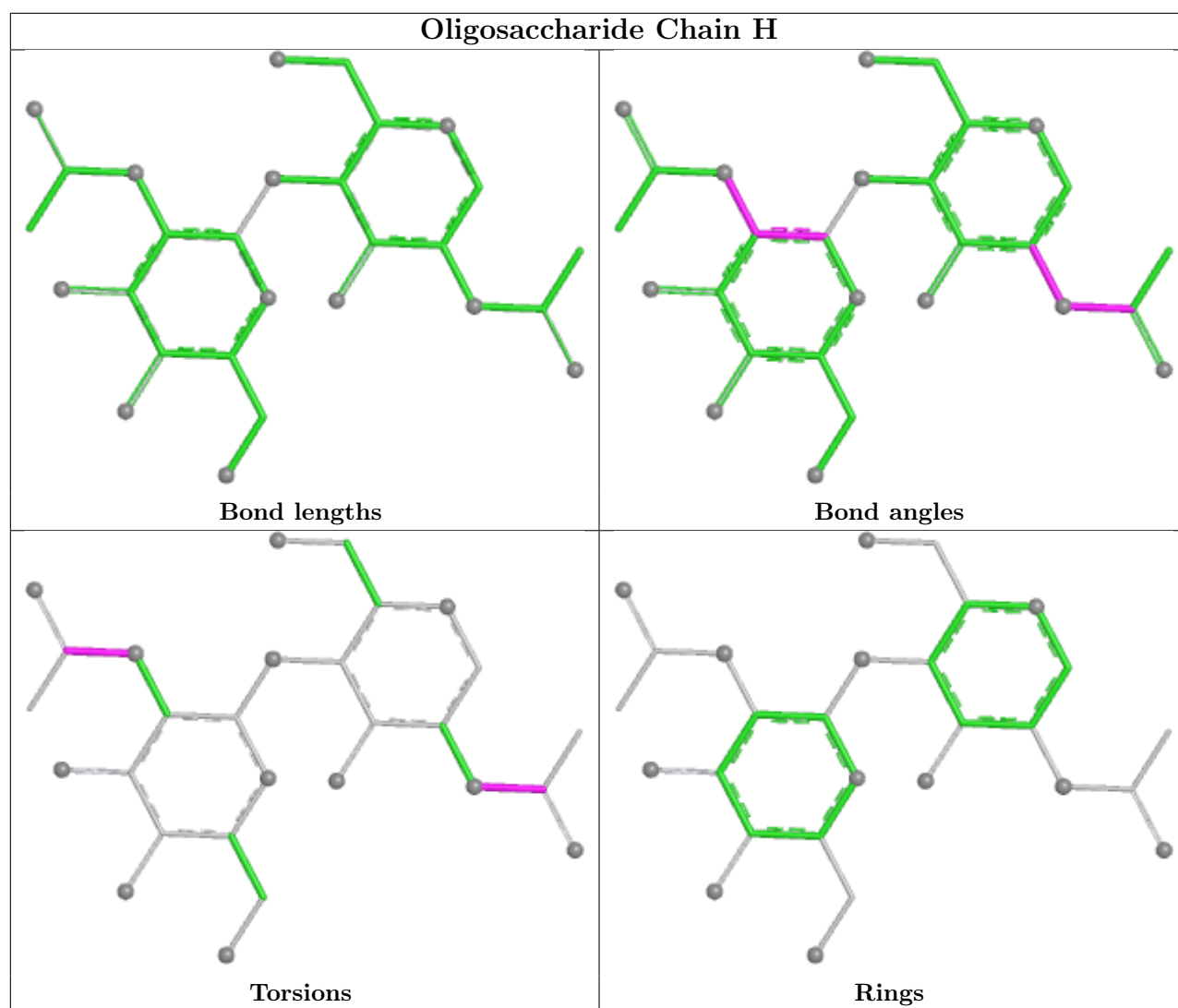
Oligosaccharide Chain E

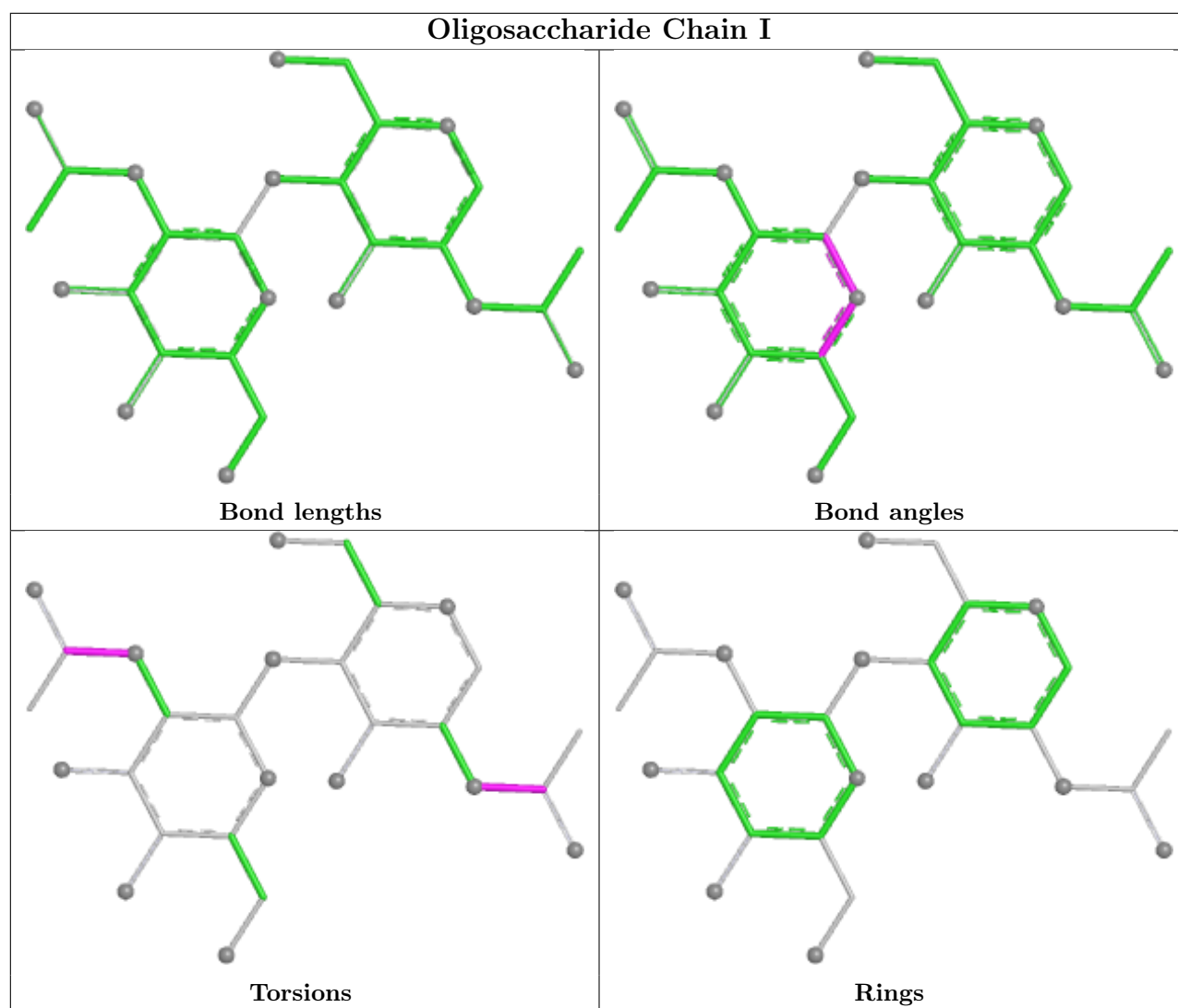


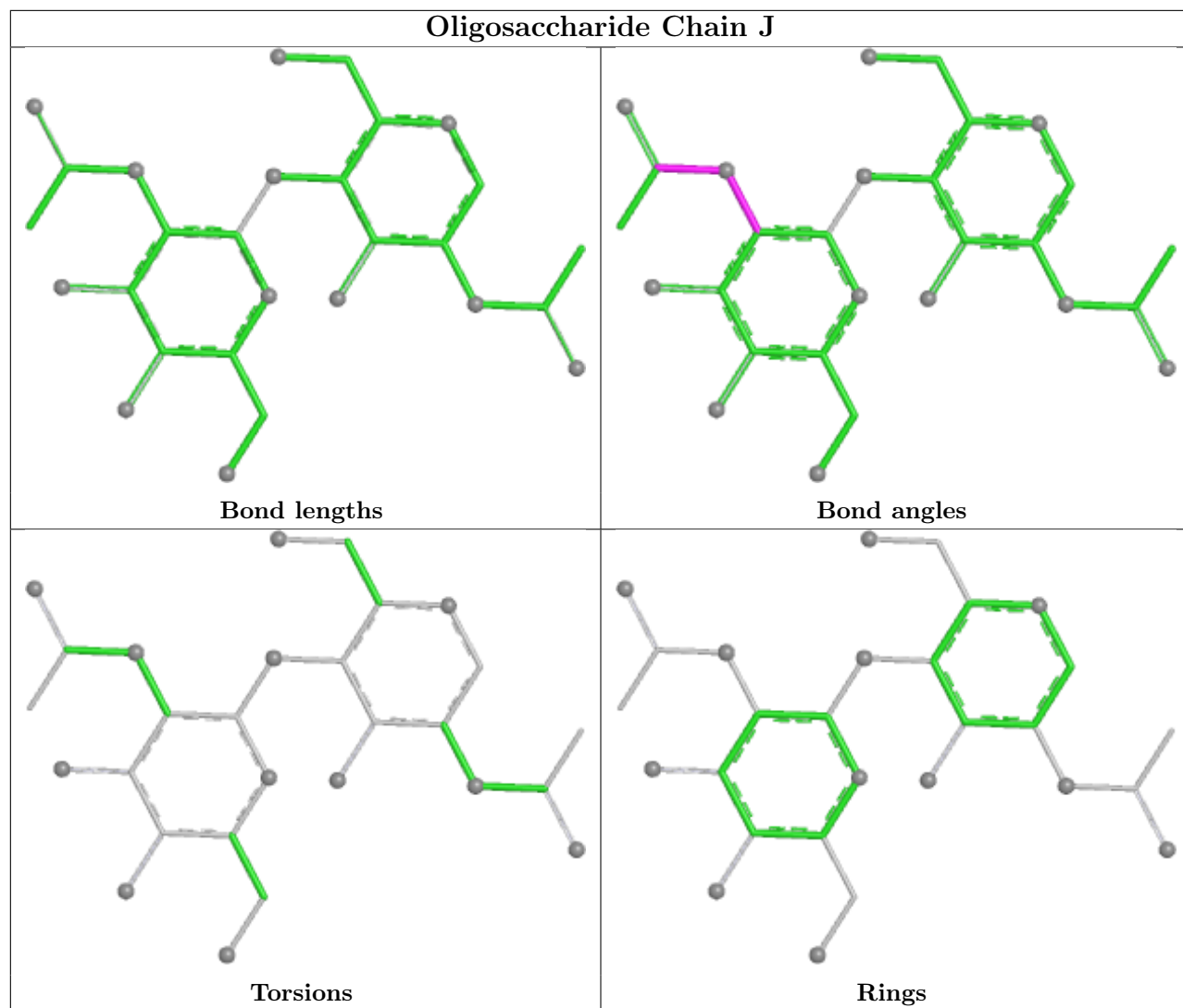


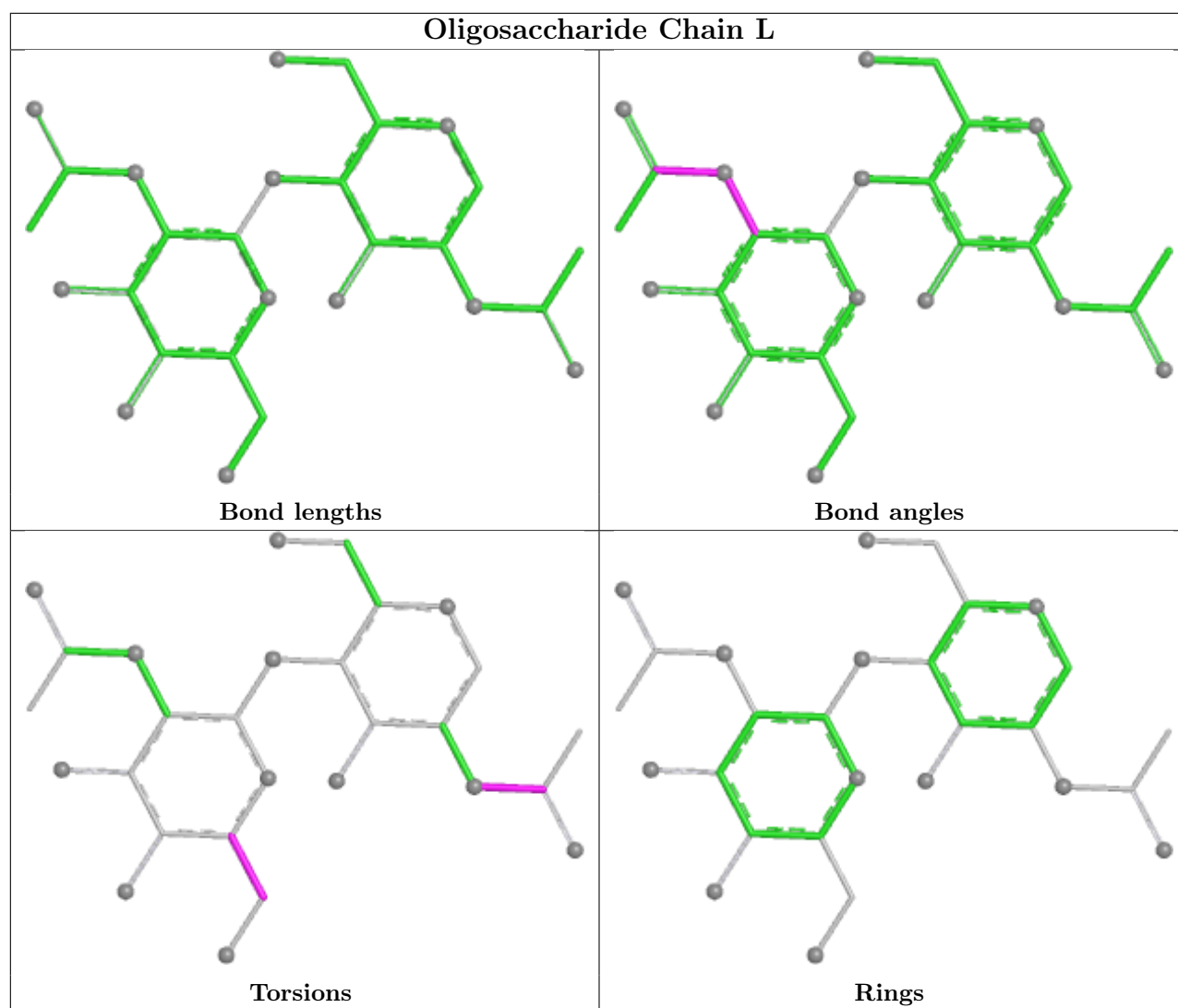


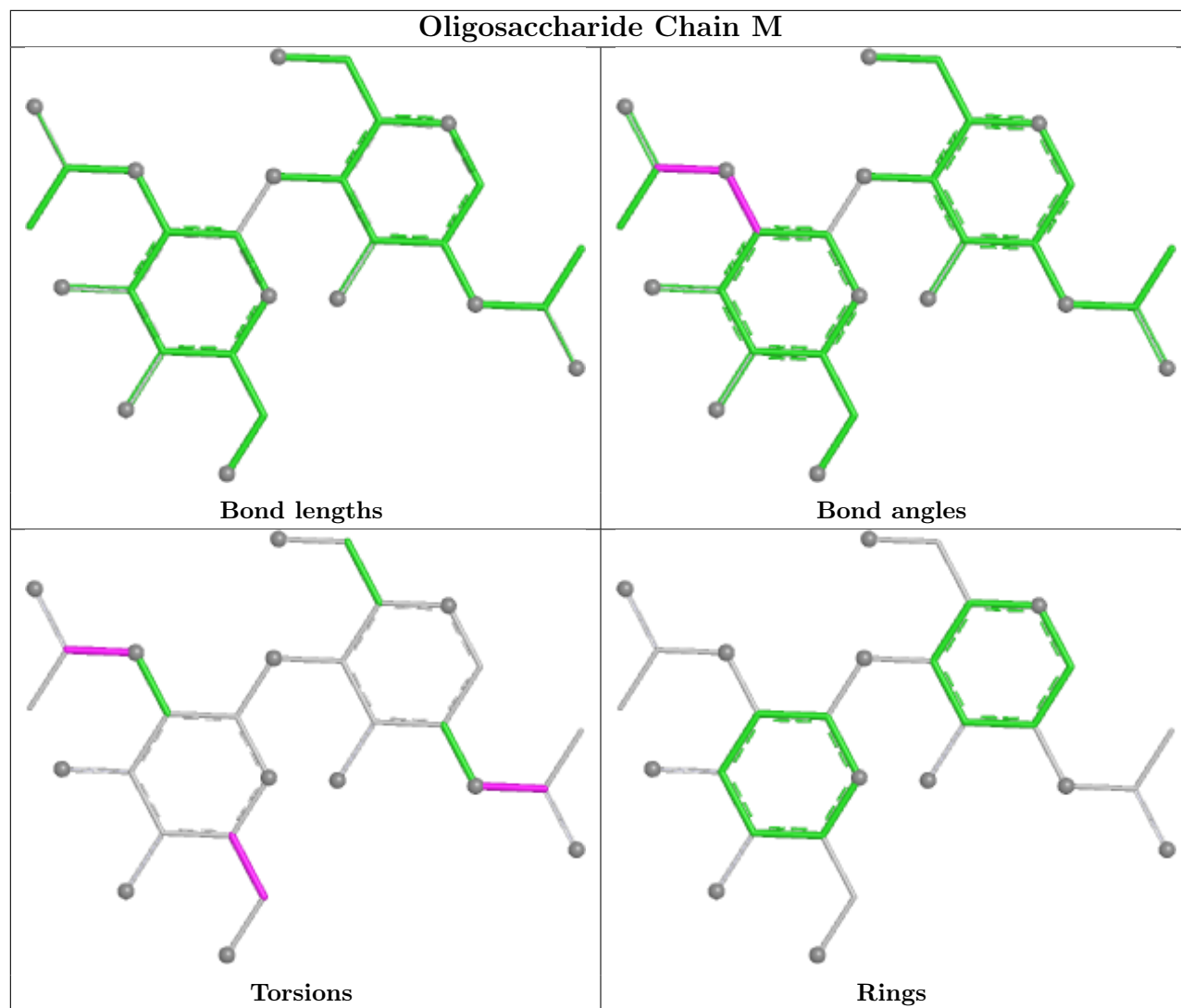


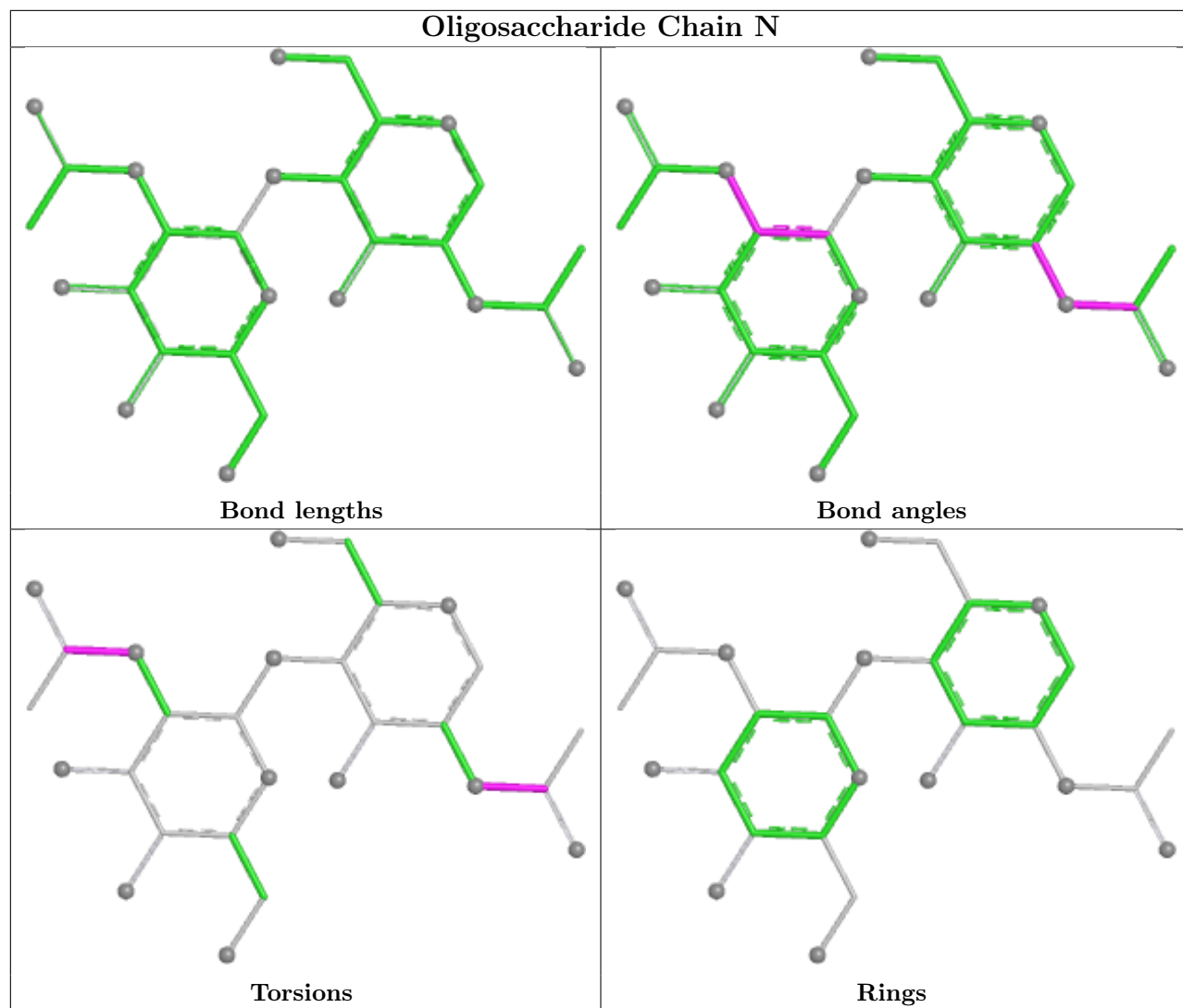


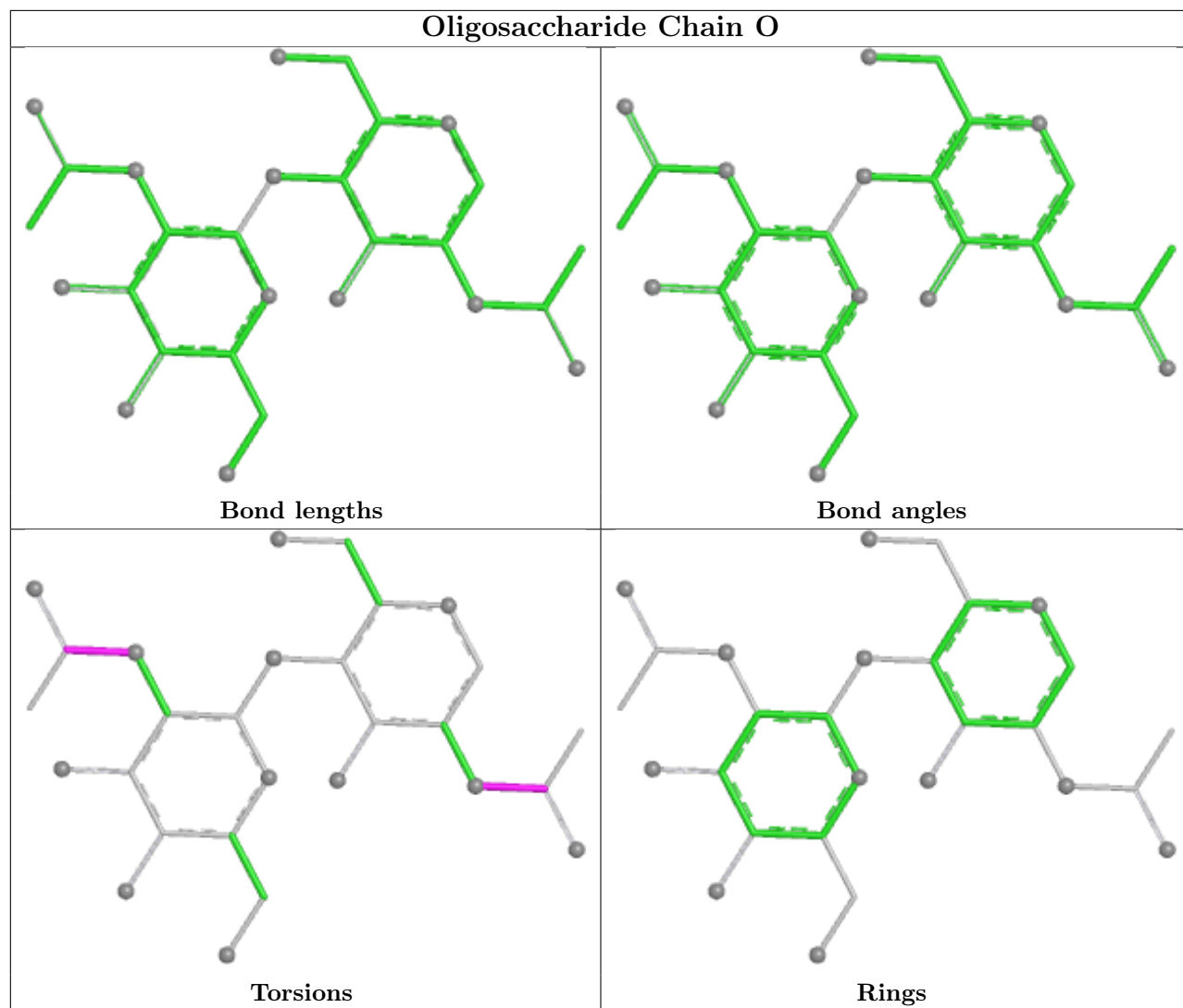


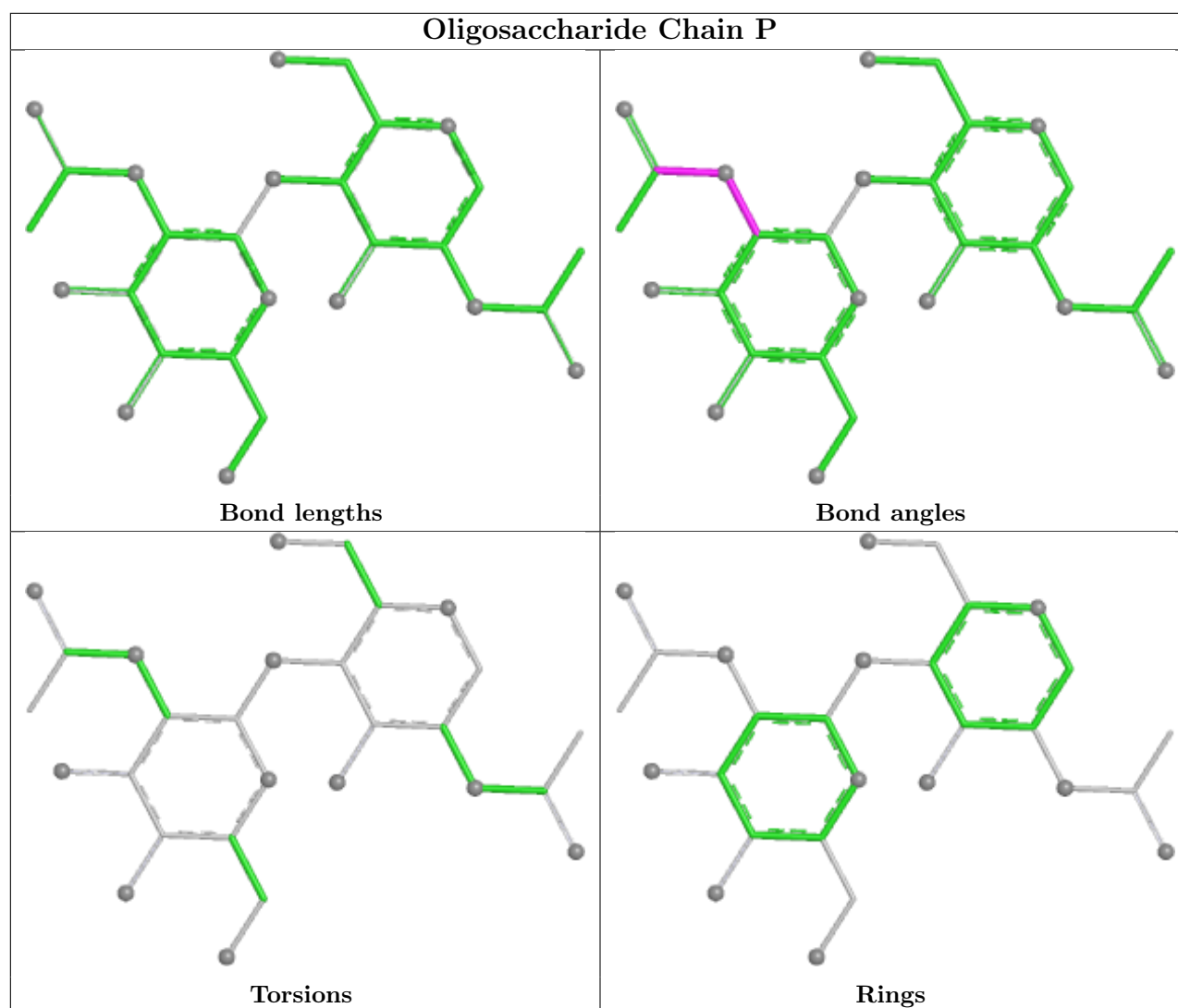












5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
5	NAG	C	3022	1	14,14,15	0.44	0	17,19,21	1.09	2 (11%)
5	NAG	A	3019	1	14,14,15	0.44	0	17,19,21	0.96	1 (5%)
5	NAG	C	3014	1	14,14,15	0.49	0	17,19,21	1.34	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	3014	1	14,14,15	0.50	0	17,19,21	1.34	2 (11%)
5	NAG	A	3011	1	14,14,15	0.44	0	17,19,21	0.81	2 (11%)
5	NAG	C	3019	1	14,14,15	0.45	0	17,19,21	0.96	1 (5%)
5	NAG	C	3011	1	14,14,15	0.45	0	17,19,21	0.81	2 (11%)
5	NAG	A	3022	1	14,14,15	0.43	0	17,19,21	0.90	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
5	NAG	C	3022	1	-	2/6/23/26	0/1/1/1
5	NAG	A	3019	1	-	2/6/23/26	0/1/1/1
5	NAG	C	3014	1	-	5/6/23/26	0/1/1/1
5	NAG	A	3014	1	-	5/6/23/26	0/1/1/1
5	NAG	A	3011	1	-	4/6/23/26	0/1/1/1
5	NAG	C	3019	1	-	2/6/23/26	0/1/1/1
5	NAG	C	3011	1	-	4/6/23/26	0/1/1/1
5	NAG	A	3022	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	3014	NAG	C1-C2-N2	3.99	116.72	110.43
5	A	3014	NAG	C1-C2-N2	3.97	116.69	110.43
5	A	3014	NAG	C2-N2-C7	3.11	127.07	122.90
5	C	3014	NAG	C2-N2-C7	3.09	127.04	122.90
5	C	3022	NAG	O5-C1-C2	2.72	115.50	111.29
5	A	3019	NAG	O5-C1-C2	2.40	115.00	111.29
5	C	3019	NAG	O5-C1-C2	2.38	114.98	111.29
5	A	3011	NAG	C1-O5-C5	2.20	115.14	112.19
5	C	3022	NAG	C2-N2-C7	2.17	125.81	122.90
5	C	3011	NAG	C1-O5-C5	2.16	115.08	112.19
5	C	3011	NAG	C1-C2-N2	2.03	113.64	110.43
5	A	3011	NAG	C1-C2-N2	2.03	113.63	110.43

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	3011	NAG	O7-C7-N2-C2
5	A	3014	NAG	C1-C2-N2-C7
5	A	3019	NAG	C8-C7-N2-C2
5	A	3019	NAG	O7-C7-N2-C2
5	A	3022	NAG	C8-C7-N2-C2
5	A	3022	NAG	O7-C7-N2-C2
5	C	3011	NAG	O7-C7-N2-C2
5	C	3014	NAG	C1-C2-N2-C7
5	C	3019	NAG	C8-C7-N2-C2
5	C	3019	NAG	O7-C7-N2-C2
5	C	3022	NAG	O7-C7-N2-C2
5	A	3011	NAG	C8-C7-N2-C2
5	C	3011	NAG	C8-C7-N2-C2
5	C	3022	NAG	C8-C7-N2-C2
5	A	3014	NAG	O7-C7-N2-C2
5	C	3014	NAG	O7-C7-N2-C2
5	A	3014	NAG	C8-C7-N2-C2
5	C	3014	NAG	C8-C7-N2-C2
5	A	3011	NAG	O5-C5-C6-O6
5	A	3014	NAG	O5-C5-C6-O6
5	C	3011	NAG	O5-C5-C6-O6
5	C	3014	NAG	O5-C5-C6-O6
5	C	3011	NAG	C4-C5-C6-O6
5	A	3011	NAG	C4-C5-C6-O6
5	A	3014	NAG	C4-C5-C6-O6
5	C	3014	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	1752/1756 (99%)	-0.03	46 (2%) 57 35	25, 88, 193, 273	1 (0%)
1	C	1752/1756 (99%)	0.01	50 (2%) 53 32	39, 92, 181, 246	1 (0%)
2	B	96/108 (88%)	0.15	2 (2%) 63 39	52, 86, 159, 237	0
2	D	96/108 (88%)	-0.01	2 (2%) 63 39	52, 84, 163, 228	0
All	All	3696/3728 (99%)	-0.01	100 (2%) 56 34	25, 89, 186, 273	2 (0%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1895	PHE	5.1
1	A	2167	ILE	5.0
1	C	1618	GLU	4.5
2	B	31	GLU	4.5
1	C	1542	ALA	4.5
1	C	2585	ALA	4.3
1	C	1095	ILE	4.2
1	C	1543	GLY	3.9
1	C	2586	GLY	3.9
1	C	1563	ASP	3.8
1	C	1074	ARG	3.7
1	C	2588	TRP	3.6
1	C	1871	GLY	3.6
1	C	2499	ASP	3.6
1	C	2552	THR	3.5
1	A	1392	ASP	3.4
1	A	1563	ASP	3.4
1	C	1226	ASN	3.4
2	D	31	GLU	3.4
1	C	2026	PHE	3.3
1	A	1398	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	2586	GLY	3.3
1	A	1821	HIS	3.3
1	A	2499	ASP	3.3
1	A	1610	GLN	3.3
1	A	1875	LEU	3.2
1	C	1998	ALA	3.2
1	C	2580	SER	3.2
1	A	2686	ILE	3.1
1	A	1424	THR	3.1
1	C	1821	HIS	3.1
1	A	1587	ILE	3.1
1	C	2587	HIS	3.1
1	A	2523	PRO	3.1
1	C	1354	SER	3.0
1	C	2497	GLU	3.0
1	A	1095	ILE	2.9
1	A	2687	ASN	2.9
1	A	2497	GLU	2.9
1	A	2587	HIS	2.9
1	A	1543	GLY	2.9
1	A	2026	PHE	2.9
1	C	2486	TYR	2.9
1	A	1074	ARG	2.9
1	A	1474	VAL	2.9
1	A	2419	TYR	2.8
1	A	2585	ALA	2.8
1	C	2028	TYR	2.7
1	A	1225	GLY	2.7
1	C	1725	GLY	2.7
1	C	1228	GLU	2.7
1	C	1636	LEU	2.7
1	C	1071	ALA	2.7
1	C	1541	LEU	2.6
1	C	2465	TRP	2.6
1	C	1090	VAL	2.6
1	A	2643	GLY	2.6
1	C	2046	VAL	2.6
1	A	1423	LEU	2.5
1	C	2483	PHE	2.5
1	C	2011	ILE	2.5
1	C	1610	GLN	2.5
1	C	1230	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	2174	ALA	2.5
1	A	1542	ALA	2.4
1	A	2501	LYS	2.4
1	C	1517	TYR	2.4
1	A	1623	VAL	2.4
1	C	2479	GLU	2.4
1	C	1994	MET	2.4
1	A	2160	PHE	2.4
1	C	1390	ALA	2.4
1	A	2028	TYR	2.4
1	C	2514	PHE	2.4
1	A	2038	SER	2.3
1	C	1421	ASN	2.3
1	C	1877	ILE	2.3
1	A	2168	ASN	2.2
1	A	1478	ALA	2.2
1	A	2620	ASP	2.2
1	A	1385	SER	2.2
1	A	1370	ALA	2.2
1	C	2032	GLY	2.2
1	C	1424	THR	2.1
1	A	2498	LEU	2.1
1	A	1618	GLU	2.1
1	A	1378	ALA	2.1
1	A	1322	ASP	2.1
1	C	1895	PHE	2.1
1	C	2559	GLU	2.1
1	A	1845	ASN	2.1
1	C	2332	GLY	2.1
2	B	102	PRO	2.1
2	D	46	ASP	2.1
1	A	2514	PHE	2.1
1	C	1378	ALA	2.0
1	C	1783	ALA	2.0
1	C	1772	VAL	2.0
1	A	2439	PHE	2.0
1	A	2453	PHE	2.0

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

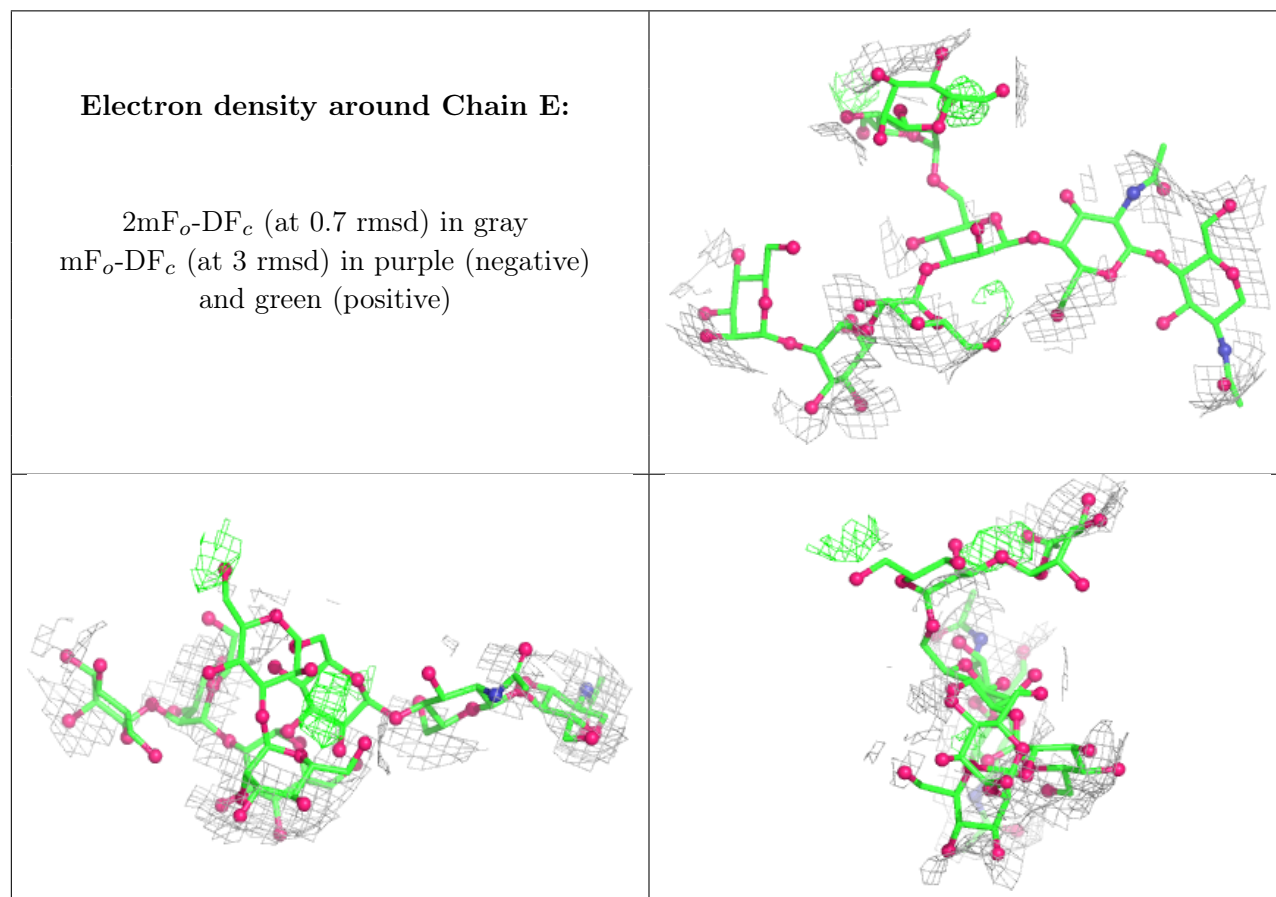
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

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

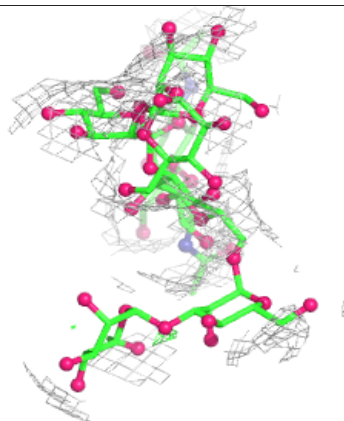
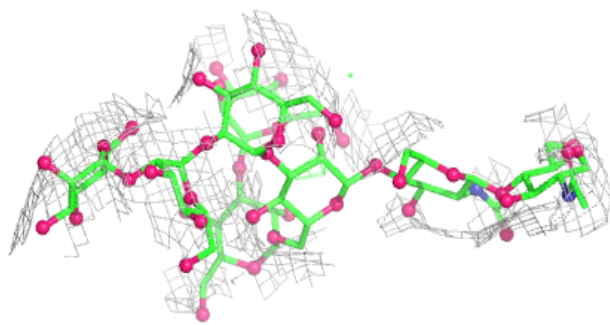
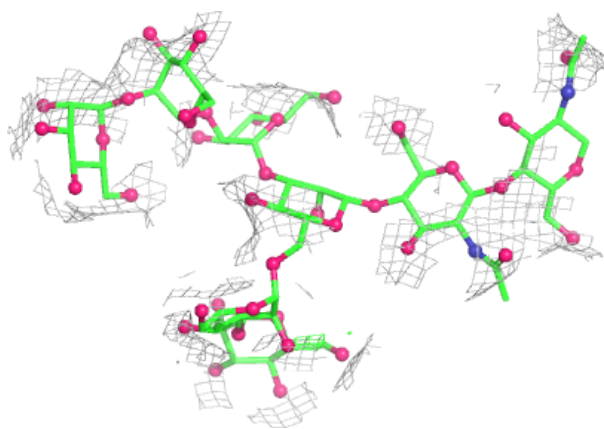
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	O	2	14/15	-0.10	0.11	167,175,200,221	0
3	MAN	K	6	11/12	0.23	0.10	167,172,180,180	0
3	MAN	E	7	11/12	0.24	0.09	180,189,196,196	0
4	NAG	J	2	14/15	0.32	0.12	144,152,161,161	0
4	NAG	I	2	14/15	0.36	0.10	157,162,169,171	0
4	NAG	H	2	14/15	0.37	0.10	153,159,168,170	0
3	MAN	E	8	11/12	0.37	0.10	197,201,210,217	0
3	MAN	K	8	11/12	0.39	0.09	204,209,219,229	0
4	NAG	P	2	14/15	0.48	0.11	163,173,226,239	0
3	MAN	K	7	11/12	0.50	0.07	183,191,199,201	0
4	NAG	N	2	14/15	0.54	0.08	162,169,178,181	0
4	NAG	P	1	14/15	0.58	0.11	123,144,158,161	0
3	MAN	E	6	11/12	0.58	0.08	163,168,175,175	0
3	BMA	K	3	11/12	0.65	0.07	143,148,162,171	0
4	NAG	N	1	14/15	0.66	0.07	108,129,143,151	0
3	BMA	E	3	11/12	0.66	0.06	140,144,160,169	0
4	NAG	O	1	14/15	0.66	0.09	124,148,159,160	0
4	NAG	M	1	14/15	0.69	0.11	84,88,92,96	0
4	NAG	G	2	14/15	0.70	0.10	102,109,115,117	0
4	NAG	M	2	14/15	0.70	0.10	101,107,114,115	0
3	NAG	K	2	14/15	0.71	0.09	122,131,137,141	0
4	NAG	L	2	14/15	0.71	0.07	136,152,164,168	0
4	NAG	I	1	14/15	0.72	0.11	113,135,147,148	0
3	MAN	E	4	11/12	0.72	0.08	125,137,143,143	0
4	NAG	G	1	14/15	0.72	0.12	89,92,95,99	0
4	NAG	J	1	14/15	0.74	0.08	99,118,131,137	0
4	NAG	L	1	14/15	0.76	0.07	116,124,130,135	0
4	NAG	H	1	14/15	0.76	0.06	103,122,135,143	0
4	NAG	F	2	14/15	0.77	0.10	133,145,156,159	0
3	NAG	E	2	14/15	0.78	0.10	119,126,132,137	0
3	MAN	K	5	11/12	0.80	0.09	141,145,152,158	0
3	NAG	E	1	14/15	0.82	0.10	93,102,115,116	0
3	MAN	E	5	11/12	0.82	0.07	139,143,149,155	0
3	MAN	K	4	11/12	0.83	0.06	129,143,148,149	0
4	NAG	F	1	14/15	0.84	0.07	111,118,123,129	0
3	NAG	K	1	14/15	0.86	0.08	96,105,119,123	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.



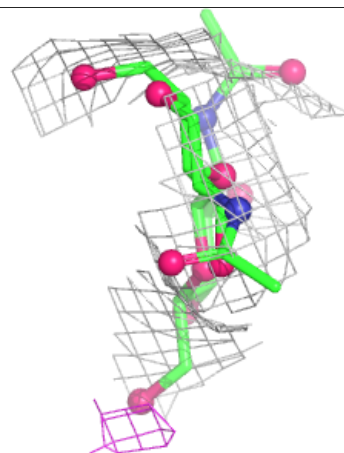
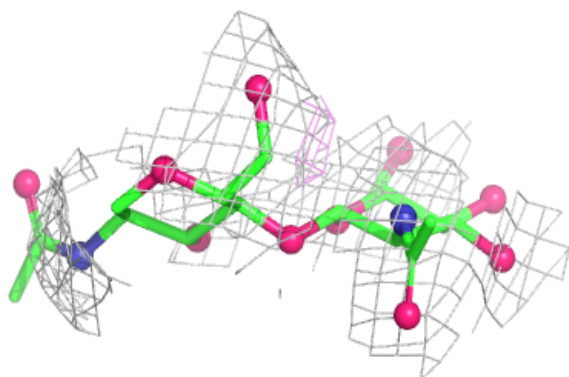
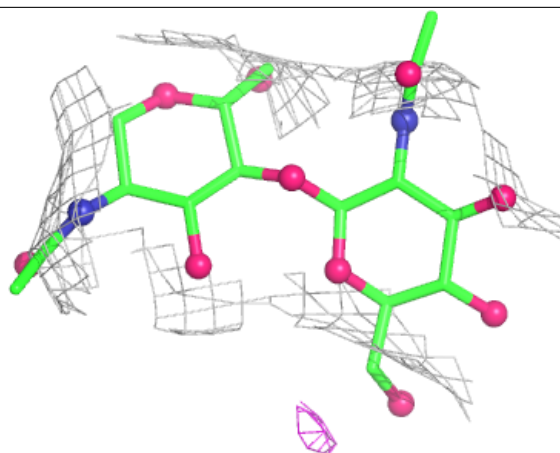
Electron density around Chain K:

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

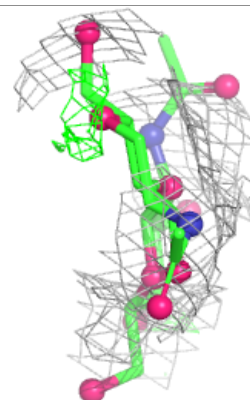
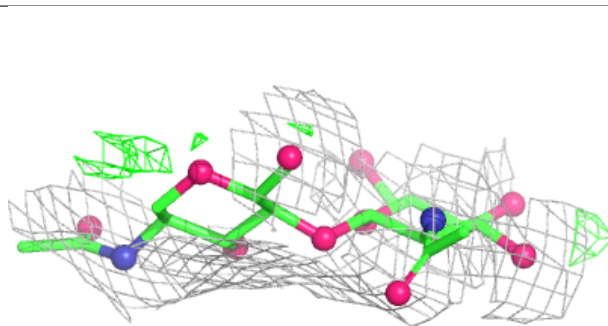
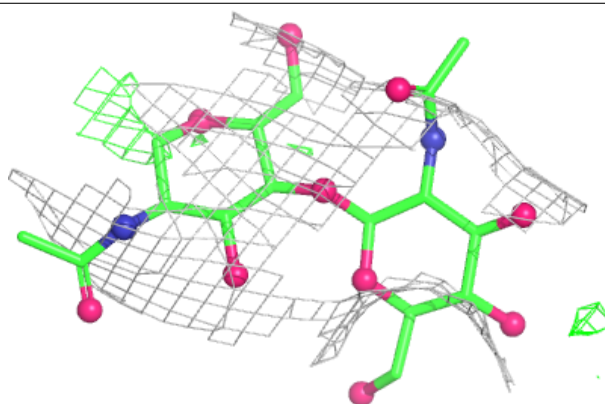


Electron density around Chain F:

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

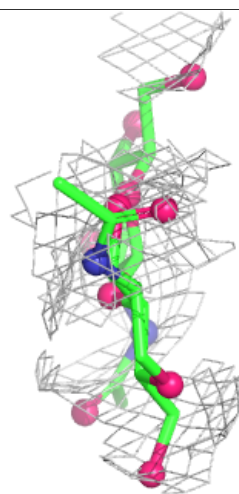
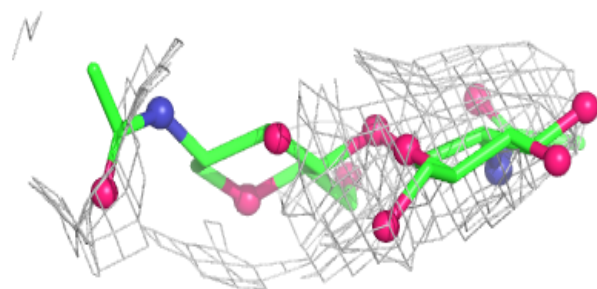
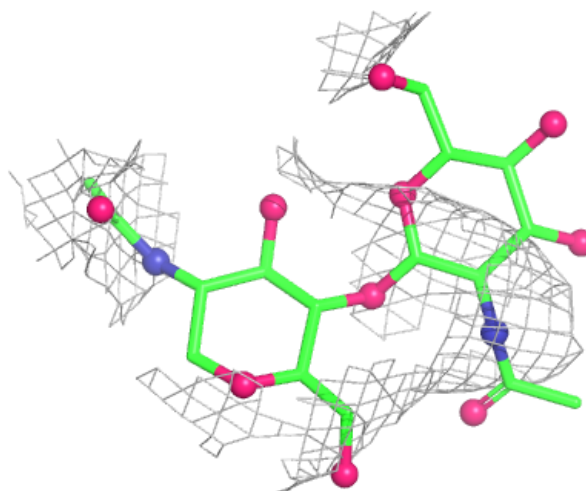
**Electron density around Chain G:**

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



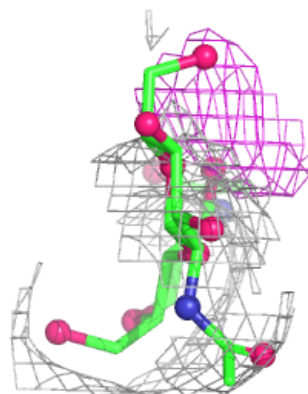
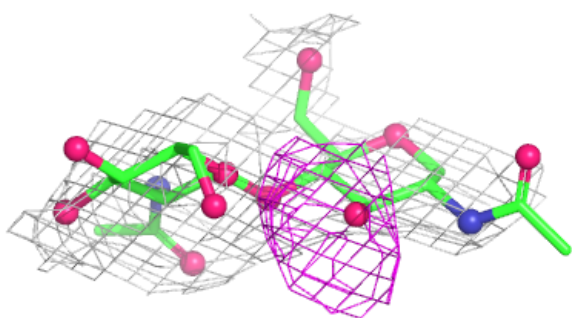
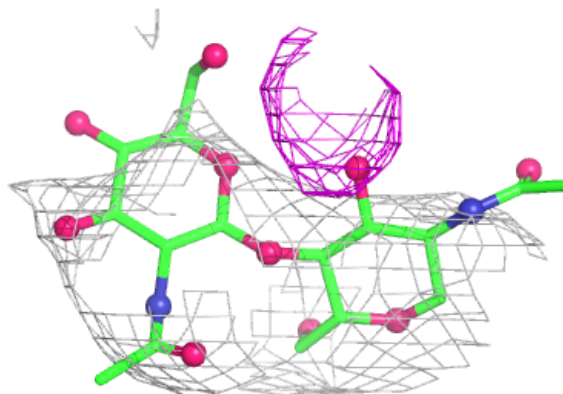
Electron density around Chain H:

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



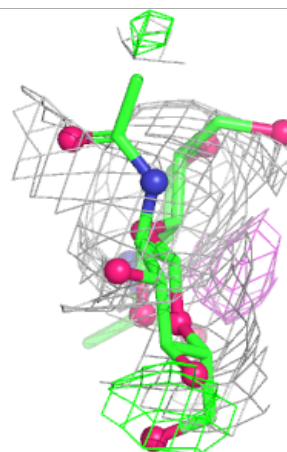
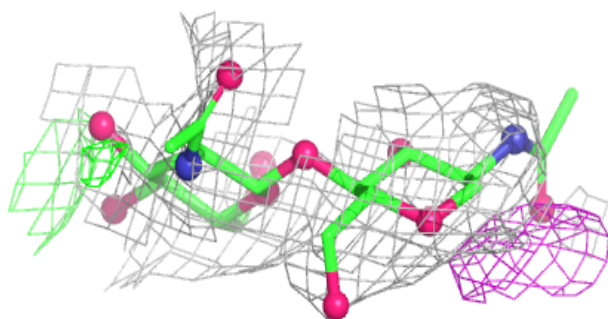
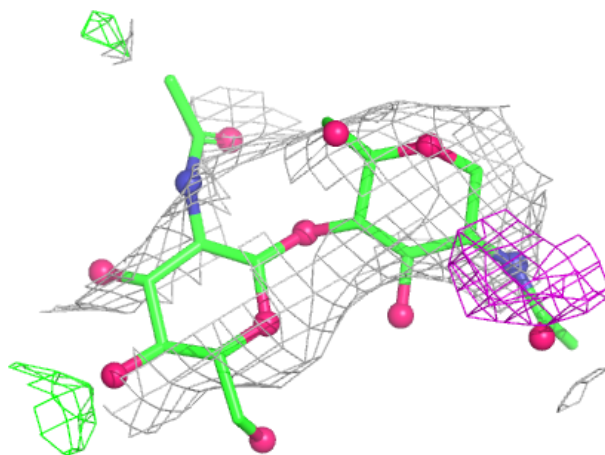
Electron density around Chain I:

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



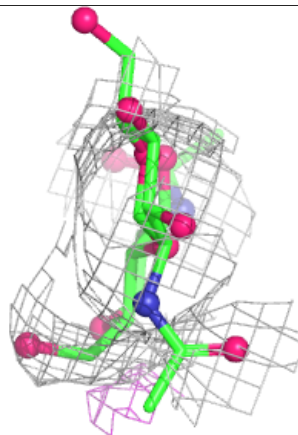
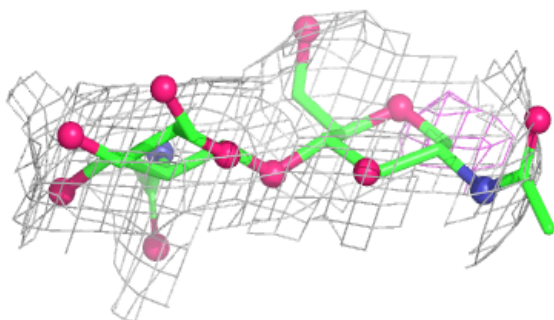
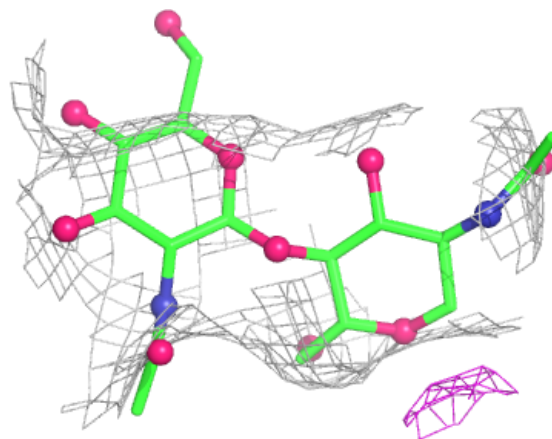
Electron density around Chain J:

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



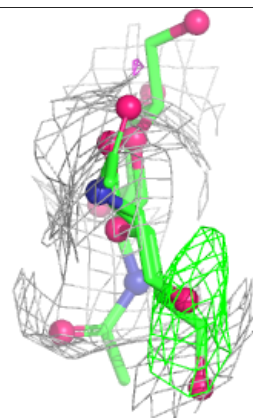
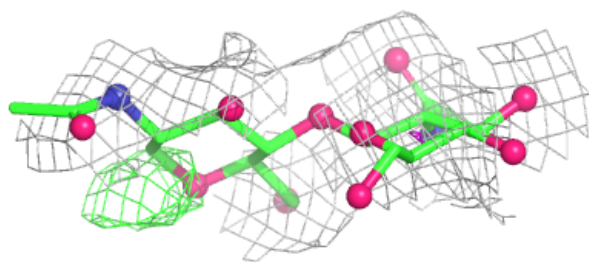
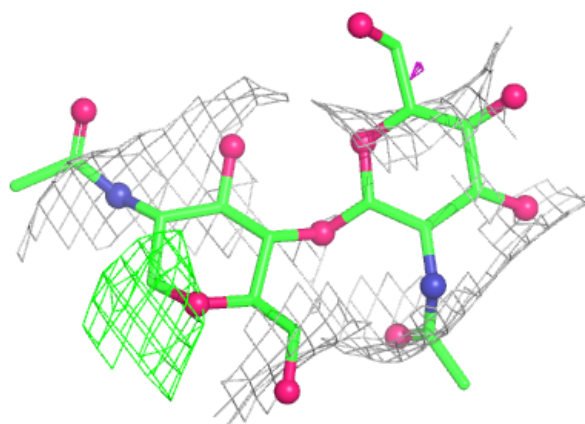
Electron density around Chain L:

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



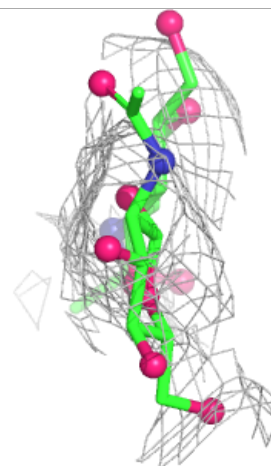
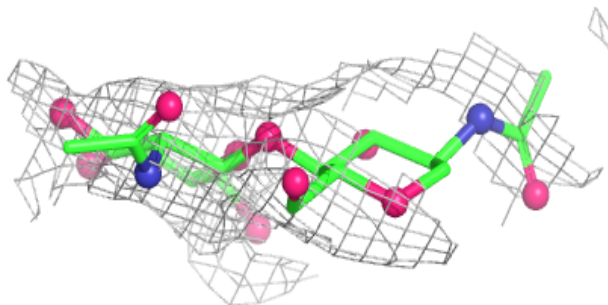
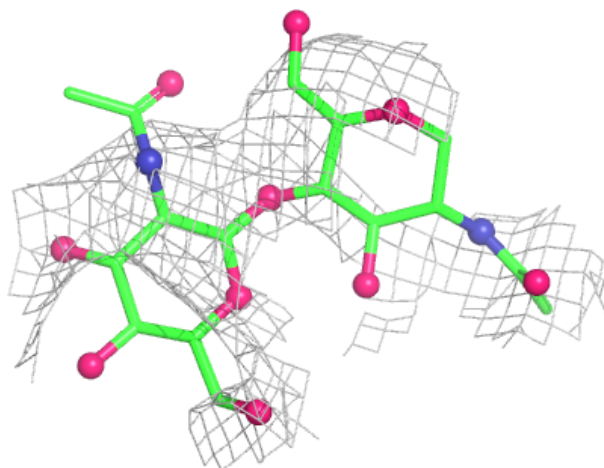
Electron density around Chain M:

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



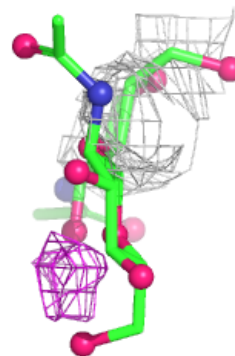
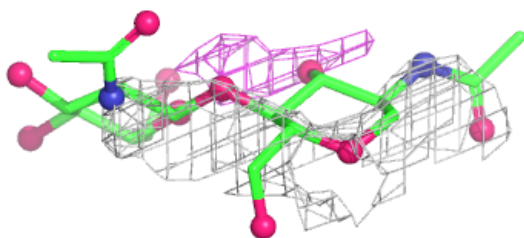
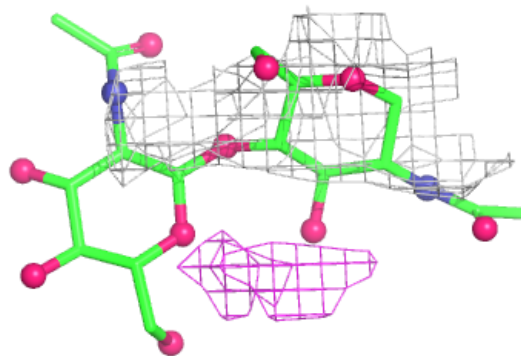
Electron density around Chain N:

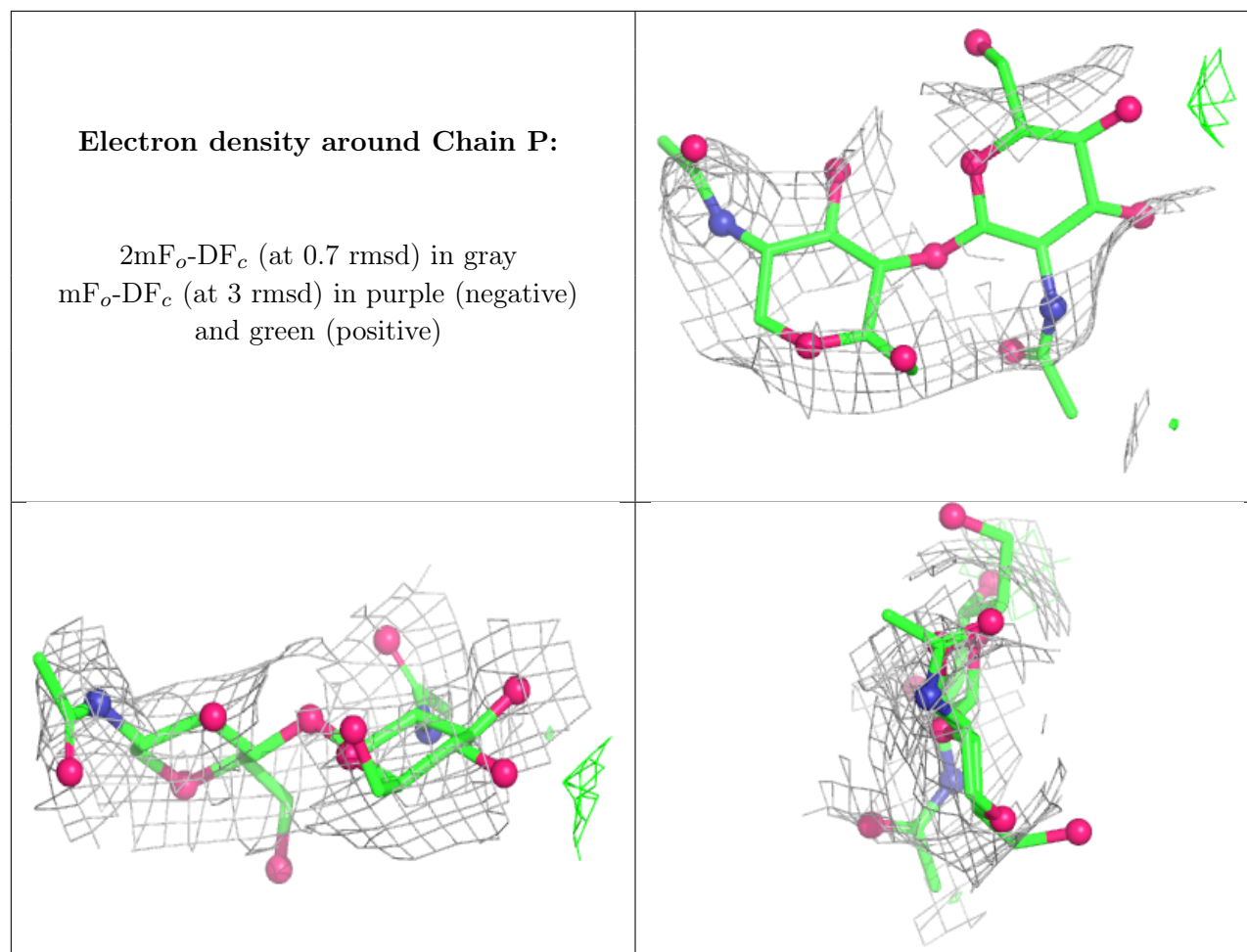
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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
5	NAG	C	3019	14/15	-0.04	0.11	183,235,245,248	0
5	NAG	A	3011	14/15	0.02	0.16	89,95,98,98	0
5	NAG	C	3011	14/15	0.21	0.15	112,119,124,124	0
5	NAG	A	3019	14/15	0.33	0.11	182,188,197,212	0
5	NAG	A	3014	14/15	0.43	0.12	111,115,122,123	0
5	NAG	A	3022	14/15	0.52	0.11	175,228,235,236	0
5	NAG	C	3014	14/15	0.62	0.13	108,112,119,119	0
5	NAG	C	3022	14/15	0.76	0.05	158,165,172,190	0

6.5 Other polymers ⓘ

There are no such residues in this entry.