



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 11:18 AM UTC

PDB ID : 6X91 / pdb_00006x91
Title : Crystal structure of MBP-fused human APOBEC1
Authors : Wolfe, A.D.; Li, S.-X.; Chen, X.S.
Deposited on : 2020-06-02
Resolution : 3.51 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

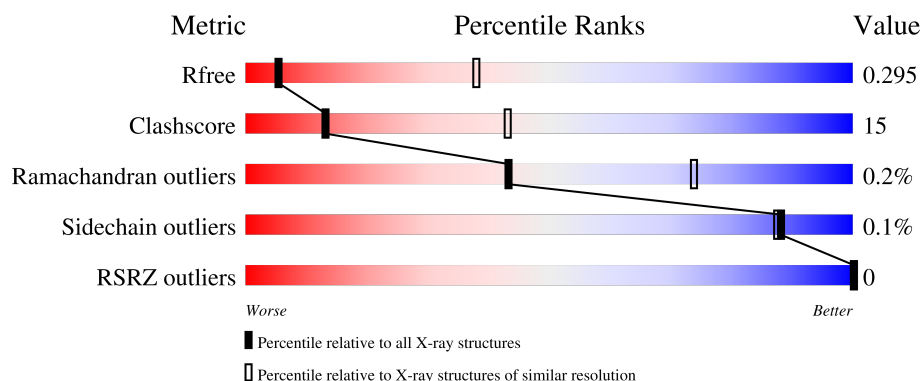
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.51 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.



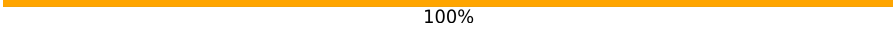
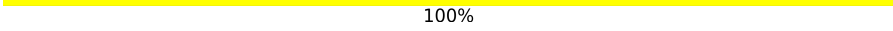
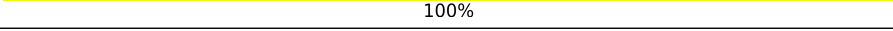
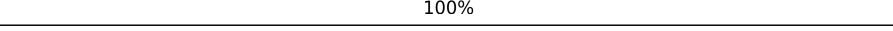
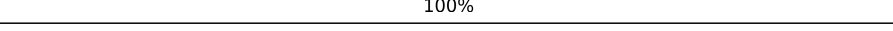
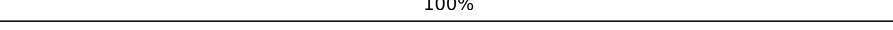
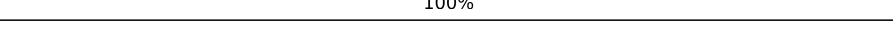
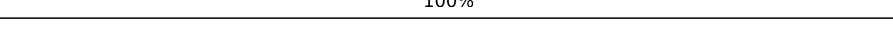
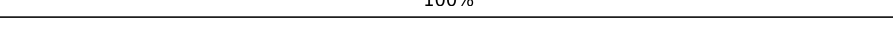
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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	593	 70% 30%
1	B	593	 67% 33%
1	C	593	 70% 30%
1	D	593	 63% 30% 6%
1	E	593	 69% 30%

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Mol	Chain	Length	Quality of chain
1	F	593	 69% 31%
1	G	593	 67% 33%
1	H	593	 64% 30% 6%
2	I	2	 50% 50%
2	J	2	 50% 50%
2	K	2	 100%
2	L	2	 100%
2	M	2	 50% 50%
2	N	2	 100%
2	O	2	 100%
2	P	2	 50% 50%
2	Q	2	 100%
2	R	2	 100%
2	S	2	 100%
2	T	2	 100%
2	U	2	 100%
2	V	2	 100%

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
2	GLC	M	1	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 37624 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 Maltodextrin-binding protein, C->U-editing enzyme APOBEC-1 chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	592	Total	C	N	O	S	0	0	0
			4725	3042	801	864	18			
1	B	592	Total	C	N	O	S	0	0	0
			4725	3042	801	864	18			
1	C	592	Total	C	N	O	S	0	0	0
			4725	3042	801	864	18			
1	D	557	Total	C	N	O	S	0	0	0
			4452	2865	756	815	16			
1	E	592	Total	C	N	O	S	0	0	0
			4725	3042	801	864	18			
1	F	592	Total	C	N	O	S	0	0	0
			4725	3042	801	864	18			
1	G	592	Total	C	N	O	S	0	0	0
			4725	3042	801	864	18			
1	H	558	Total	C	N	O	S	0	0	0
			4452	2864	756	816	16			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A4Z0THX4
A	313	VAL	ALA	engineered mutation	UNP A0A4Z0THX4
A	368	ASN	-	linker	UNP A0A4Z0THX4
A	369	SER	-	linker	UNP A0A4Z0THX4
A	370	SER	-	linker	UNP A0A4Z0THX4
A	371	SER	-	linker	UNP A0A4Z0THX4
A	1046	ALA	MET	engineered mutation	UNP P41238
A	1048	SER	ARG	engineered mutation	UNP P41238
A	1063	ALA	GLU	engineered mutation	UNP P41238
A	1080	THR	MET	engineered mutation	UNP P41238
A	1121	ALA	TRP	conflict	UNP P41238
A	1146	ASP	ALA	engineered mutation	UNP P41238

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1173	ALA	LEU	engineered mutation	UNP P41238
A	1199	ALA	TRP	engineered mutation	UNP P41238
A	1205	ALA	PHE	engineered mutation	UNP P41238
B	1	MET	-	initiating methionine	UNP A0A4Z0THX4
B	313	VAL	ALA	engineered mutation	UNP A0A4Z0THX4
B	368	ASN	-	linker	UNP A0A4Z0THX4
B	369	SER	-	linker	UNP A0A4Z0THX4
B	370	SER	-	linker	UNP A0A4Z0THX4
B	371	SER	-	linker	UNP A0A4Z0THX4
B	1046	ALA	MET	engineered mutation	UNP P41238
B	1048	SER	ARG	engineered mutation	UNP P41238
B	1063	ALA	GLU	engineered mutation	UNP P41238
B	1080	THR	MET	engineered mutation	UNP P41238
B	1121	ALA	TRP	conflict	UNP P41238
B	1146	ASP	ALA	engineered mutation	UNP P41238
B	1173	ALA	LEU	engineered mutation	UNP P41238
B	1199	ALA	TRP	engineered mutation	UNP P41238
B	1205	ALA	PHE	engineered mutation	UNP P41238
C	1	MET	-	initiating methionine	UNP A0A4Z0THX4
C	313	VAL	ALA	engineered mutation	UNP A0A4Z0THX4
C	368	ASN	-	linker	UNP A0A4Z0THX4
C	369	SER	-	linker	UNP A0A4Z0THX4
C	370	SER	-	linker	UNP A0A4Z0THX4
C	371	SER	-	linker	UNP A0A4Z0THX4
C	1046	ALA	MET	engineered mutation	UNP P41238
C	1048	SER	ARG	engineered mutation	UNP P41238
C	1063	ALA	GLU	engineered mutation	UNP P41238
C	1080	THR	MET	engineered mutation	UNP P41238
C	1121	ALA	TRP	conflict	UNP P41238
C	1146	ASP	ALA	engineered mutation	UNP P41238
C	1173	ALA	LEU	engineered mutation	UNP P41238
C	1199	ALA	TRP	engineered mutation	UNP P41238
C	1205	ALA	PHE	engineered mutation	UNP P41238
D	1	MET	-	initiating methionine	UNP A0A4Z0THX4
D	313	VAL	ALA	engineered mutation	UNP A0A4Z0THX4
D	368	ASN	-	linker	UNP A0A4Z0THX4
D	369	SER	-	linker	UNP A0A4Z0THX4
D	370	SER	-	linker	UNP A0A4Z0THX4
D	371	SER	-	linker	UNP A0A4Z0THX4
D	1046	ALA	MET	engineered mutation	UNP P41238
D	1048	SER	ARG	engineered mutation	UNP P41238
D	1063	ALA	GLU	engineered mutation	UNP P41238

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1080	THR	MET	engineered mutation	UNP P41238
D	1121	ALA	TRP	conflict	UNP P41238
D	1146	ASP	ALA	engineered mutation	UNP P41238
D	1173	ALA	LEU	engineered mutation	UNP P41238
D	1199	ALA	TRP	engineered mutation	UNP P41238
D	1205	ALA	PHE	engineered mutation	UNP P41238
E	1	MET	-	initiating methionine	UNP A0A4Z0THX4
E	313	VAL	ALA	engineered mutation	UNP A0A4Z0THX4
E	368	ASN	-	linker	UNP A0A4Z0THX4
E	369	SER	-	linker	UNP A0A4Z0THX4
E	370	SER	-	linker	UNP A0A4Z0THX4
E	371	SER	-	linker	UNP A0A4Z0THX4
E	1046	ALA	MET	engineered mutation	UNP P41238
E	1048	SER	ARG	engineered mutation	UNP P41238
E	1063	ALA	GLU	engineered mutation	UNP P41238
E	1080	THR	MET	engineered mutation	UNP P41238
E	1121	ALA	TRP	conflict	UNP P41238
E	1146	ASP	ALA	engineered mutation	UNP P41238
E	1173	ALA	LEU	engineered mutation	UNP P41238
E	1199	ALA	TRP	engineered mutation	UNP P41238
E	1205	ALA	PHE	engineered mutation	UNP P41238
F	1	MET	-	initiating methionine	UNP A0A4Z0THX4
F	313	VAL	ALA	engineered mutation	UNP A0A4Z0THX4
F	368	ASN	-	linker	UNP A0A4Z0THX4
F	369	SER	-	linker	UNP A0A4Z0THX4
F	370	SER	-	linker	UNP A0A4Z0THX4
F	371	SER	-	linker	UNP A0A4Z0THX4
F	1046	ALA	MET	engineered mutation	UNP P41238
F	1048	SER	ARG	engineered mutation	UNP P41238
F	1063	ALA	GLU	engineered mutation	UNP P41238
F	1080	THR	MET	engineered mutation	UNP P41238
F	1121	ALA	TRP	conflict	UNP P41238
F	1146	ASP	ALA	engineered mutation	UNP P41238
F	1173	ALA	LEU	engineered mutation	UNP P41238
F	1199	ALA	TRP	engineered mutation	UNP P41238
F	1205	ALA	PHE	engineered mutation	UNP P41238
G	1	MET	-	initiating methionine	UNP A0A4Z0THX4
G	313	VAL	ALA	engineered mutation	UNP A0A4Z0THX4
G	368	ASN	-	linker	UNP A0A4Z0THX4
G	369	SER	-	linker	UNP A0A4Z0THX4
G	370	SER	-	linker	UNP A0A4Z0THX4
G	371	SER	-	linker	UNP A0A4Z0THX4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1046	ALA	MET	engineered mutation	UNP P41238
G	1048	SER	ARG	engineered mutation	UNP P41238
G	1063	ALA	GLU	engineered mutation	UNP P41238
G	1080	THR	MET	engineered mutation	UNP P41238
G	1121	ALA	TRP	conflict	UNP P41238
G	1146	ASP	ALA	engineered mutation	UNP P41238
G	1173	ALA	LEU	engineered mutation	UNP P41238
G	1199	ALA	TRP	engineered mutation	UNP P41238
G	1205	ALA	PHE	engineered mutation	UNP P41238
H	1	MET	-	initiating methionine	UNP A0A4Z0THX4
H	313	VAL	ALA	engineered mutation	UNP A0A4Z0THX4
H	368	ASN	-	linker	UNP A0A4Z0THX4
H	369	SER	-	linker	UNP A0A4Z0THX4
H	370	SER	-	linker	UNP A0A4Z0THX4
H	371	SER	-	linker	UNP A0A4Z0THX4
H	1046	ALA	MET	engineered mutation	UNP P41238
H	1048	SER	ARG	engineered mutation	UNP P41238
H	1063	ALA	GLU	engineered mutation	UNP P41238
H	1080	THR	MET	engineered mutation	UNP P41238
H	1121	ALA	TRP	conflict	UNP P41238
H	1146	ASP	ALA	engineered mutation	UNP P41238
H	1173	ALA	LEU	engineered mutation	UNP P41238
H	1199	ALA	TRP	engineered mutation	UNP P41238
H	1205	ALA	PHE	engineered mutation	UNP P41238

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	I	2	Total	C	O	0	0	0
			23	12	11			
2	J	2	Total	C	O	0	0	0
			23	12	11			
2	K	2	Total	C	O	0	0	0
			23	12	11			
2	L	2	Total	C	O	0	0	0
			23	12	11			
2	M	2	Total	C	O	0	0	0
			23	12	11			

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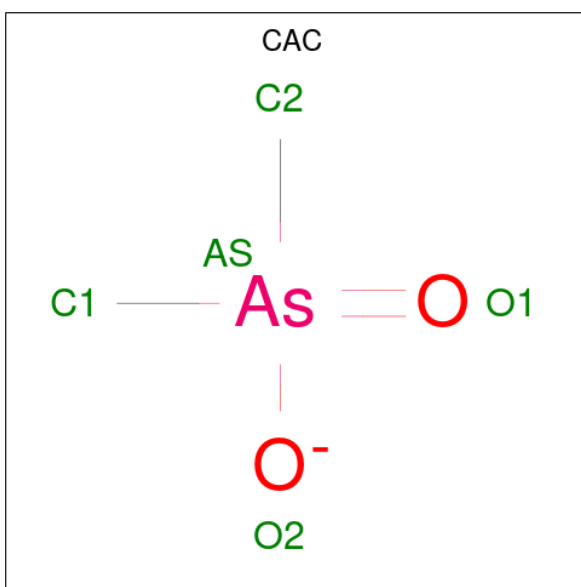
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	N	2	Total	C	O	0	0	0
			23	12	11			
2	O	2	Total	C	O	0	0	0
			23	12	11			
2	P	2	Total	C	O	0	0	0
			23	12	11			
2	Q	2	Total	C	O	0	0	0
			23	12	11			
2	R	2	Total	C	O	0	0	0
			23	12	11			
2	S	2	Total	C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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		
3	G	1	Total	Zn	0	0
			1	1		
3	H	1	Total	Zn	0	0
			1	1		

- Molecule 4 is CACODYLATE ION (CCD ID: CAC) (formula: C₂H₆AsO₂).

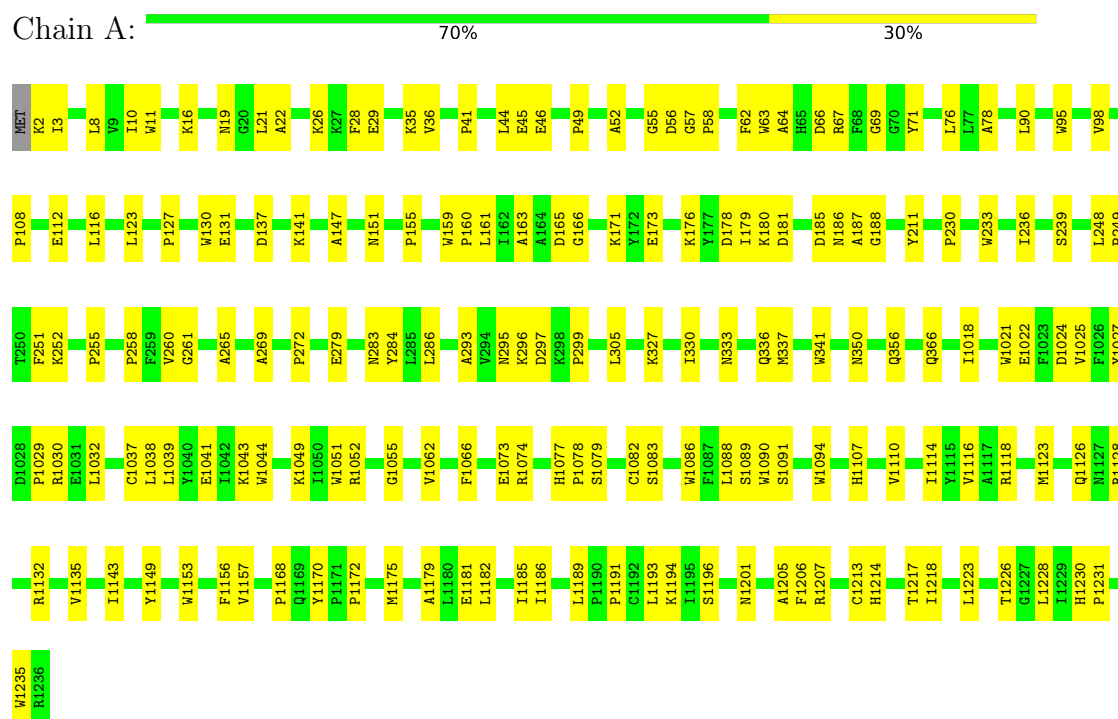


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		
4	C	1	Total	As	C	O	0	0
			5	1	2	2		
4	D	1	Total	As	C	O	0	0
			5	1	2	2		
4	E	1	Total	As	C	O	0	0
			5	1	2	2		
4	F	1	Total	As	C	O	0	0
			5	1	2	2		
4	G	1	Total	As	C	O	0	0
			5	1	2	2		
4	H	1	Total	As	C	O	0	0
			5	1	2	2		

3 Residue-property plots

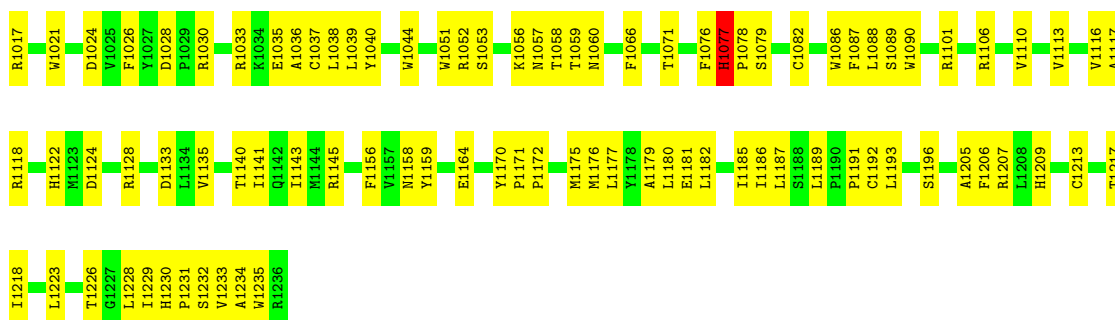
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Maltodextrin-binding protein, C->U-editing enzyme APOBEC-1 chimera



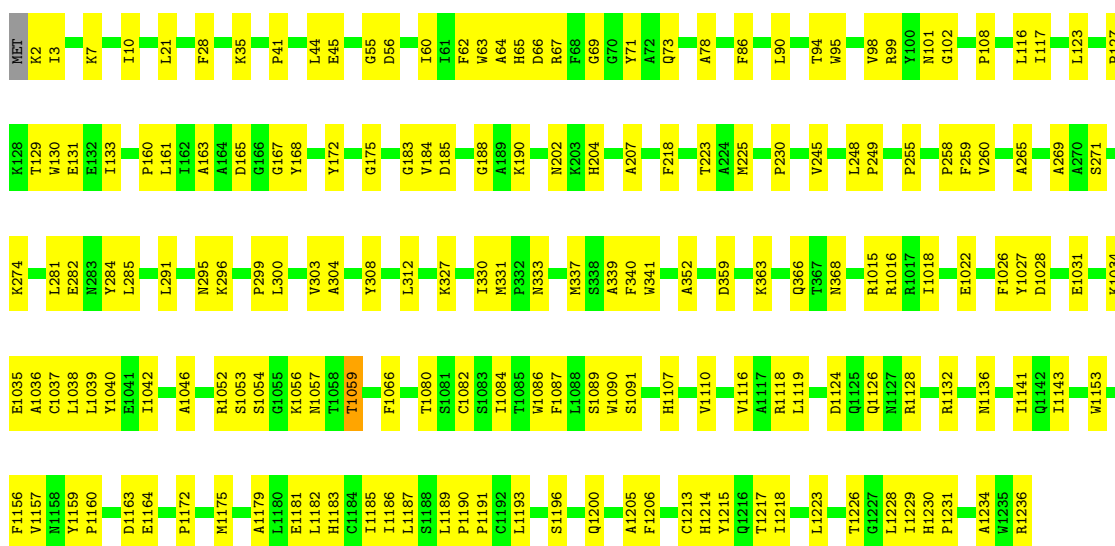
- Molecule 1: Maltodextrin-binding protein, C->U-editing enzyme APOBEC-1 chimera





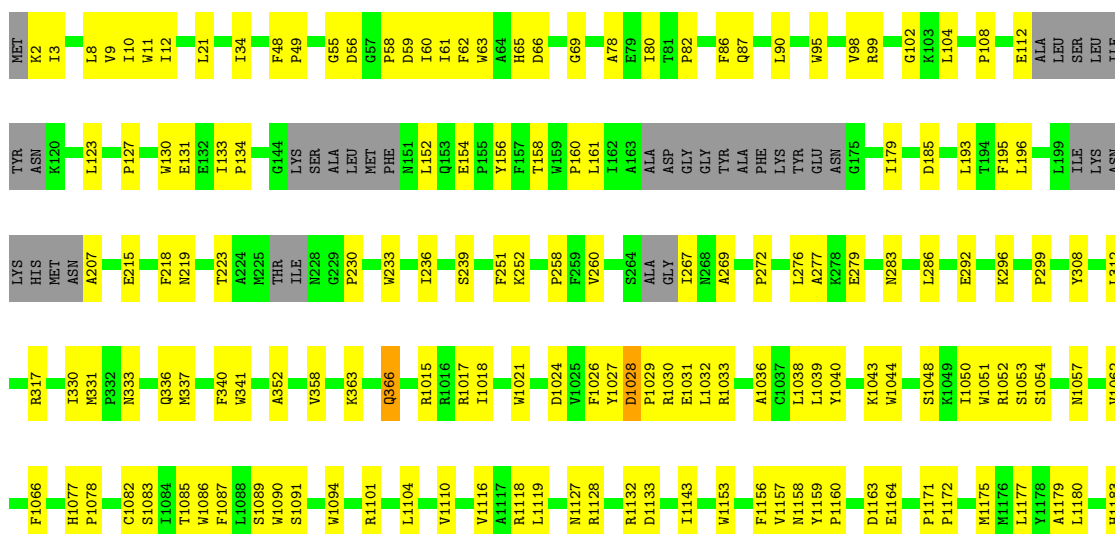
- Molecule 1: Maltodextrin-binding protein, C->U-editing enzyme APOBEC-1 chimera

Chain C: 70% 30%



- Molecule 1: Maltodextrin-binding protein, C->U-editing enzyme APOBEC-1 chimera

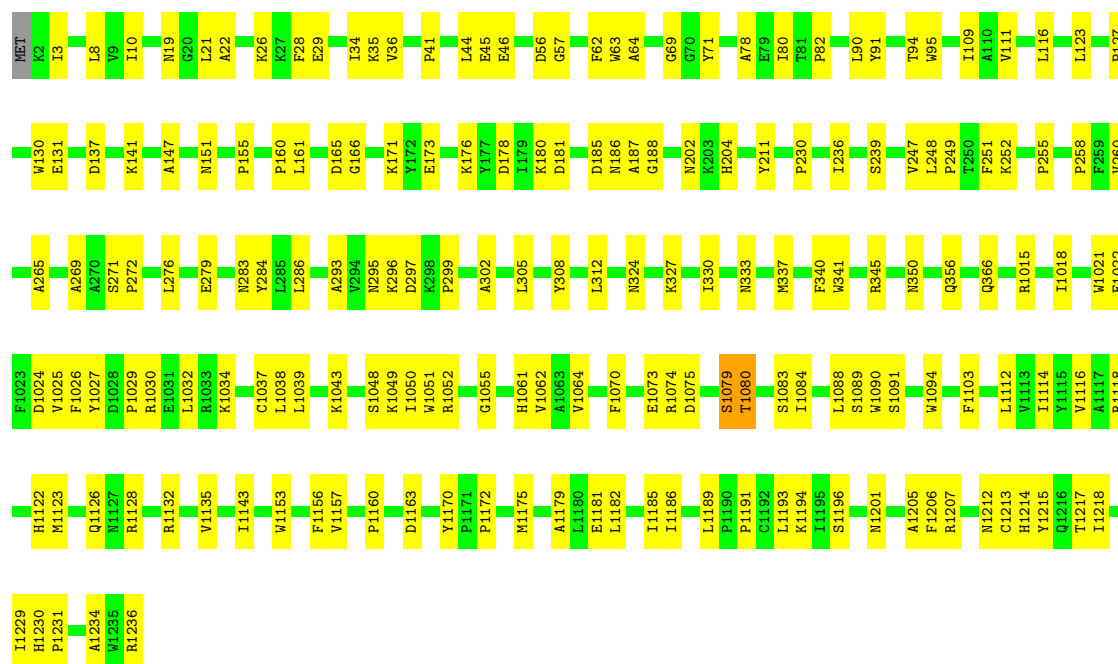
Chain D: 63% 30% 6%





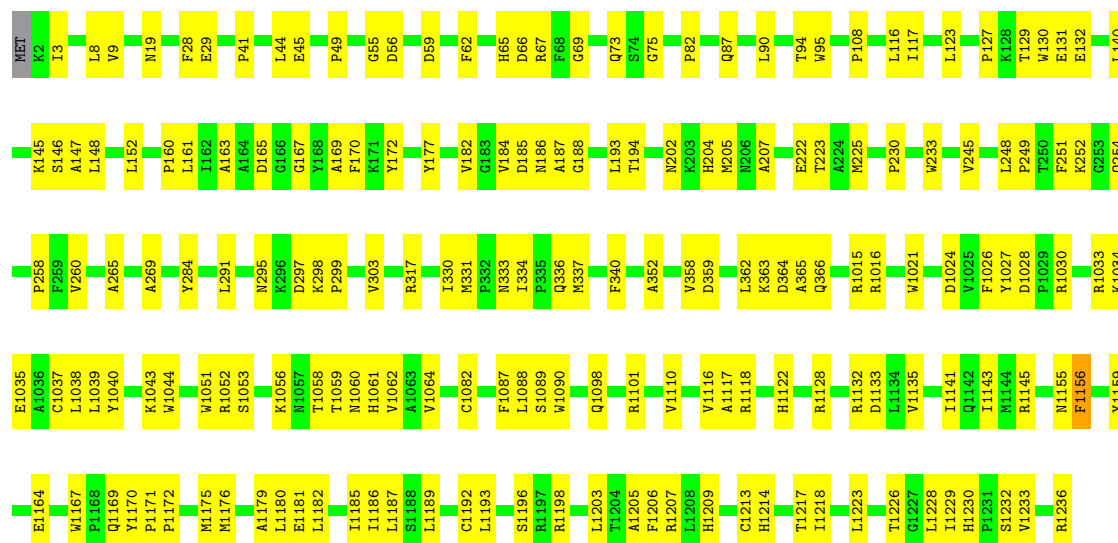
- Molecule 1: Maltodextrin-binding protein, C->U-editing enzyme APOBEC-1 chimera

Chain E: 69% 30%



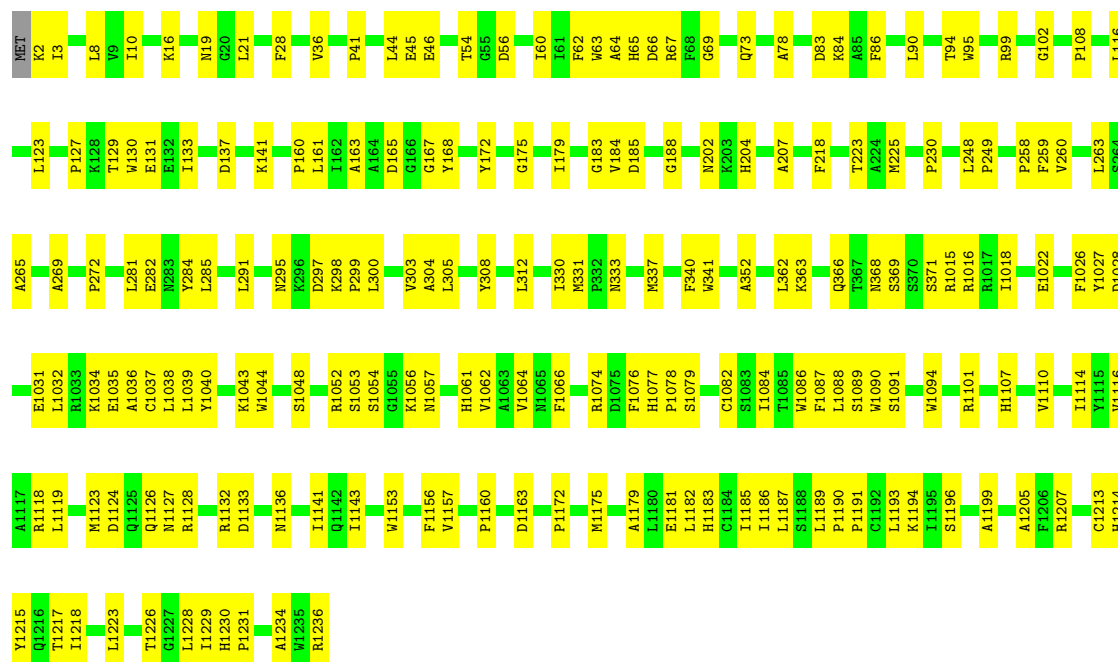
- Molecule 1: Maltodextrin-binding protein, C->U-editing enzyme APOBEC-1 chimera

Chain F: 69% 31%



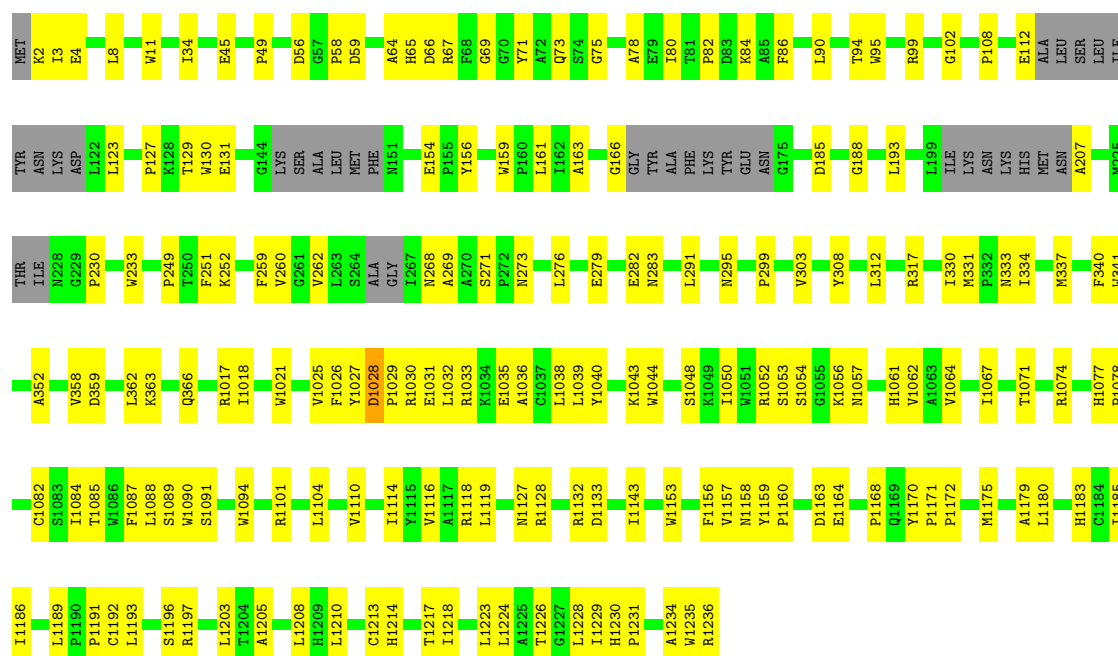
- Molecule 1: Maltodextrin-binding protein, C->U-editing enzyme APOBEC-1 chimera

Chain G: 67% 33%



- Molecule 1: Maltodextrin-binding protein, C->U-editing enzyme APOBEC-1 chimera

Chain H: 64% 30% 6%



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain I: 50% 50%



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain J:  50% 50%

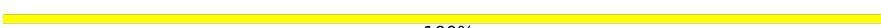
GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain K:  100%

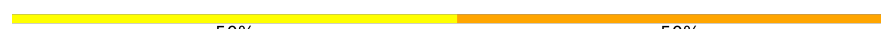
GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain L:  100%

GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain M:  50% 50%

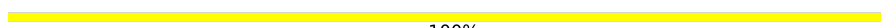
GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain N:  100%

GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain O:  100%

GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain P:  50% 50%

GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain Q:  100%

GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain R:  100%GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain S:  100%GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain T:  100%GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain U:  100%GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain V:  100%GLC1
GLC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	177.72Å 179.21Å 210.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.61 – 3.51 49.61 – 3.51	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.61-3.51) 90.1 (49.61-3.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.83 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.276 , 0.298 0.277 , 0.295	Depositor DCC
R_{free} test set	8334 reflections (9.83%)	wwPDB-VP
Wilson B-factor (Å ²)	84.6	Xtriage
Anisotropy	0.720	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 122.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.289 for k,h,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	37624	wwPDB-VP
Average B, all atoms (Å ²)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, CAC, ZN

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	0.20	0/4860	0.52	1/6609 (0.0%)
1	B	0.20	0/4860	0.54	2/6609 (0.0%)
1	C	0.22	0/4860	0.54	0/6609
1	D	0.20	0/4575	0.50	0/6217
1	E	0.19	0/4860	0.51	0/6609
1	F	0.21	0/4860	0.54	0/6609
1	G	0.21	0/4860	0.53	0/6609
1	H	0.19	0/4575	0.51	1/6218 (0.0%)
All	All	0.20	0/38310	0.53	4/52089 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1077	HIS	CA-C-N	-6.57	111.63	119.84
1	B	1077	HIS	C-N-CA	-6.57	111.63	119.84
1	A	1079	SER	N-CA-C	5.41	122.32	110.80
1	H	1028	ASP	N-CA-C	5.34	121.62	109.81

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4725	0	4643	150	0
1	B	4725	0	4643	151	0
1	C	4725	0	4643	131	0
1	D	4452	0	4364	138	0
1	E	4725	0	4643	137	0
1	F	4725	0	4643	155	0
1	G	4725	0	4643	137	0
1	H	4452	0	4359	148	0
2	I	23	0	20	2	0
2	J	23	0	20	1	0
2	K	23	0	20	3	0
2	L	23	0	21	0	0
2	M	23	0	20	9	0
2	N	23	0	20	6	0
2	O	23	0	20	0	0
2	P	23	0	20	1	0
2	Q	23	0	20	0	0
2	R	23	0	20	3	0
2	S	23	0	20	2	0
2	T	23	0	21	2	0
2	U	23	0	20	6	0
2	V	23	0	20	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	1	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
All	All	37624	0	36863	1110	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 15.

The worst 5 of 1110 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:C:1034:LYS:HG3	2:M:1:GLC:H1	1.27	1.15
1:B:1077:HIS:HB3	1:B:1078:PRO:HD2	1.38	1.05
1:G:168:TYR:HB2	1:G:183:GLY:HA3	1.46	0.97
1:B:1033:ARG:HD2	2:K:2:GLC:H3	1.46	0.95
1:B:1159:TYR:HE2	1:B:1164:GLU:HG2	1.28	0.94

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	590/593 (100%)	560 (95%)	30 (5%)	0	100	100
1	B	590/593 (100%)	558 (95%)	29 (5%)	3 (0%)	24	58
1	C	590/593 (100%)	563 (95%)	26 (4%)	1 (0%)	43	74
1	D	543/593 (92%)	518 (95%)	25 (5%)	0	100	100
1	E	590/593 (100%)	566 (96%)	22 (4%)	2 (0%)	36	66
1	F	590/593 (100%)	561 (95%)	28 (5%)	1 (0%)	43	74
1	G	590/593 (100%)	560 (95%)	29 (5%)	1 (0%)	43	74
1	H	544/593 (92%)	522 (96%)	21 (4%)	1 (0%)	43	74
All	All	4627/4744 (98%)	4408 (95%)	210 (4%)	9 (0%)	43	74

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1077	HIS
1	E	1080	THR
1	B	1059	THR
1	F	1059	THR

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Mol	Chain	Res	Type
1	G	84	LYS

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	500/501 (100%)	500 (100%)	0	100	100
1	B	500/501 (100%)	499 (100%)	1 (0%)	87	85
1	C	500/501 (100%)	500 (100%)	0	100	100
1	D	473/501 (94%)	471 (100%)	2 (0%)	84	82
1	E	500/501 (100%)	500 (100%)	0	100	100
1	F	500/501 (100%)	499 (100%)	1 (0%)	87	85
1	G	500/501 (100%)	500 (100%)	0	100	100
1	H	472/501 (94%)	472 (100%)	0	100	100
All	All	3945/4008 (98%)	3941 (100%)	4 (0%)	88	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1077	HIS
1	D	366	GLN
1	D	1028	ASP
1	F	1156	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	119	ASN
1	H	73	GLN
1	E	1212	ASN
1	H	1129	GLN
1	G	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 ⓘ

28 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	GLC	I	1	2	12,12,12	1.18	1 (8%)	17,17,17	0.78	0
2	GLC	I	2	2	11,11,12	1.80	3 (27%)	15,15,17	1.30	2 (13%)
2	GLC	J	1	2	12,12,12	1.13	1 (8%)	17,17,17	0.94	0
2	GLC	J	2	2	11,11,12	1.46	2 (18%)	15,15,17	1.54	2 (13%)
2	GLC	K	1	2	12,12,12	1.25	1 (8%)	17,17,17	1.76	6 (35%)
2	GLC	K	2	2	11,11,12	1.45	2 (18%)	15,15,17	1.68	3 (20%)
2	GLC	L	1	2	12,12,12	1.05	1 (8%)	17,17,17	1.48	3 (17%)
2	GLC	L	2	2	11,11,12	1.62	3 (27%)	15,15,17	0.63	0
2	GLC	M	1	2	12,12,12	1.12	1 (8%)	17,17,17	1.12	1 (5%)
2	GLC	M	2	2	11,11,12	1.53	3 (27%)	15,15,17	1.04	0
2	GLC	N	1	2	12,12,12	1.19	1 (8%)	17,17,17	1.75	3 (17%)
2	GLC	N	2	2	11,11,12	1.60	3 (27%)	15,15,17	0.98	1 (6%)
2	GLC	O	1	2	12,12,12	1.05	1 (8%)	17,17,17	1.39	3 (17%)
2	GLC	O	2	2	11,11,12	1.62	3 (27%)	15,15,17	1.51	1 (6%)
2	GLC	P	1	2	12,12,12	1.13	1 (8%)	17,17,17	0.98	1 (5%)
2	GLC	P	2	2	11,11,12	1.68	3 (27%)	15,15,17	0.90	0
2	GLC	Q	1	2	12,12,12	1.30	1 (8%)	17,17,17	1.07	1 (5%)
2	GLC	Q	2	2	11,11,12	1.58	3 (27%)	15,15,17	1.12	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	R	1	2	12,12,12	1.06	1 (8%)	17,17,17	1.33	2 (11%)
2	GLC	R	2	2	11,11,12	1.74	3 (27%)	15,15,17	1.60	3 (20%)
2	GLC	S	1	2	12,12,12	1.20	1 (8%)	17,17,17	0.84	0
2	GLC	S	2	2	11,11,12	1.71	3 (27%)	15,15,17	1.22	1 (6%)
2	GLC	T	1	2	12,12,12	1.18	1 (8%)	17,17,17	1.18	3 (17%)
2	GLC	T	2	2	11,11,12	1.50	3 (27%)	15,15,17	0.93	1 (6%)
2	GLC	U	1	2	12,12,12	0.97	1 (8%)	17,17,17	2.88	8 (47%)
2	GLC	U	2	2	11,11,12	1.75	3 (27%)	15,15,17	1.83	4 (26%)
2	GLC	V	1	2	12,12,12	1.13	1 (8%)	17,17,17	0.80	0
2	GLC	V	2	2	11,11,12	1.77	3 (27%)	15,15,17	1.61	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	I	1	2	-	2/2/22/22	0/1/1/1
2	GLC	I	2	2	-	2/2/19/22	0/1/1/1
2	GLC	J	1	2	-	0/2/22/22	0/1/1/1
2	GLC	J	2	2	-	1/2/19/22	0/1/1/1
2	GLC	K	1	2	-	2/2/22/22	0/1/1/1
2	GLC	K	2	2	-	1/2/19/22	0/1/1/1
2	GLC	L	1	2	-	0/2/22/22	0/1/1/1
2	GLC	L	2	2	-	1/2/19/22	0/1/1/1
2	GLC	M	1	2	-	0/2/22/22	0/1/1/1
2	GLC	M	2	2	-	1/2/19/22	0/1/1/1
2	GLC	N	1	2	-	2/2/22/22	0/1/1/1
2	GLC	N	2	2	-	2/2/19/22	0/1/1/1
2	GLC	O	1	2	-	0/2/22/22	0/1/1/1
2	GLC	O	2	2	-	0/2/19/22	0/1/1/1
2	GLC	P	1	2	-	0/2/22/22	0/1/1/1
2	GLC	P	2	2	-	0/2/19/22	0/1/1/1
2	GLC	Q	1	2	-	0/2/22/22	0/1/1/1
2	GLC	Q	2	2	-	0/2/19/22	0/1/1/1
2	GLC	R	1	2	-	2/2/22/22	0/1/1/1
2	GLC	R	2	2	-	2/2/19/22	0/1/1/1
2	GLC	S	1	2	-	1/2/22/22	0/1/1/1
2	GLC	S	2	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	T	1	2	-	2/2/22/22	0/1/1/1
2	GLC	T	2	2	-	2/2/19/22	0/1/1/1
2	GLC	U	1	2	-	2/2/22/22	0/1/1/1
2	GLC	U	2	2	-	2/2/19/22	0/1/1/1
2	GLC	V	1	2	-	0/2/22/22	0/1/1/1
2	GLC	V	2	2	-	1/2/19/22	0/1/1/1

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	2	GLC	O5-C1	4.29	1.50	1.43
2	R	2	GLC	O5-C1	4.00	1.50	1.43
2	U	2	GLC	O5-C1	3.94	1.50	1.43
2	S	2	GLC	O5-C1	3.90	1.50	1.43
2	O	2	GLC	O5-C1	3.78	1.50	1.43

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	1	GLC	O5-C5-C4	-6.66	97.70	109.70
2	U	1	GLC	O4-C4-C5	-5.17	96.59	109.32
2	U	1	GLC	C4-C3-C2	4.88	119.39	110.83
2	O	2	GLC	C1-C2-C3	4.87	116.73	109.64
2	U	2	GLC	O2-C2-C1	-4.23	99.53	109.22

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	2	GLC	C4-C5-C6-O6
2	T	2	GLC	C4-C5-C6-O6
2	U	2	GLC	O5-C5-C6-O6
2	I	2	GLC	O5-C5-C6-O6
2	T	1	GLC	C4-C5-C6-O6

There are no ring outliers.

18 monomers are involved in 39 short contacts:

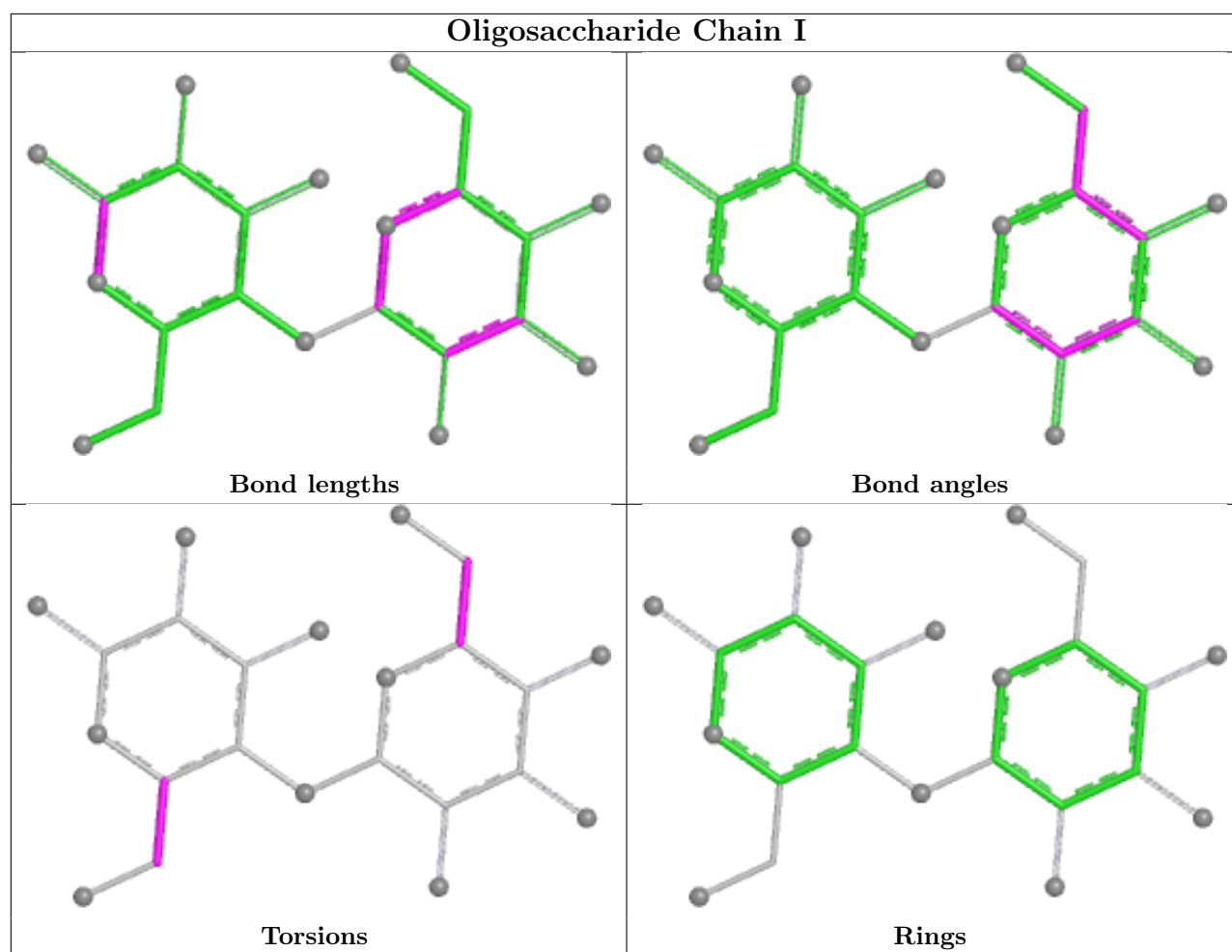
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	2	GLC	2	0

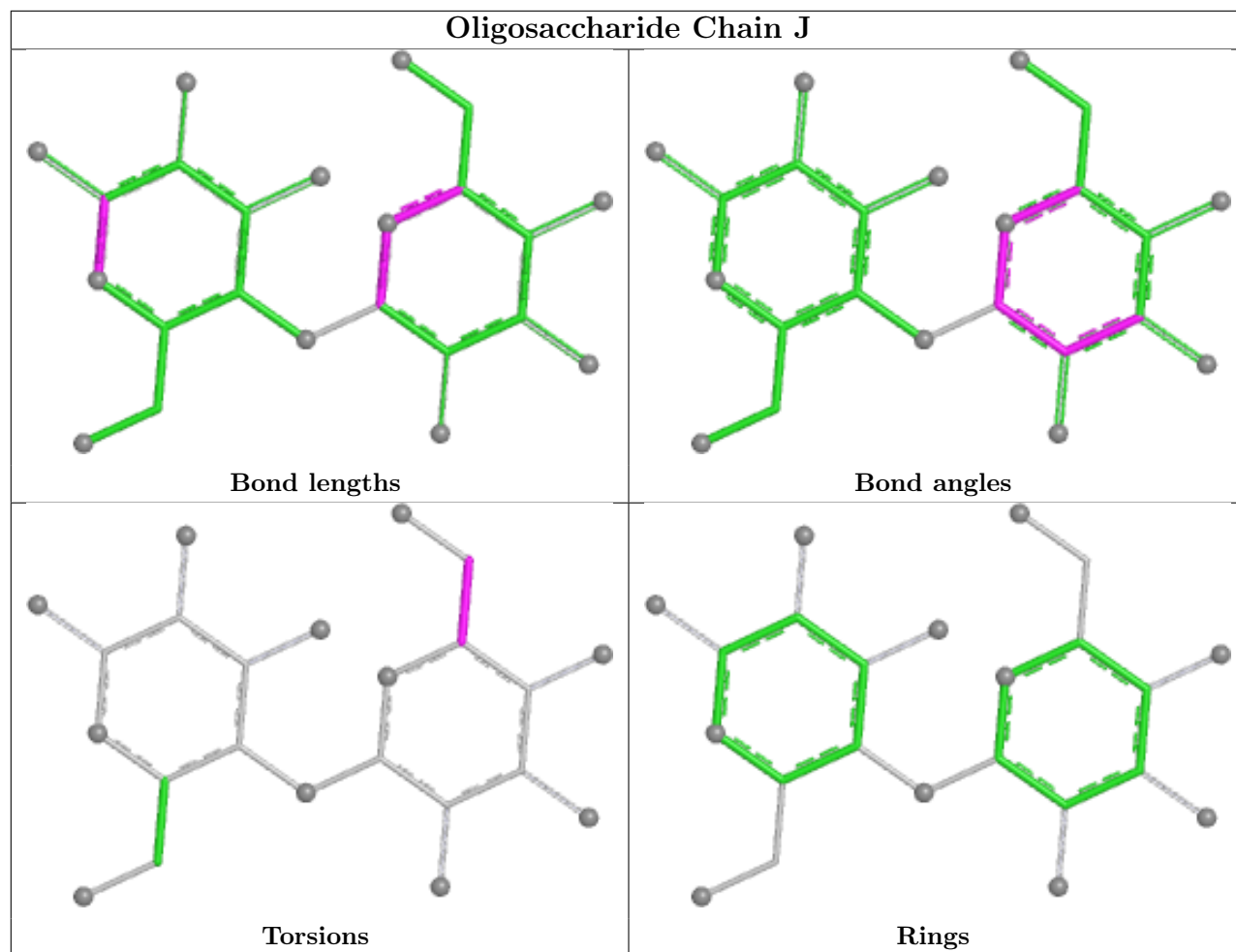
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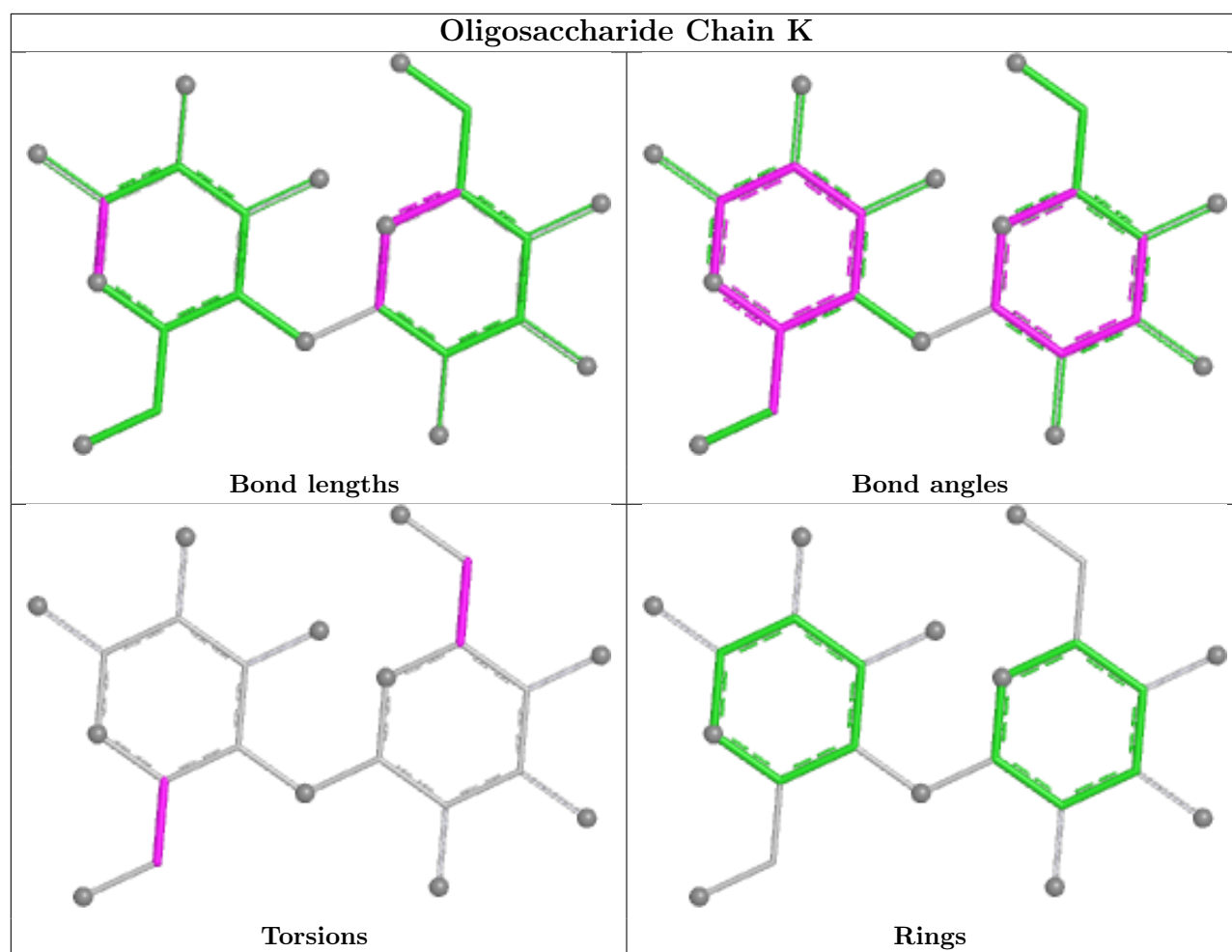
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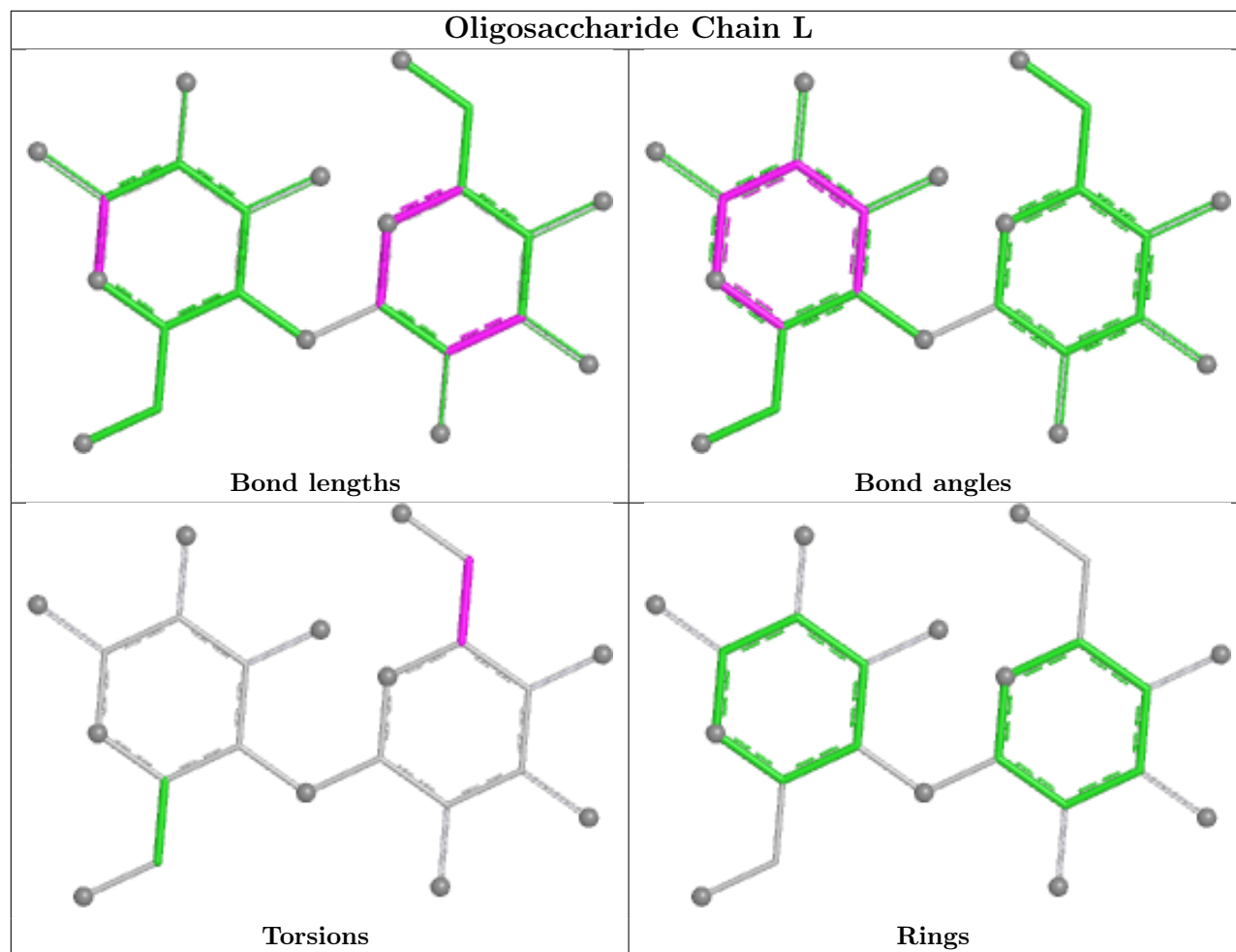
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	2	GLC	1	0
2	M	1	GLC	9	0
2	U	1	GLC	4	0
2	T	2	GLC	1	0
2	V	2	GLC	1	0
2	S	1	GLC	1	0
2	K	2	GLC	2	0
2	N	2	GLC	5	0
2	S	2	GLC	2	0
2	U	2	GLC	4	0
2	T	1	GLC	1	0
2	J	2	GLC	1	0
2	V	1	GLC	4	0
2	P	2	GLC	1	0
2	K	1	GLC	1	0
2	N	1	GLC	1	0
2	R	1	GLC	2	0

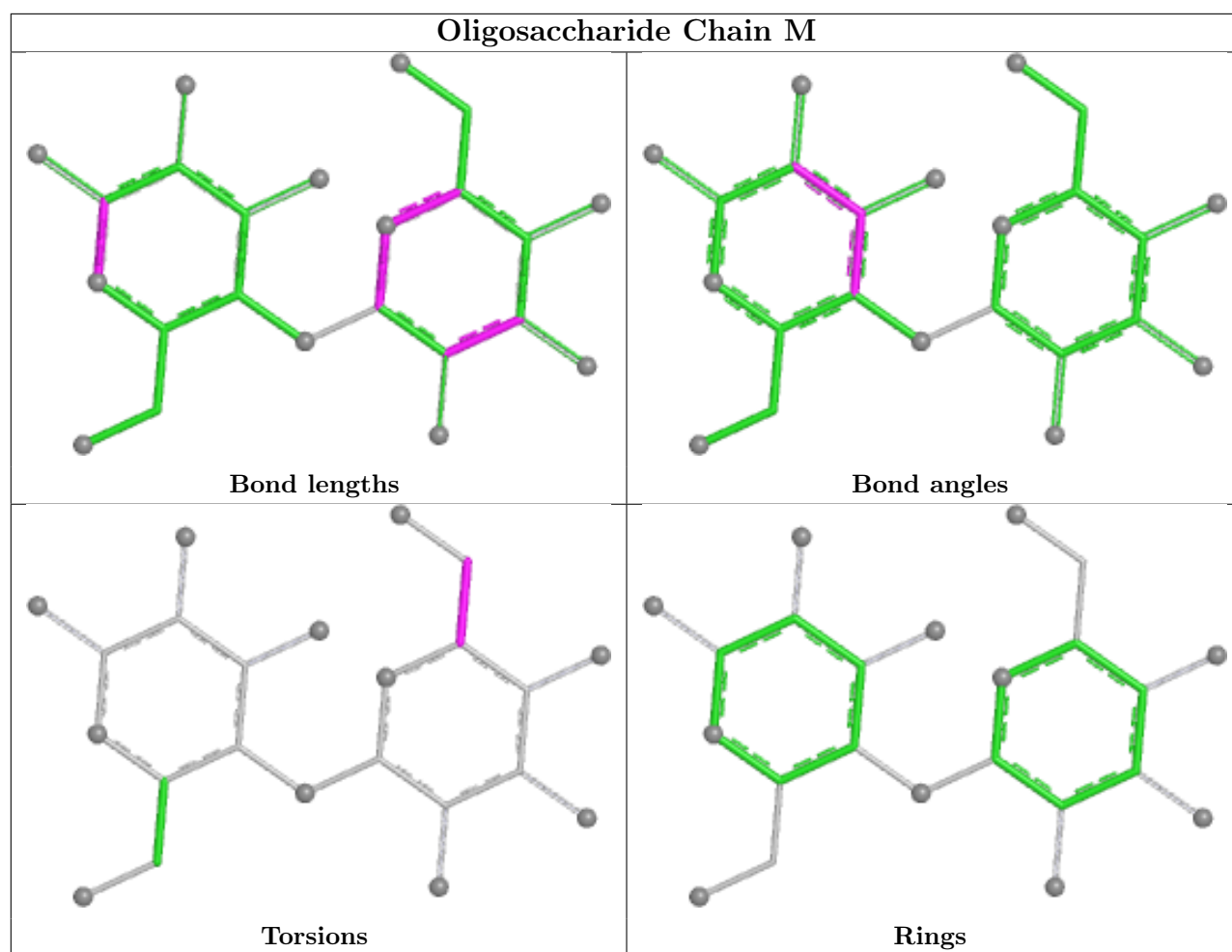
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

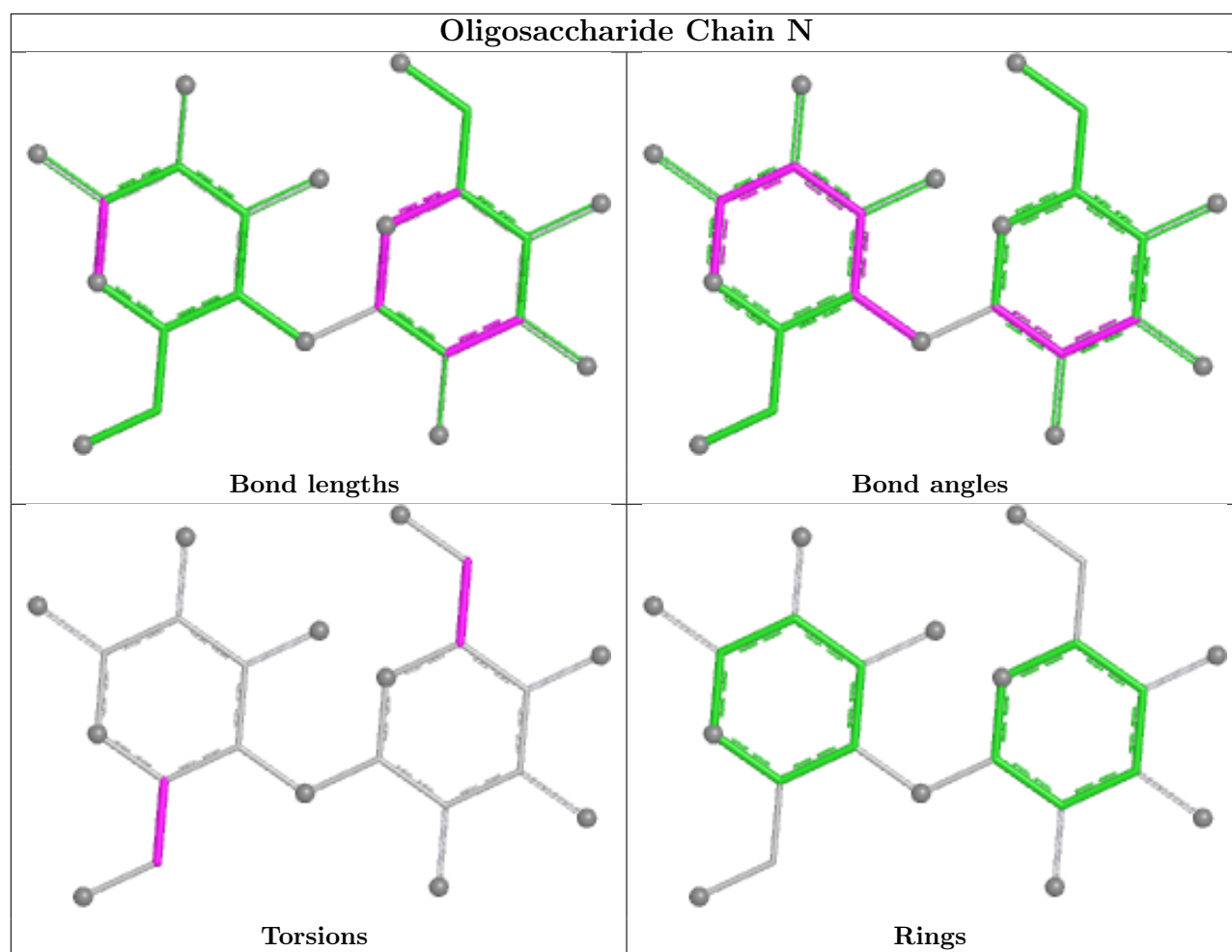


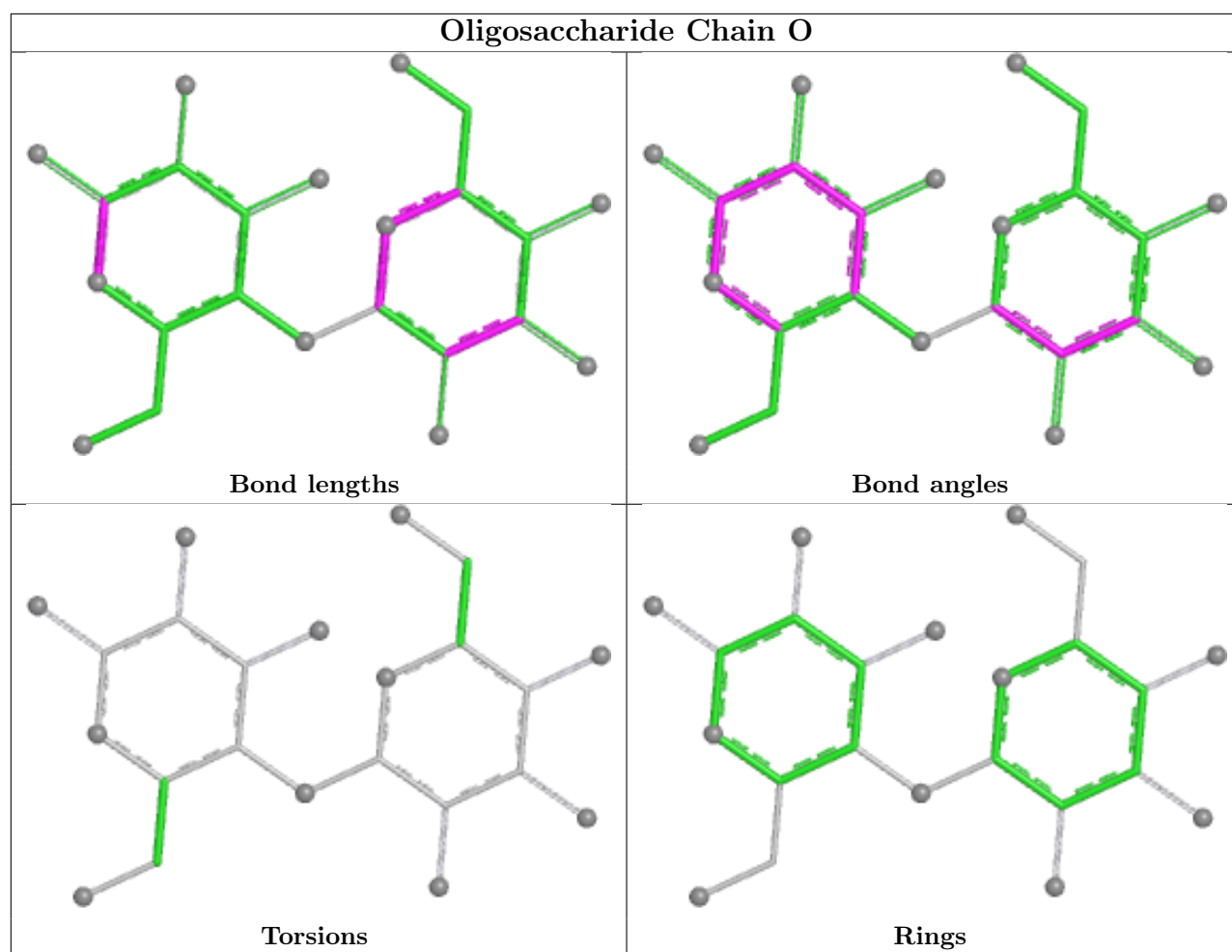


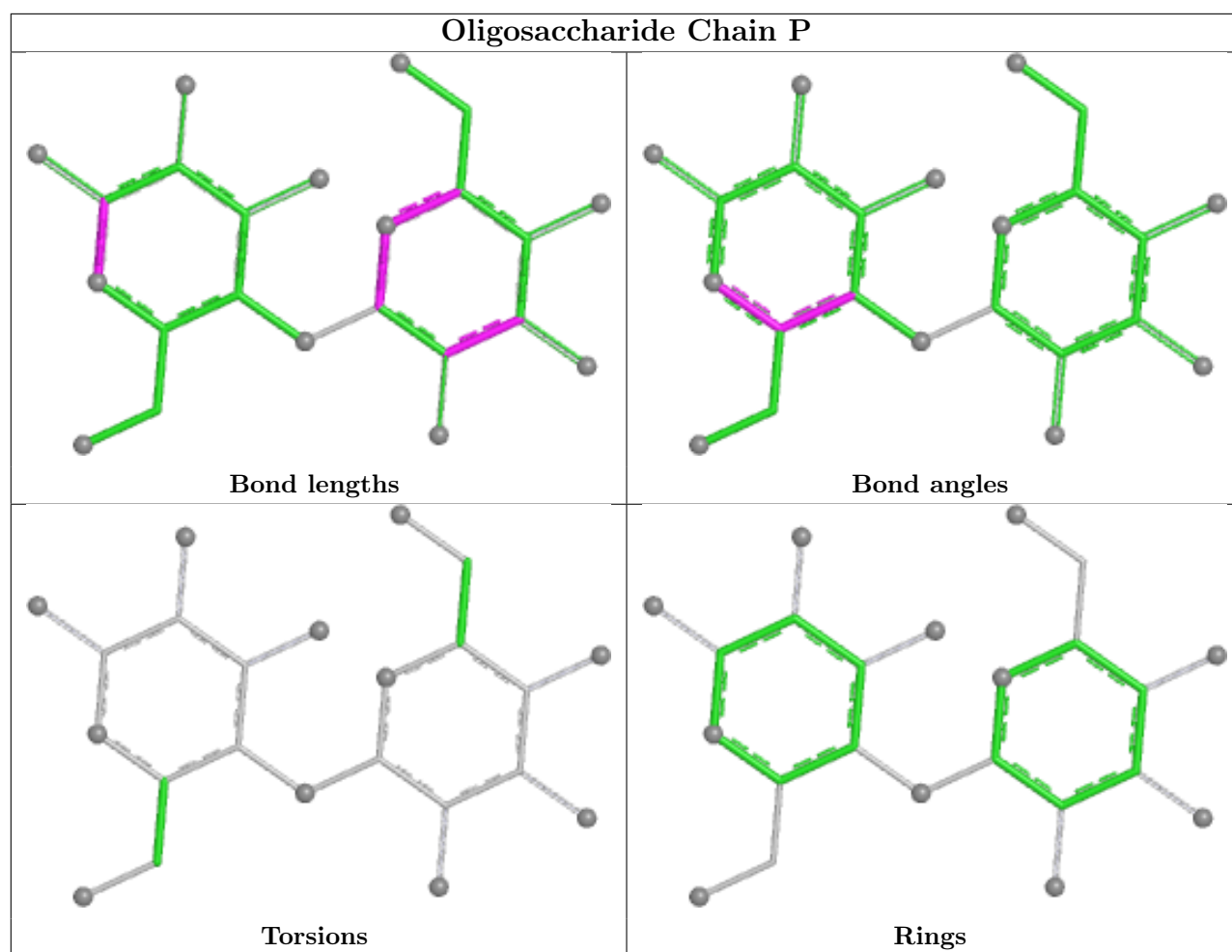


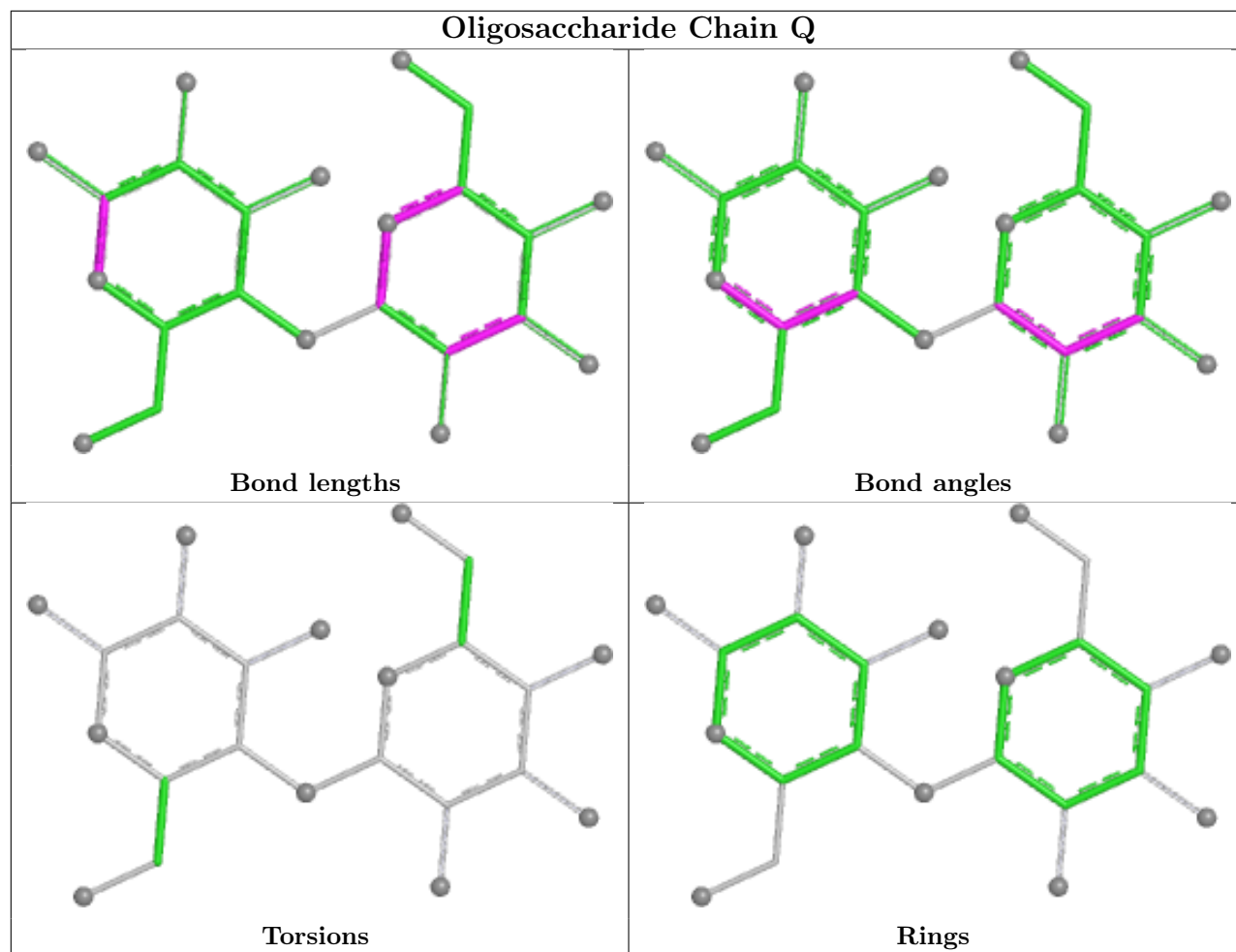


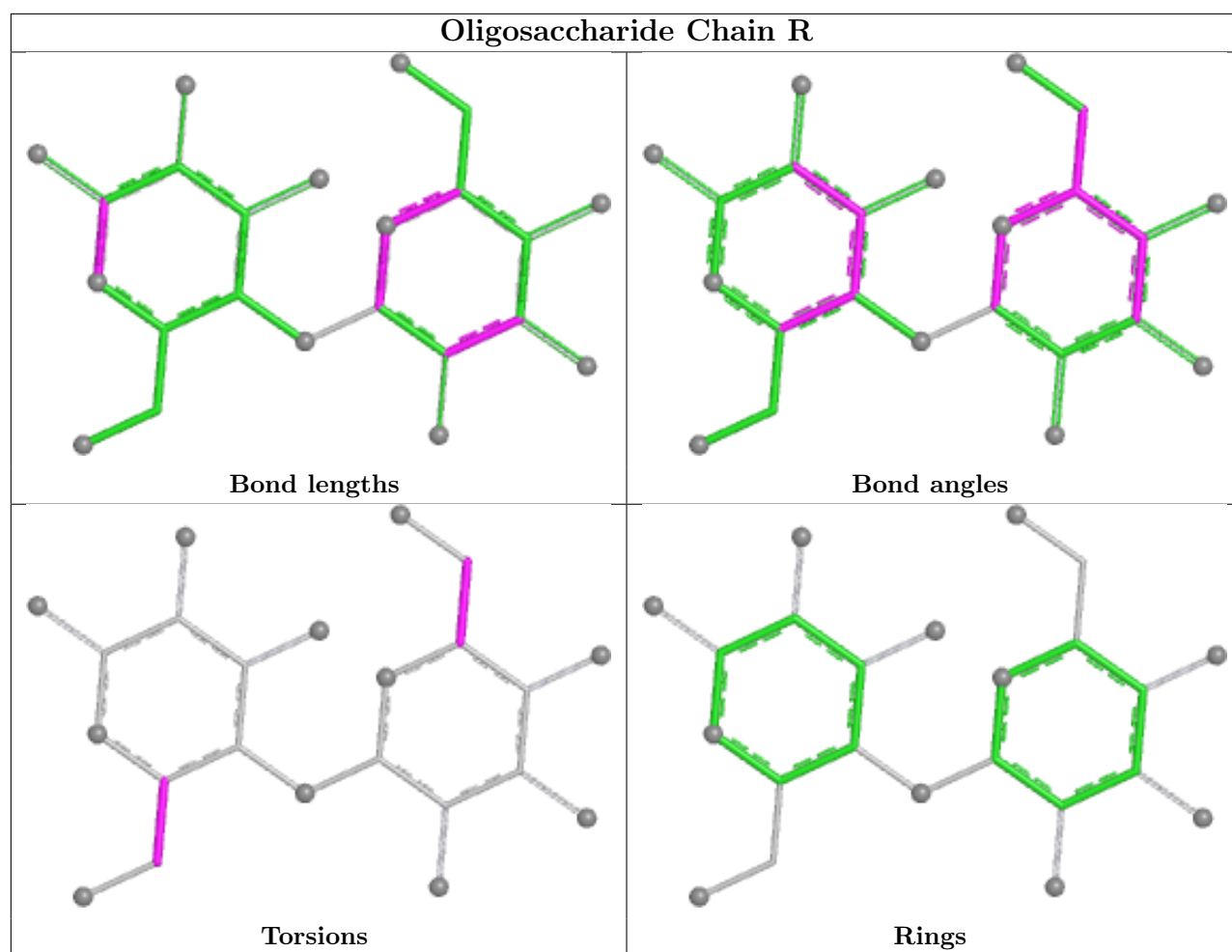


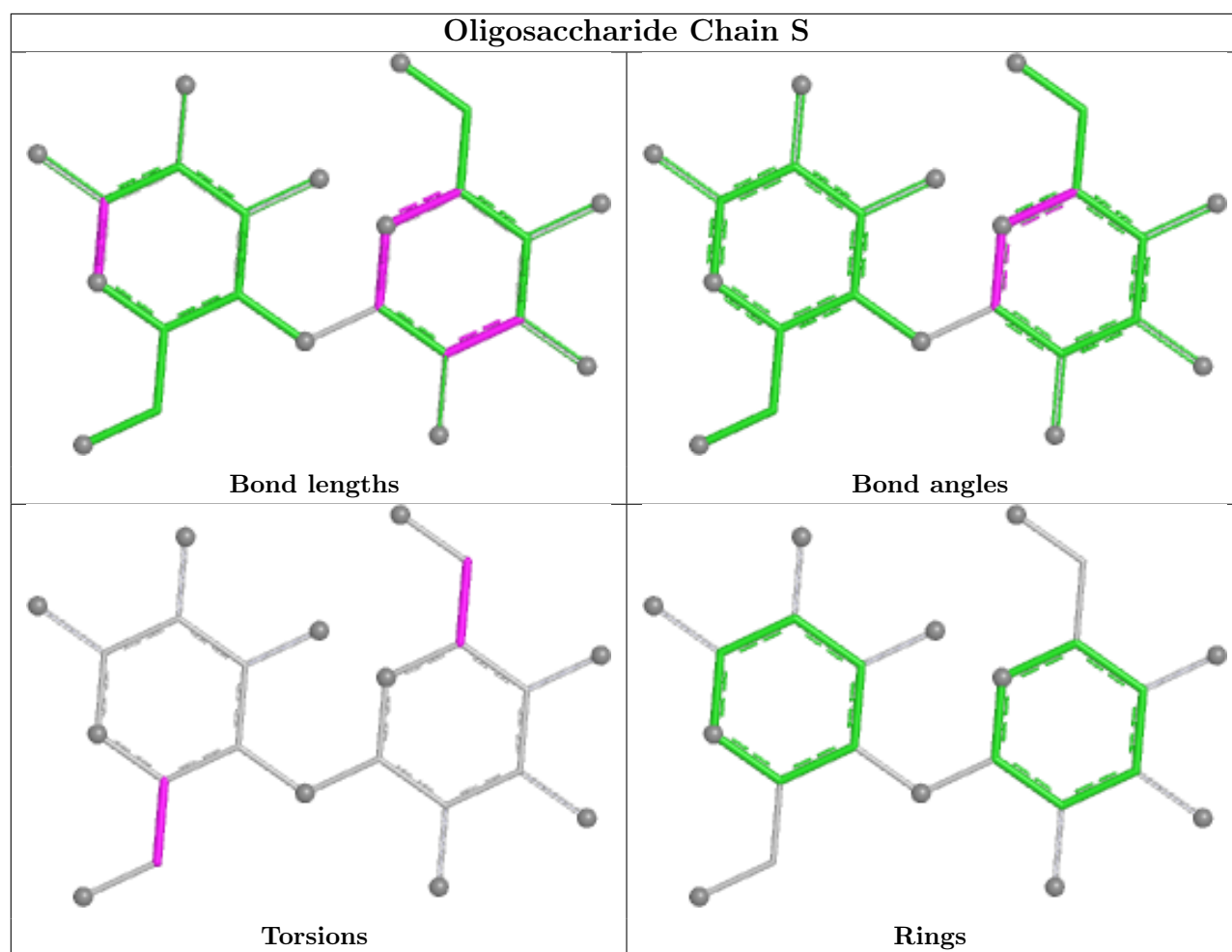


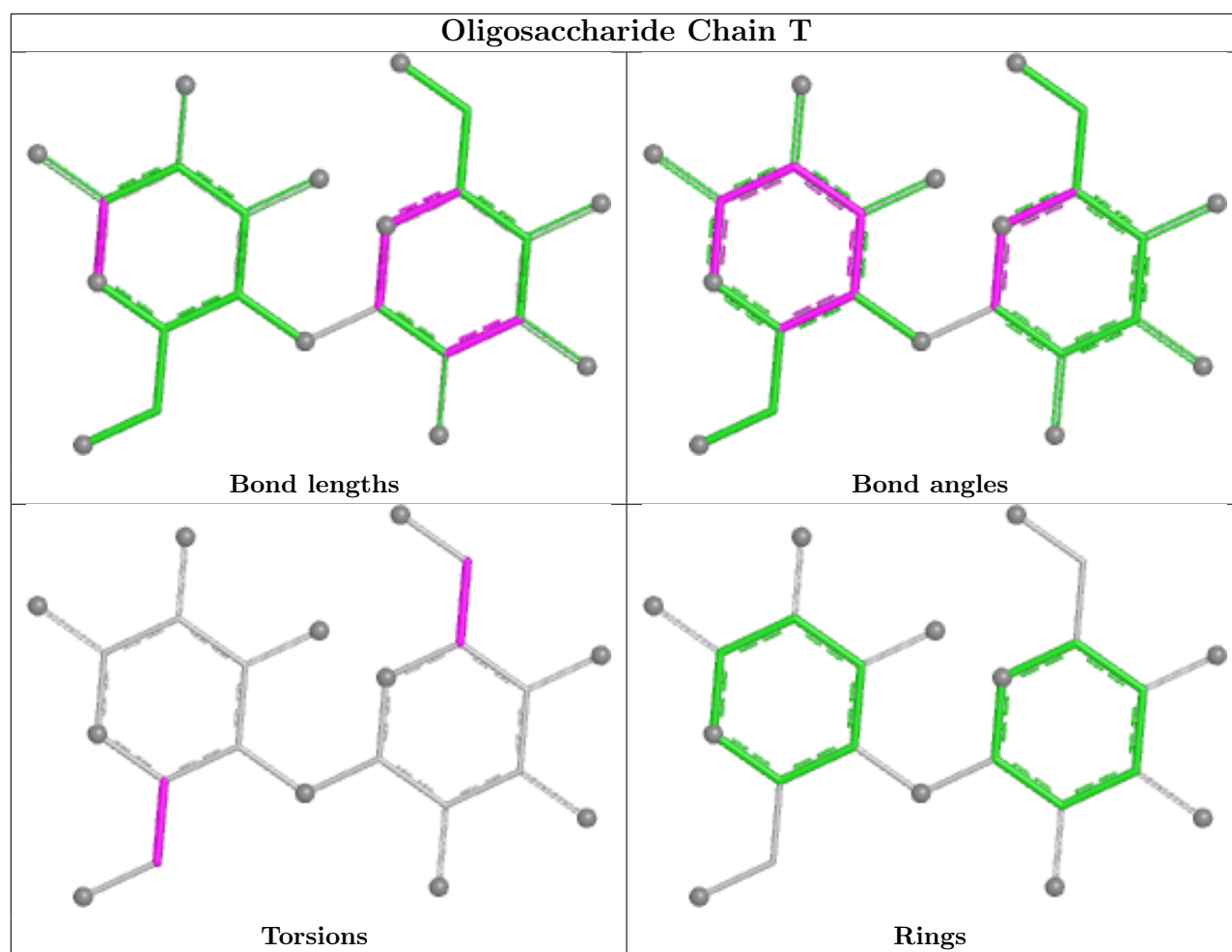


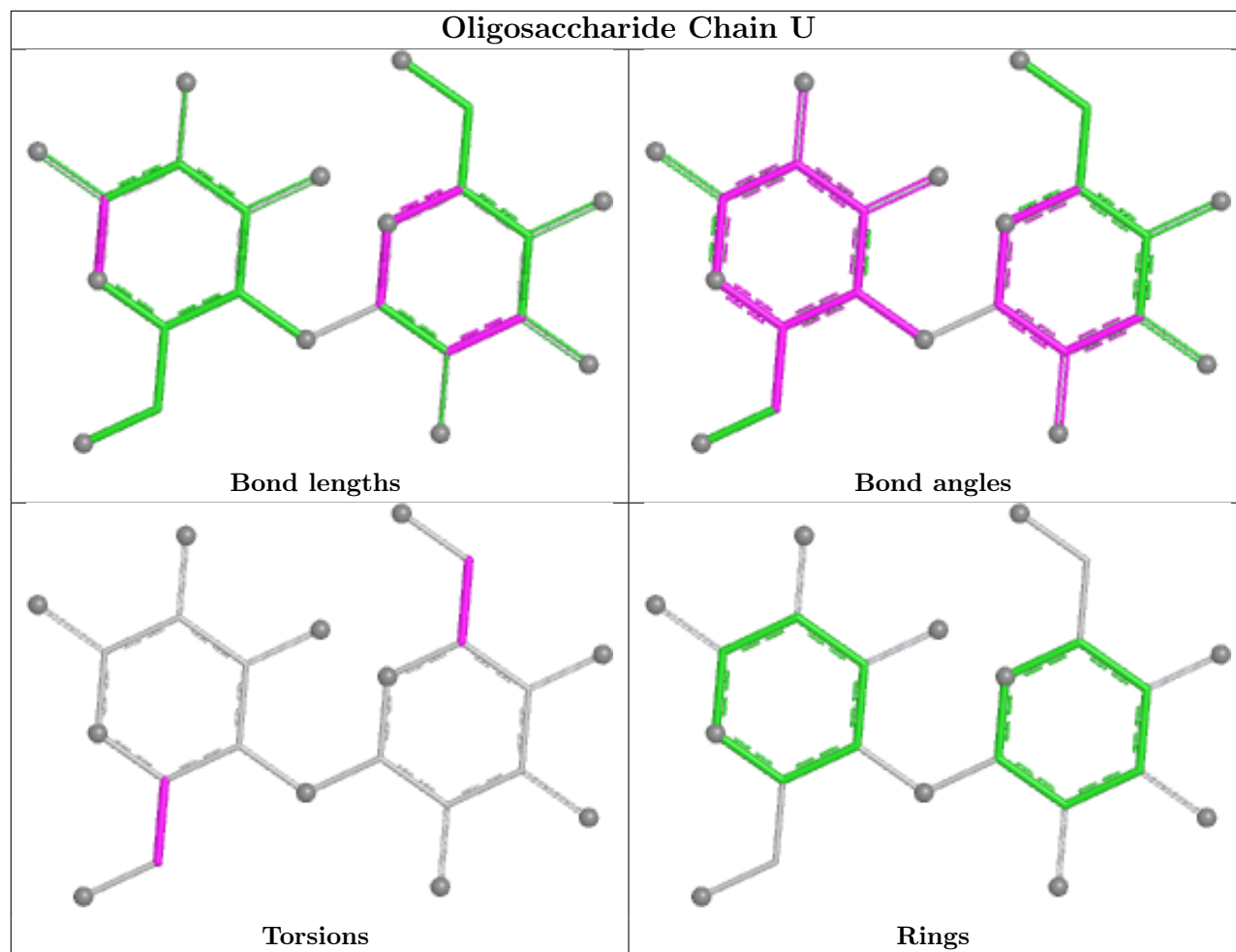


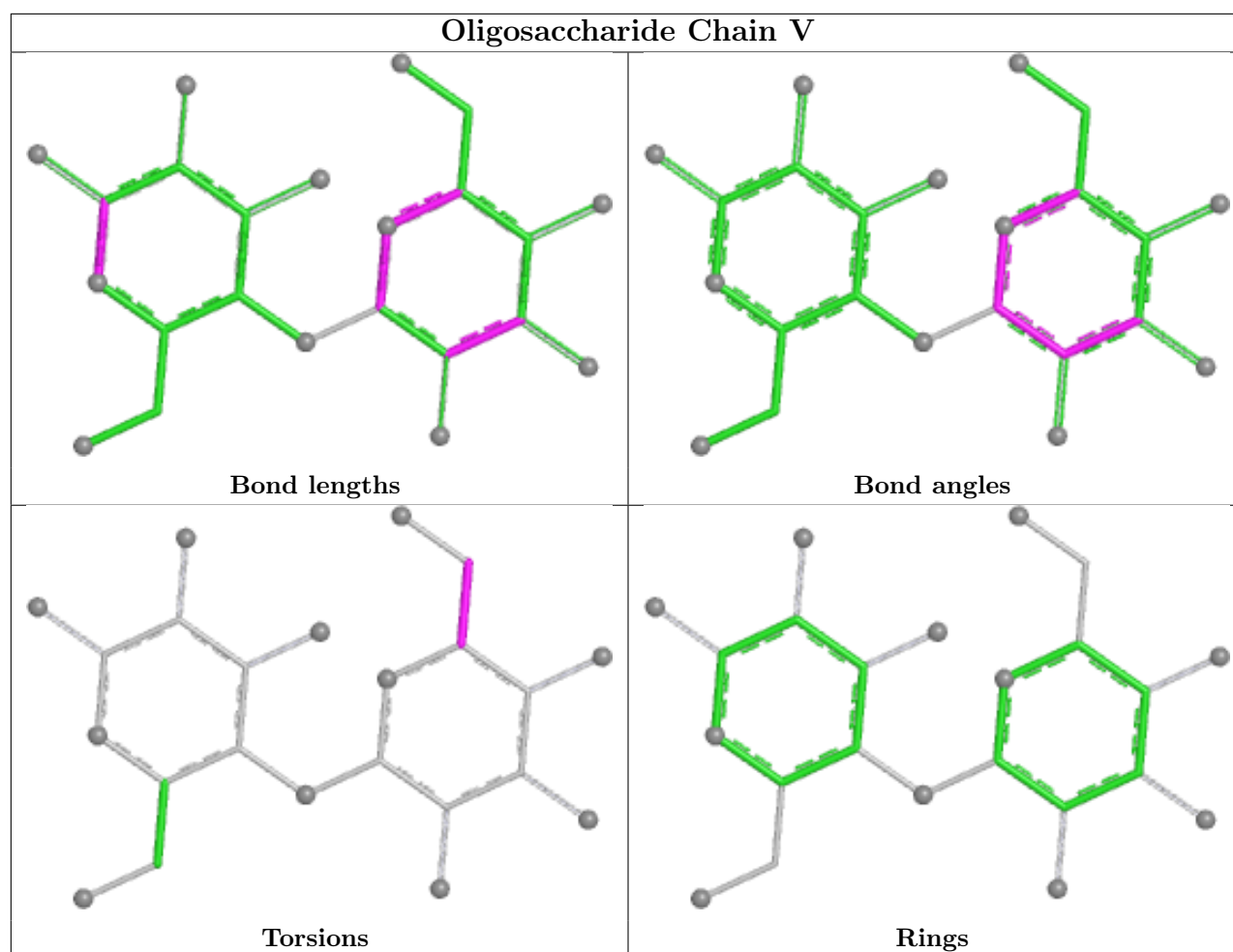












5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CAC	G	1302	3	2,4,4	2.76	2 (100%)	4,6,6	1.65	0
4	CAC	F	1302	3	2,4,4	2.70	2 (100%)	4,6,6	1.41	1 (25%)
4	CAC	C	1302	3	2,4,4	2.64	2 (100%)	4,6,6	1.55	1 (25%)
4	CAC	A	1302	3	2,4,4	2.56	2 (100%)	4,6,6	1.73	1 (25%)
4	CAC	H	1302	3	2,4,4	2.72	2 (100%)	4,6,6	1.69	1 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CAC	E	1302	3	2,4,4	2.59	2 (100%)	4,6,6	1.10	0
4	CAC	D	1302	3	2,4,4	2.62	2 (100%)	4,6,6	1.08	0
4	CAC	B	1302	3	2,4,4	2.74	2 (100%)	4,6,6	1.69	1 (25%)

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1302	CAC	AS-C2	2.80	1.96	1.90
4	D	1302	CAC	AS-C1	2.78	1.96	1.90
4	B	1302	CAC	AS-C2	2.77	1.96	1.90
4	F	1302	CAC	AS-C2	2.74	1.96	1.90
4	H	1302	CAC	AS-C1	2.72	1.96	1.90

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1302	CAC	O1-AS-C2	-2.50	108.39	111.50
4	C	1302	CAC	O1-AS-C1	-2.18	108.79	111.50
4	F	1302	CAC	O1-AS-C2	-2.06	108.94	111.50
4	H	1302	CAC	O1-AS-C2	-2.06	108.94	111.50
4	B	1302	CAC	O1-AS-C2	-2.06	108.94	111.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1302	CAC	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	592/593 (99%)	-1.21	0 100 100	76, 119, 160, 218	0
1	B	592/593 (99%)	-1.25	0 100 100	59, 123, 189, 221	0
1	C	592/593 (99%)	-1.24	0 100 100	63, 103, 154, 188	0
1	D	557/593 (93%)	-0.92	0 100 100	81, 199, 253, 274	0
1	E	592/593 (99%)	-1.12	0 100 100	87, 125, 168, 242	0
1	F	592/593 (99%)	-1.22	0 100 100	62, 119, 182, 220	0
1	G	592/593 (99%)	-1.26	0 100 100	64, 104, 151, 184	0
1	H	558/593 (94%)	-0.91	0 100 100	81, 198, 258, 279	0
All	All	4667/4744 (98%)	-1.15	0 100 100	59, 125, 234, 279	0

There are no RSRZ outliers to report.

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	GLC	N	1	12/12	0.93	0.05	167,214,228,229	0
2	GLC	N	2	11/12	0.94	0.05	180,215,239,257	0
2	GLC	O	1	12/12	0.95	0.05	153,173,206,207	0

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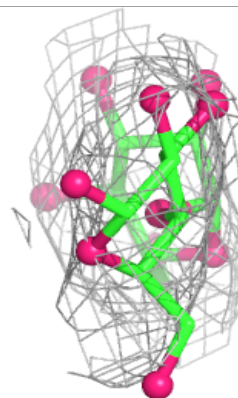
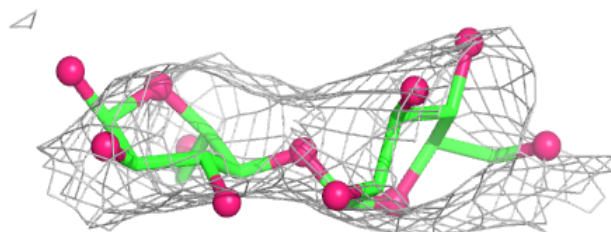
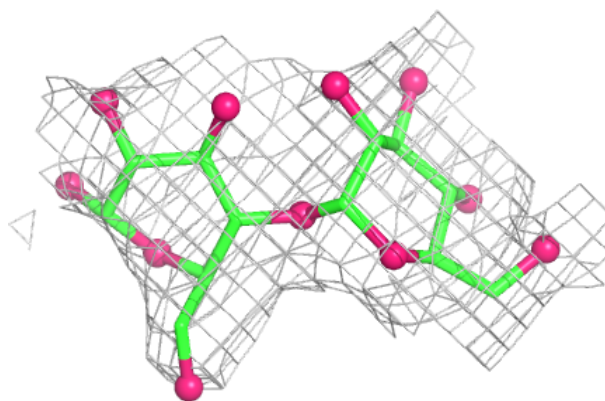
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	U	1	12/12	0.95	0.05	182,227,236,236	0
2	GLC	O	2	11/12	0.98	0.04	114,155,184,199	0
2	GLC	R	2	11/12	0.98	0.04	118,152,169,170	0
2	GLC	K	1	12/12	0.98	0.05	118,135,151,164	0
2	GLC	U	2	11/12	0.98	0.04	127,200,236,238	0
2	GLC	V	1	12/12	0.98	0.05	152,182,244,295	0
2	GLC	V	2	11/12	0.98	0.04	158,173,189,193	0
2	GLC	K	2	11/12	0.99	0.05	45,117,133,137	0
2	GLC	L	1	12/12	0.99	0.04	65,104,112,121	0
2	GLC	P	1	12/12	0.99	0.05	84,115,138,146	0
2	GLC	P	2	11/12	0.99	0.05	110,135,146,165	0
2	GLC	R	1	12/12	0.99	0.02	82,110,129,144	0
2	GLC	L	2	11/12	0.99	0.03	63,104,120,123	0
2	GLC	S	1	12/12	0.99	0.03	70,141,153,161	0
2	GLC	S	2	11/12	0.99	0.04	40,97,126,138	0
2	GLC	T	1	12/12	0.99	0.03	84,121,139,143	0
2	GLC	T	2	11/12	0.99	0.04	79,123,149,154	0
2	GLC	M	1	12/12	0.99	0.04	88,118,132,133	0
2	GLC	M	2	11/12	0.99	0.04	82,109,137,147	0
2	GLC	I	2	11/12	0.99	0.03	114,129,134,138	0
2	GLC	I	1	12/12	0.99	0.04	87,113,141,141	0
2	GLC	Q	1	12/12	1.00	0.04	115,137,160,163	0
2	GLC	Q	2	11/12	1.00	0.03	65,123,145,157	0
2	GLC	J	1	12/12	1.00	0.03	93,123,142,146	0
2	GLC	J	2	11/12	1.00	0.03	75,136,149,149	0

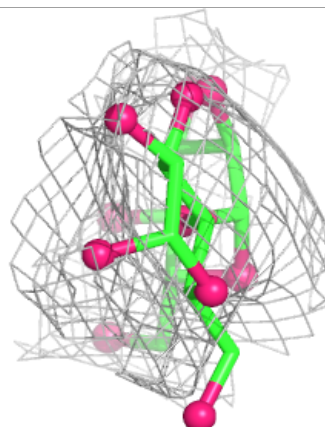
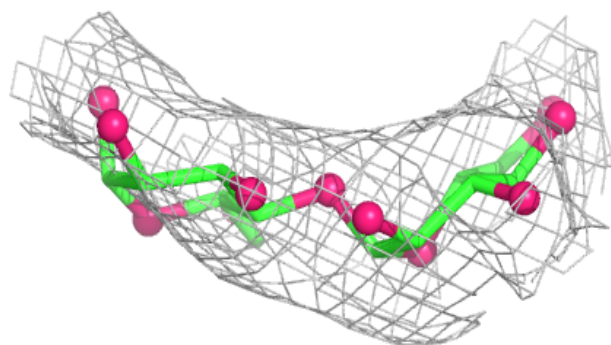
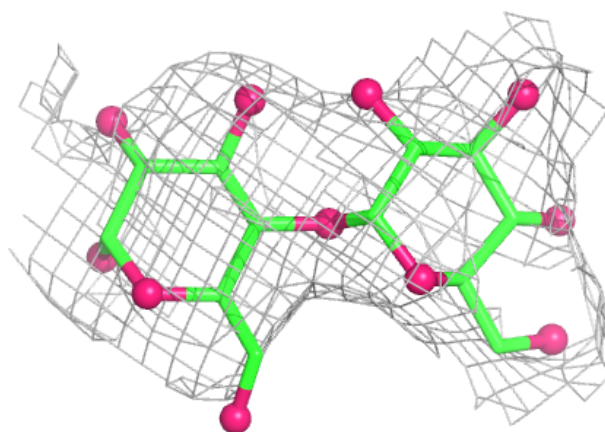
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

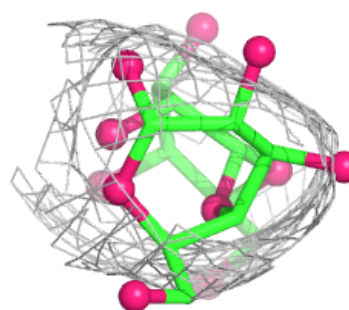
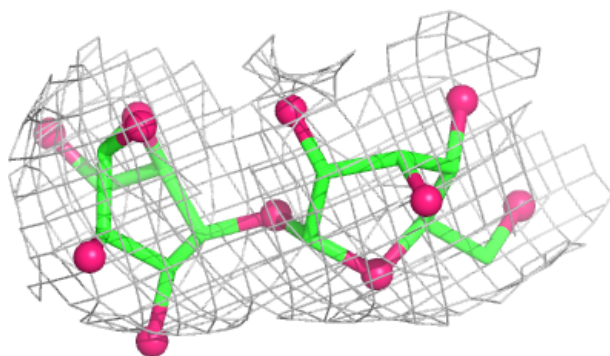
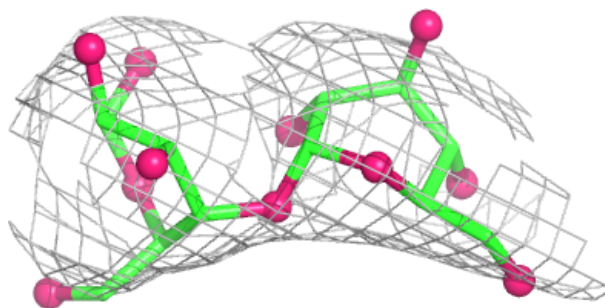
**Electron density around Chain J:**

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and green (positive)



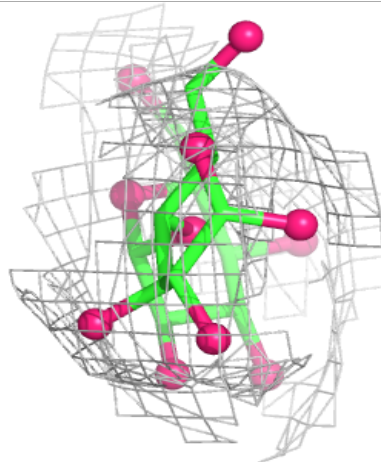
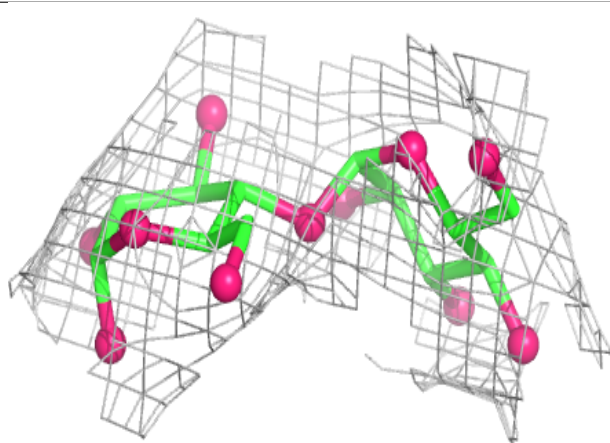
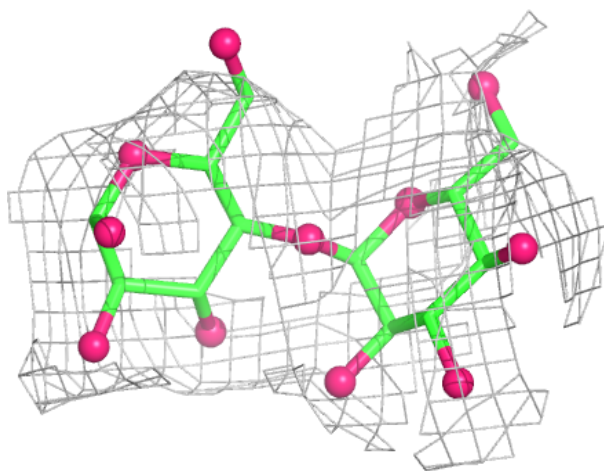
Electron density around Chain K:

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and green (positive)



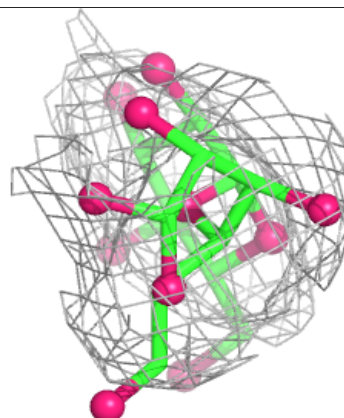
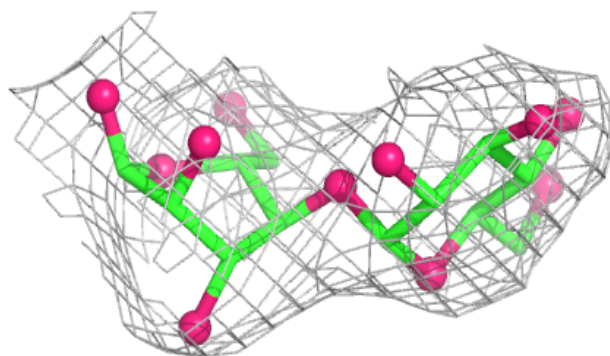
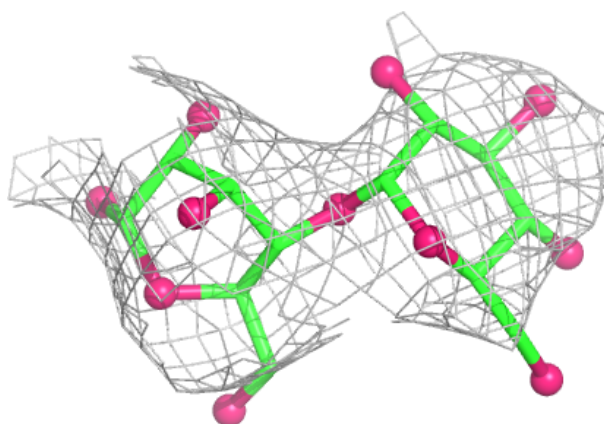
Electron density around Chain L:

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and green (positive)

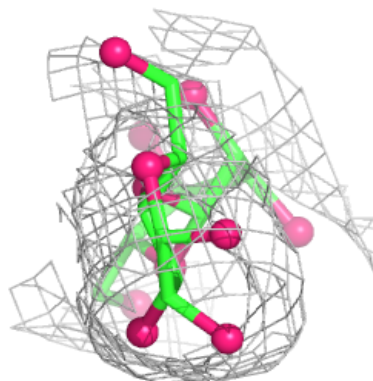
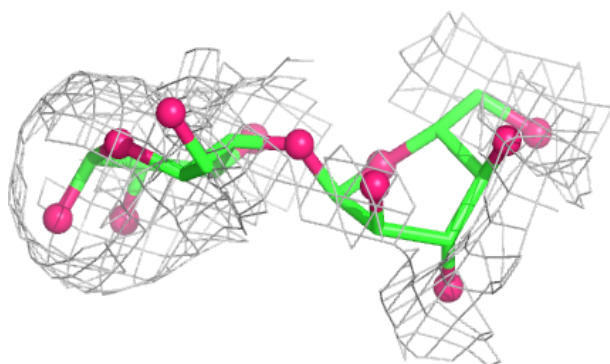
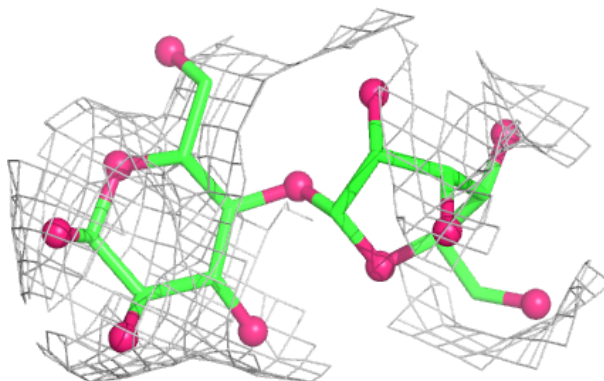


Electron density around Chain M:

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

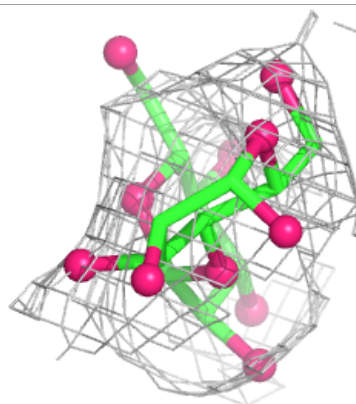
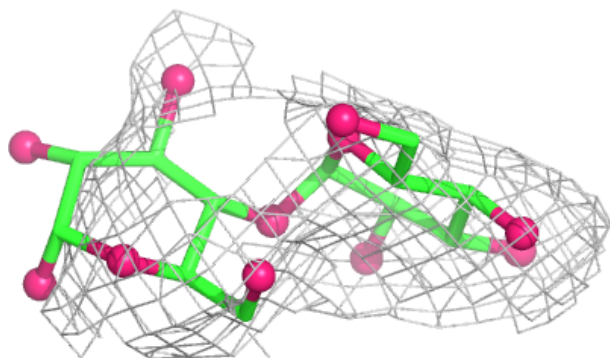
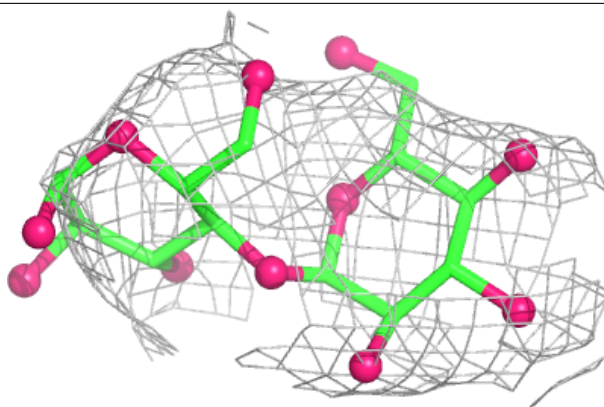
**Electron density around Chain N:**

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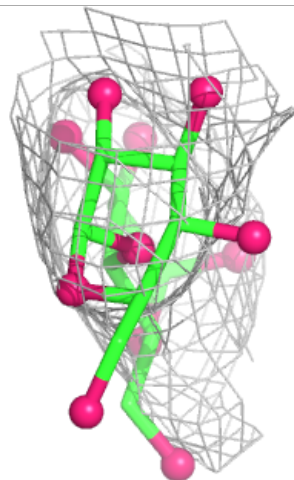
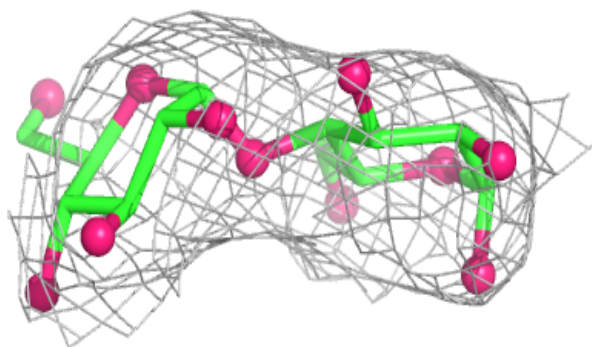
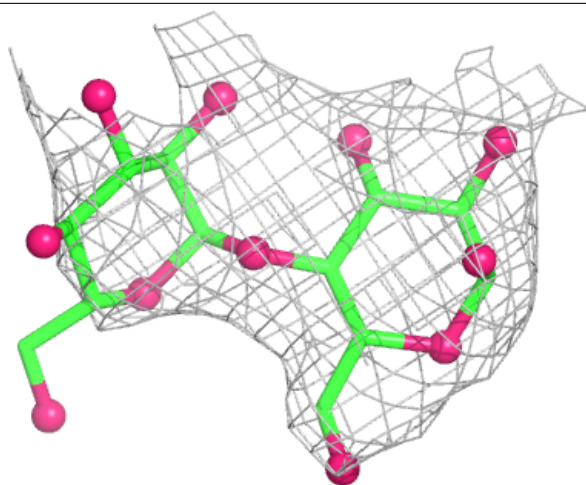
Electron density around Chain O:

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and green (positive)



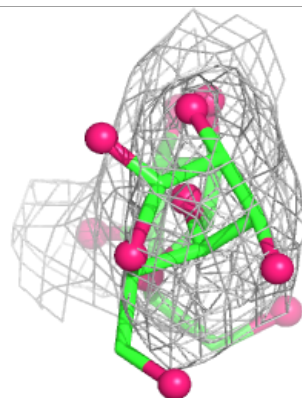
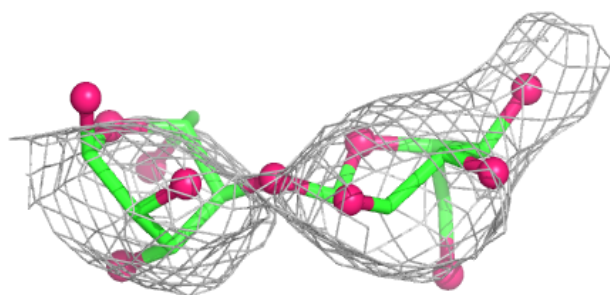
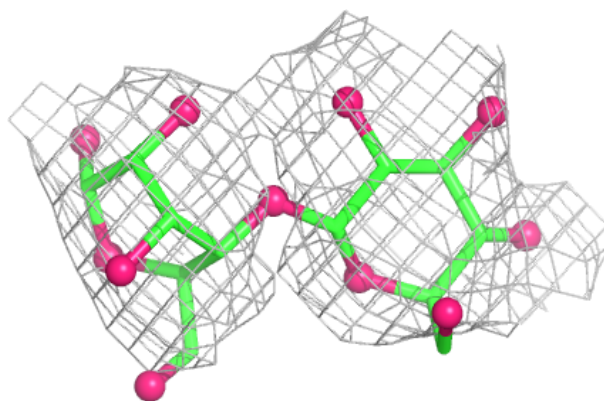
Electron density around Chain P:

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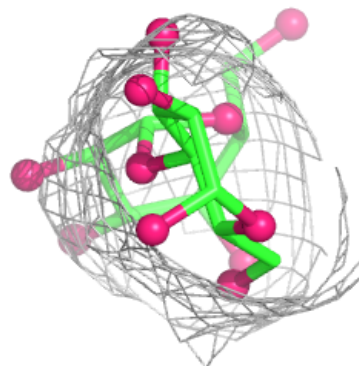
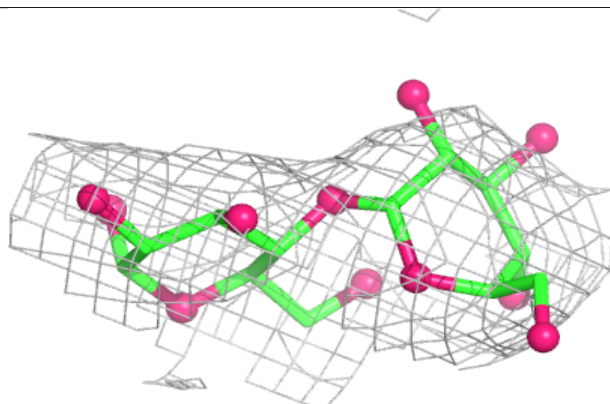
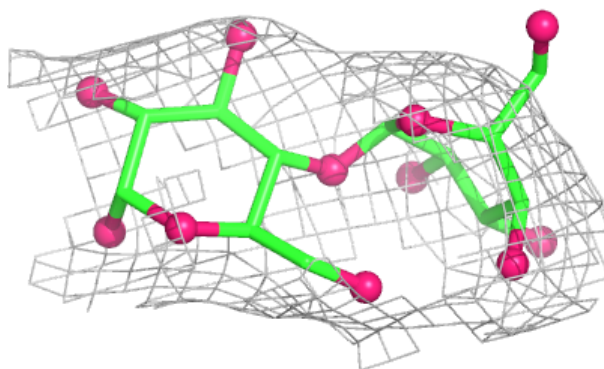


Electron density around Chain Q:

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and green (positive)

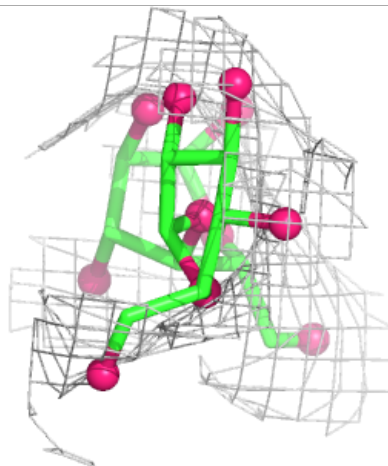
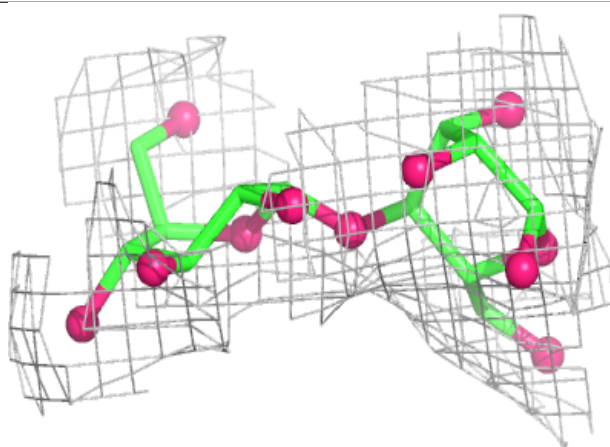
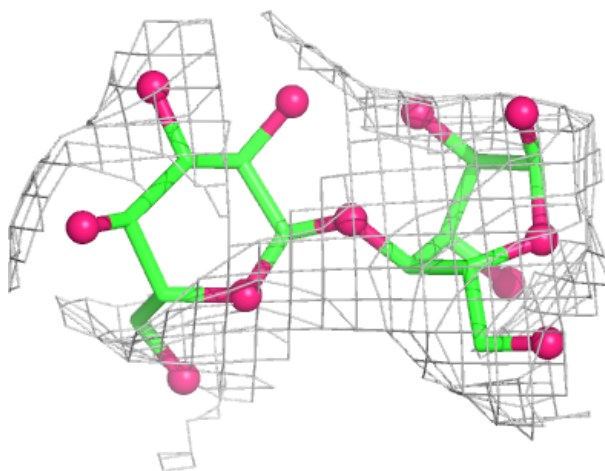
**Electron density around Chain R:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



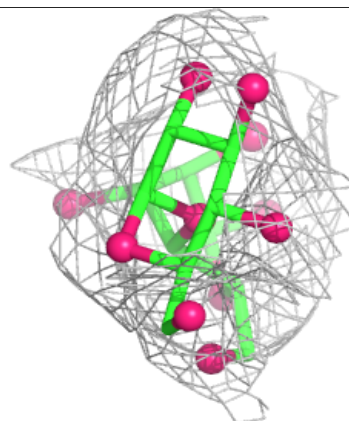
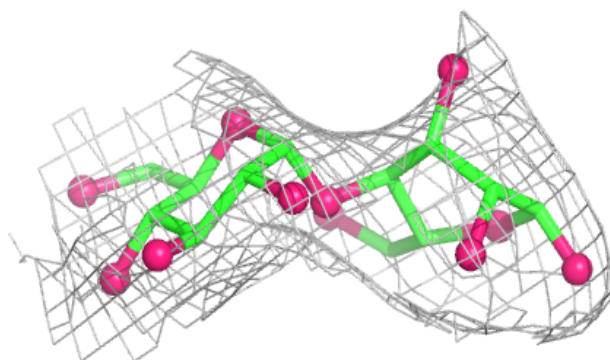
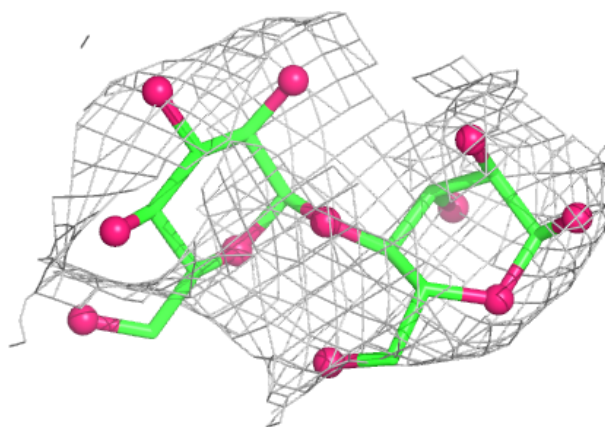
Electron density around Chain S:

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and green (positive)



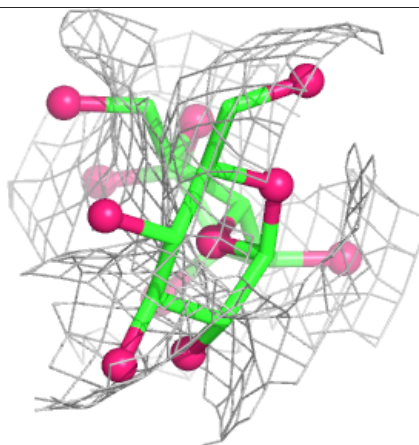
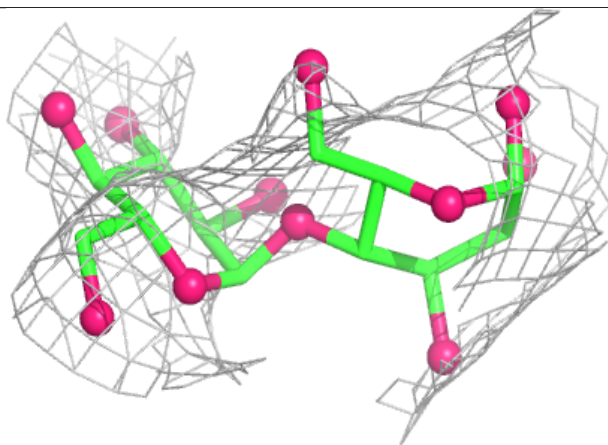
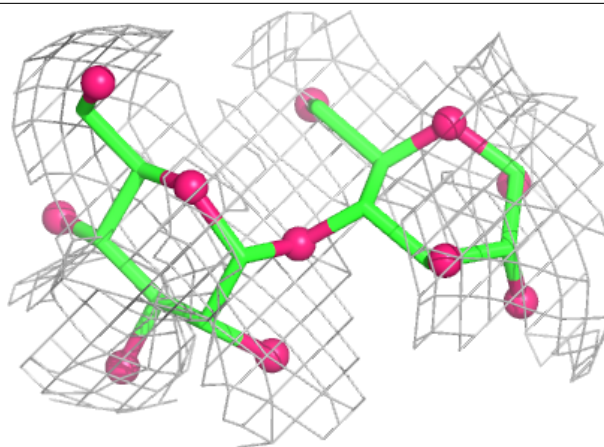
Electron density around Chain T:

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

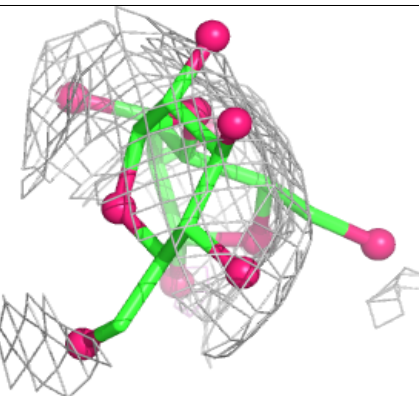
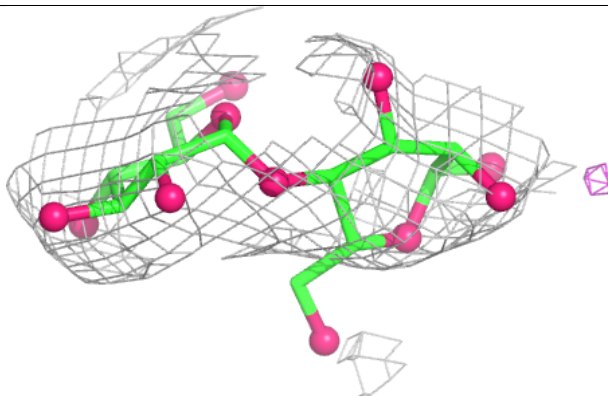
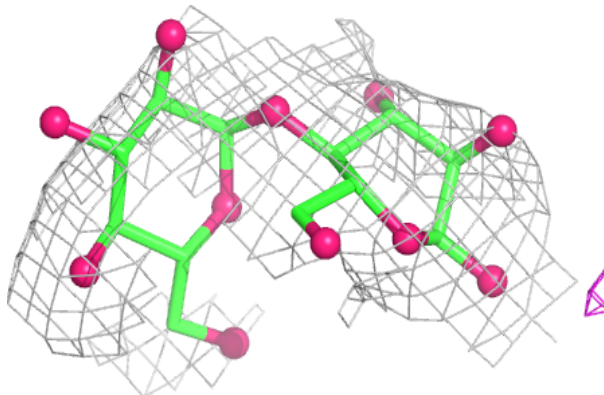


Electron density around Chain U:

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and green (positive)

**Electron density around Chain V:**

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and green (positive)



6.4 Ligands

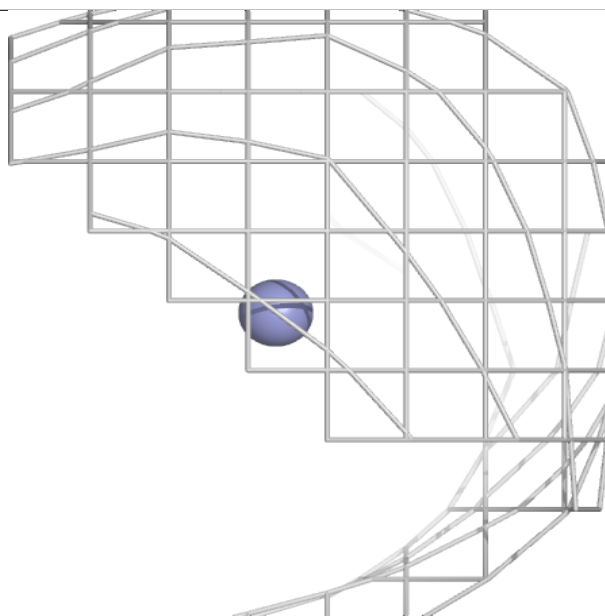
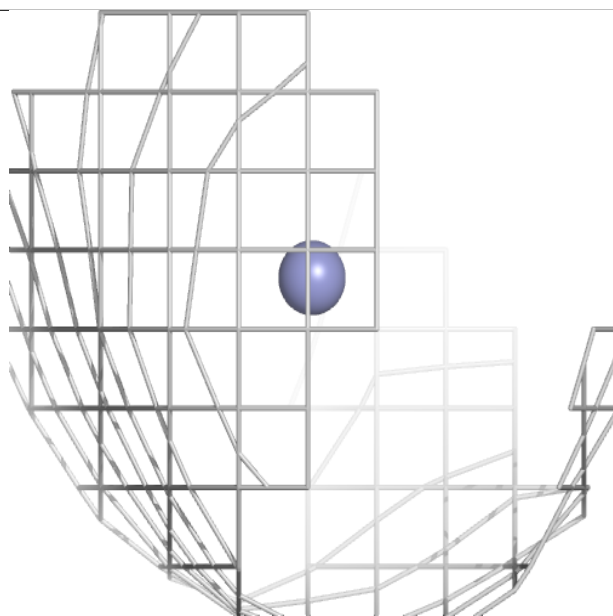
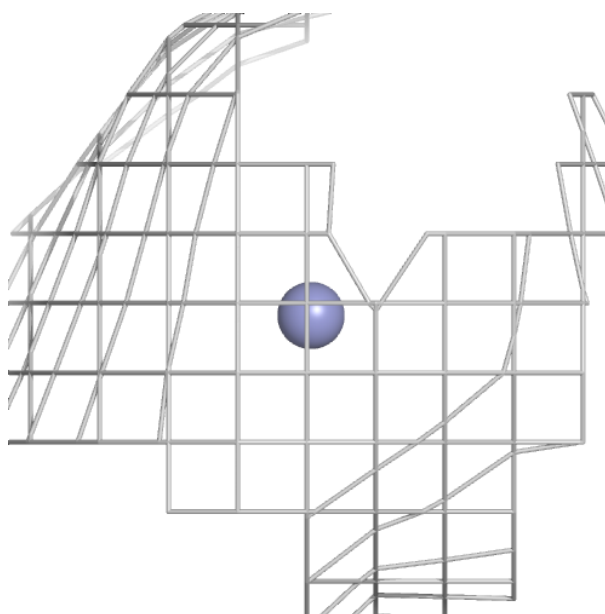
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CAC	D	1302	5/5	0.99	0.06	172,175,187,188	0
3	ZN	B	1301	1/1	1.00	0.02	157,157,157,157	0
3	ZN	C	1301	1/1	1.00	0.01	124,124,124,124	0
3	ZN	D	1301	1/1	1.00	0.01	209,209,209,209	0
3	ZN	E	1301	1/1	1.00	0.01	155,155,155,155	0
3	ZN	F	1301	1/1	1.00	0.02	158,158,158,158	0
3	ZN	G	1301	1/1	1.00	0.01	123,123,123,123	0
3	ZN	H	1301	1/1	1.00	0.02	186,186,186,186	0
4	CAC	A	1302	5/5	1.00	0.03	120,121,132,145	0
4	CAC	B	1302	5/5	1.00	0.04	91,113,122,137	0
4	CAC	C	1302	5/5	1.00	0.02	76,98,106,110	0
3	ZN	A	1301	1/1	1.00	0.01	129,129,129,129	0
4	CAC	E	1302	5/5	1.00	0.03	113,120,133,134	0
4	CAC	F	1302	5/5	1.00	0.03	94,99,120,137	0
4	CAC	G	1302	5/5	1.00	0.03	78,92,107,138	0
4	CAC	H	1302	5/5	1.00	0.04	154,186,196,230	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

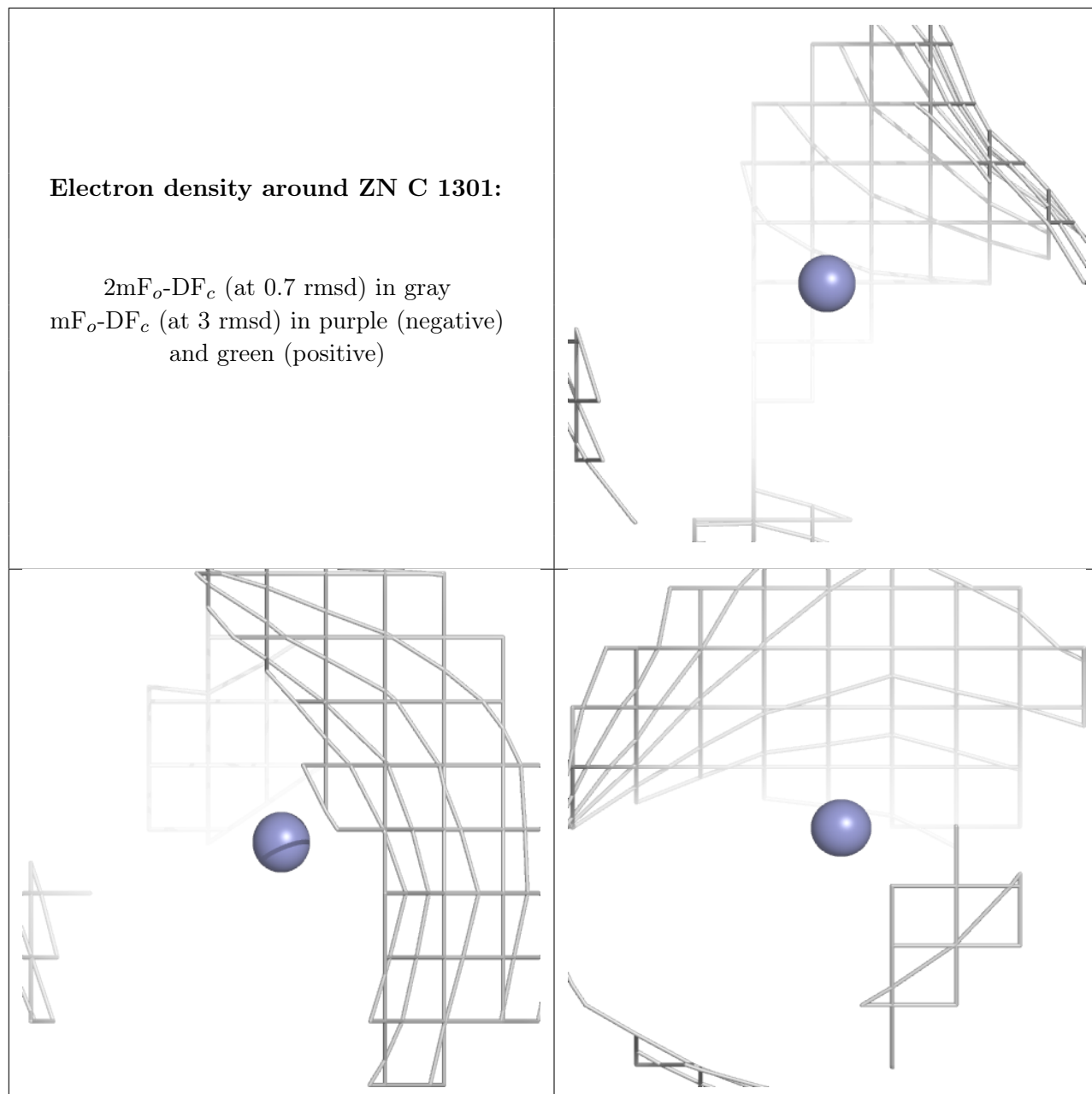
Electron density around ZN B 1301:

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



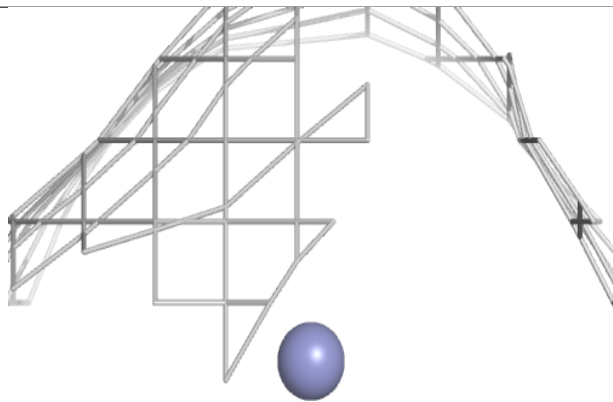
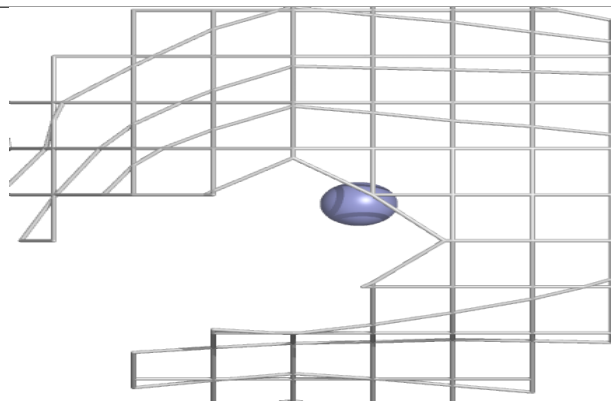
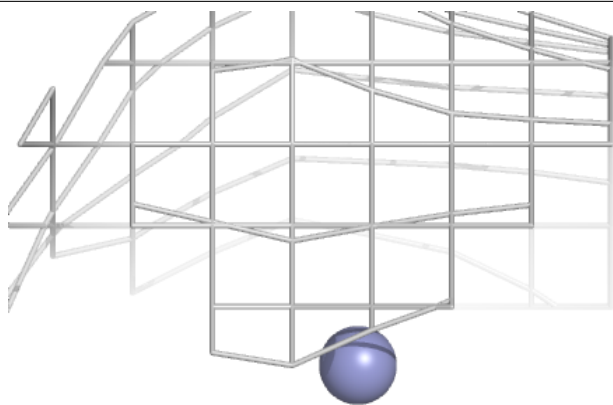
Electron density around ZN C 1301:

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



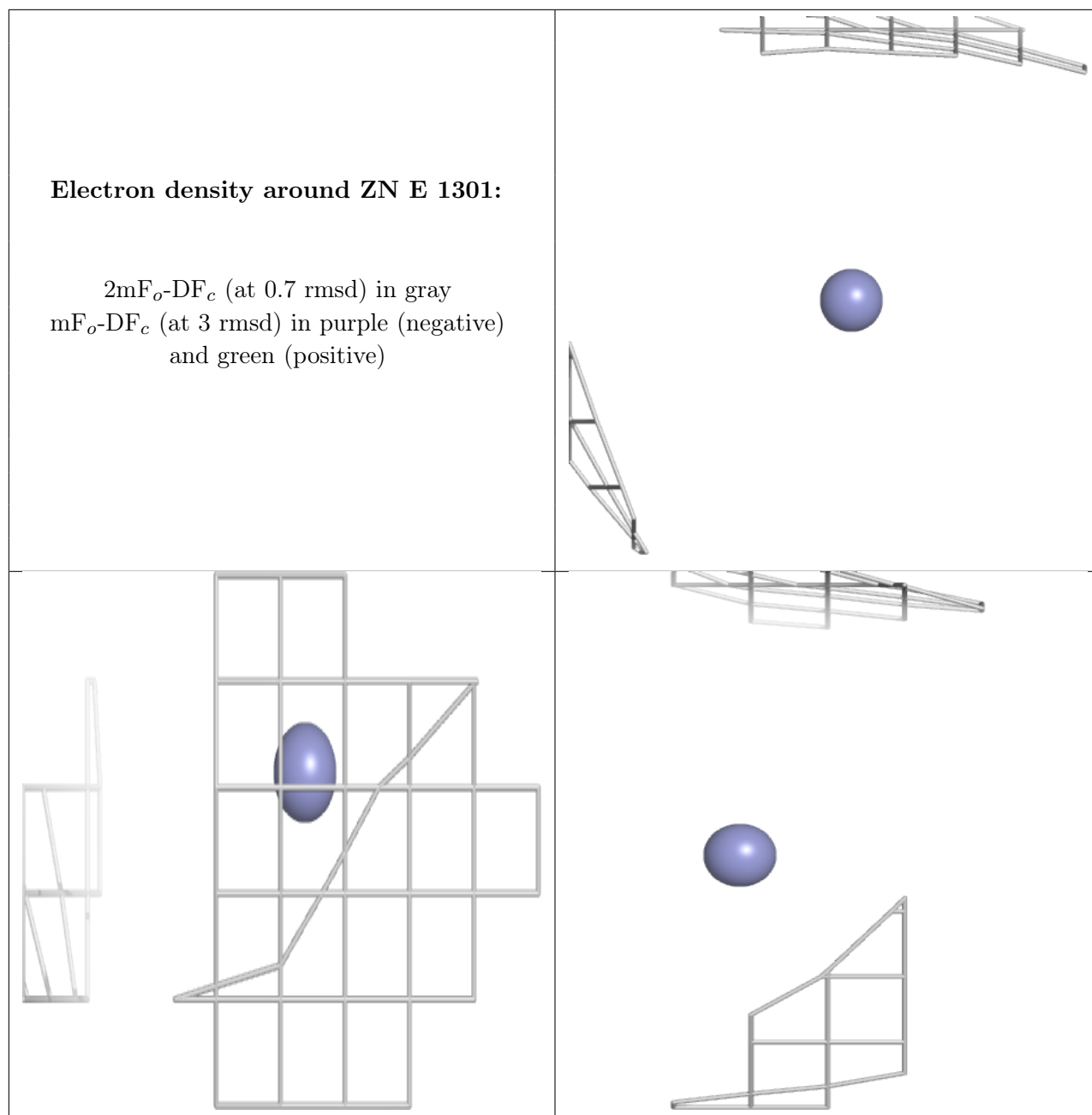
Electron density around ZN D 1301:

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



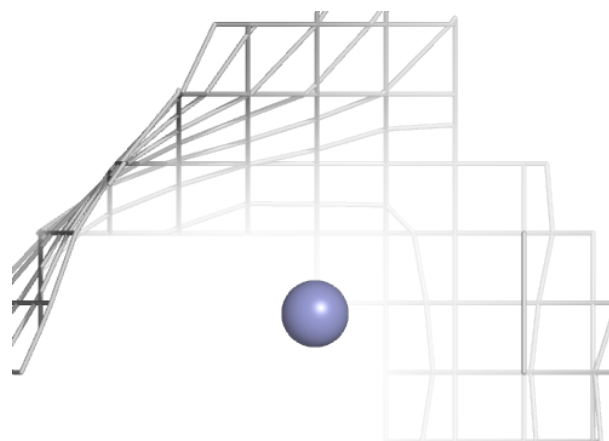
Electron density around ZN E 1301:

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

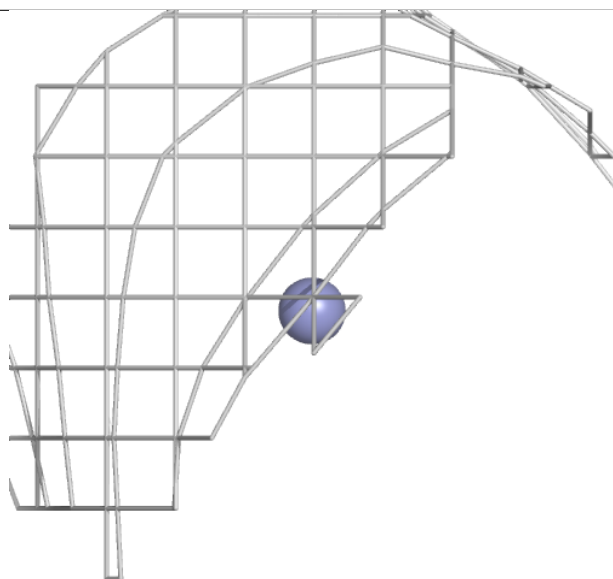


Electron density around ZN F 1301:

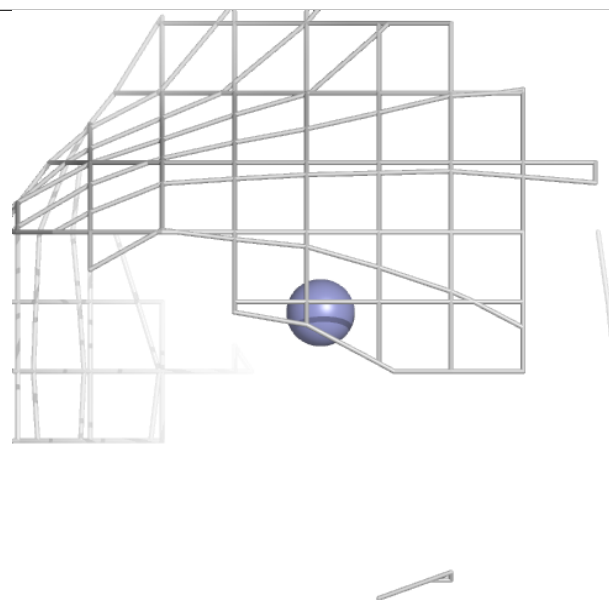
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



↑

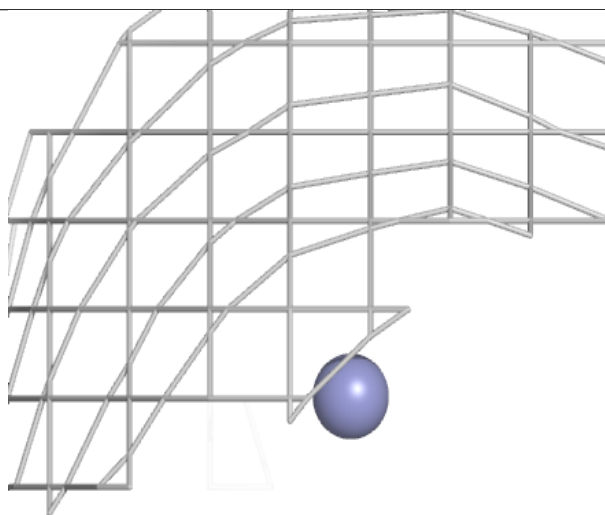
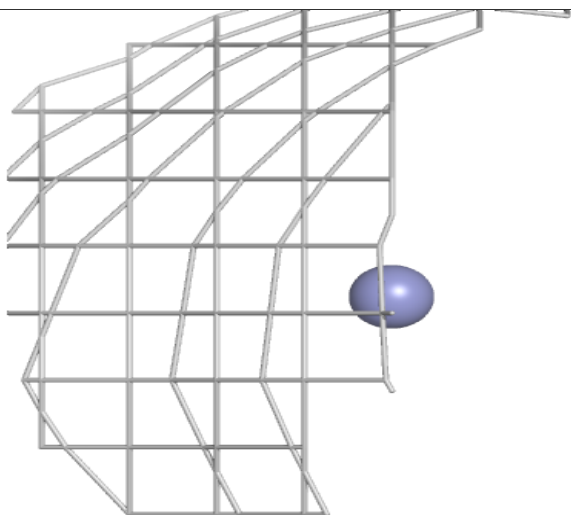
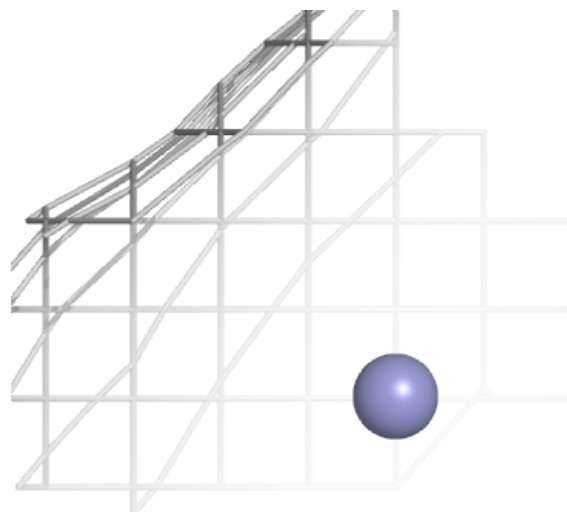


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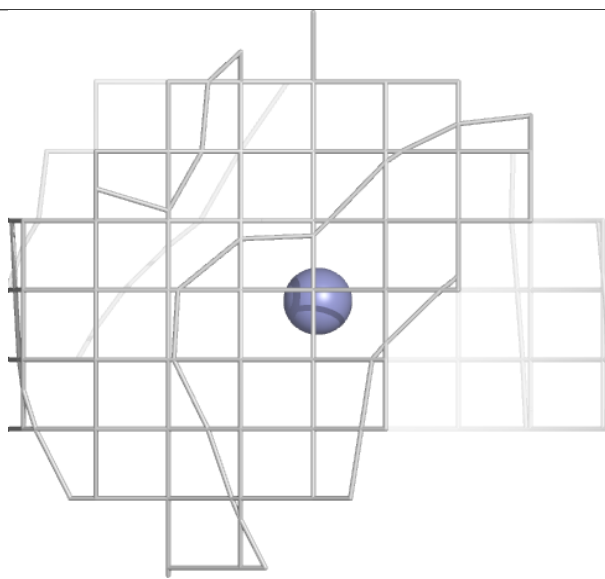
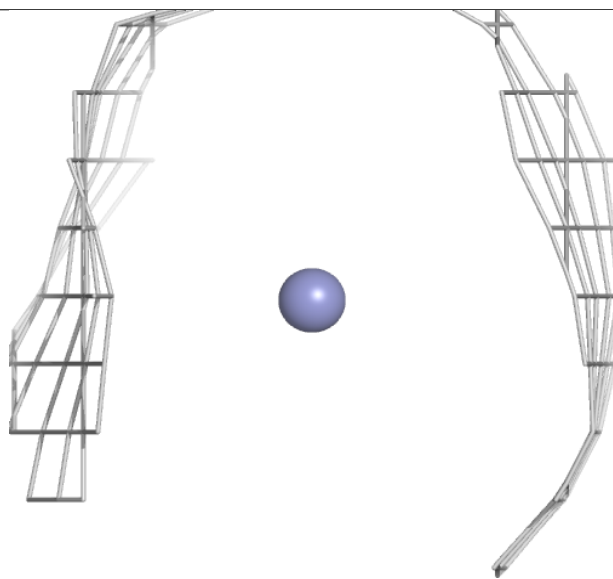
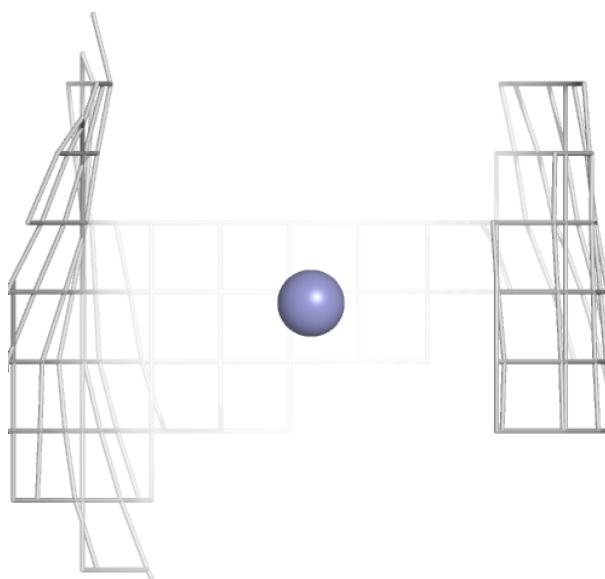
Electron density around ZN G 1301:

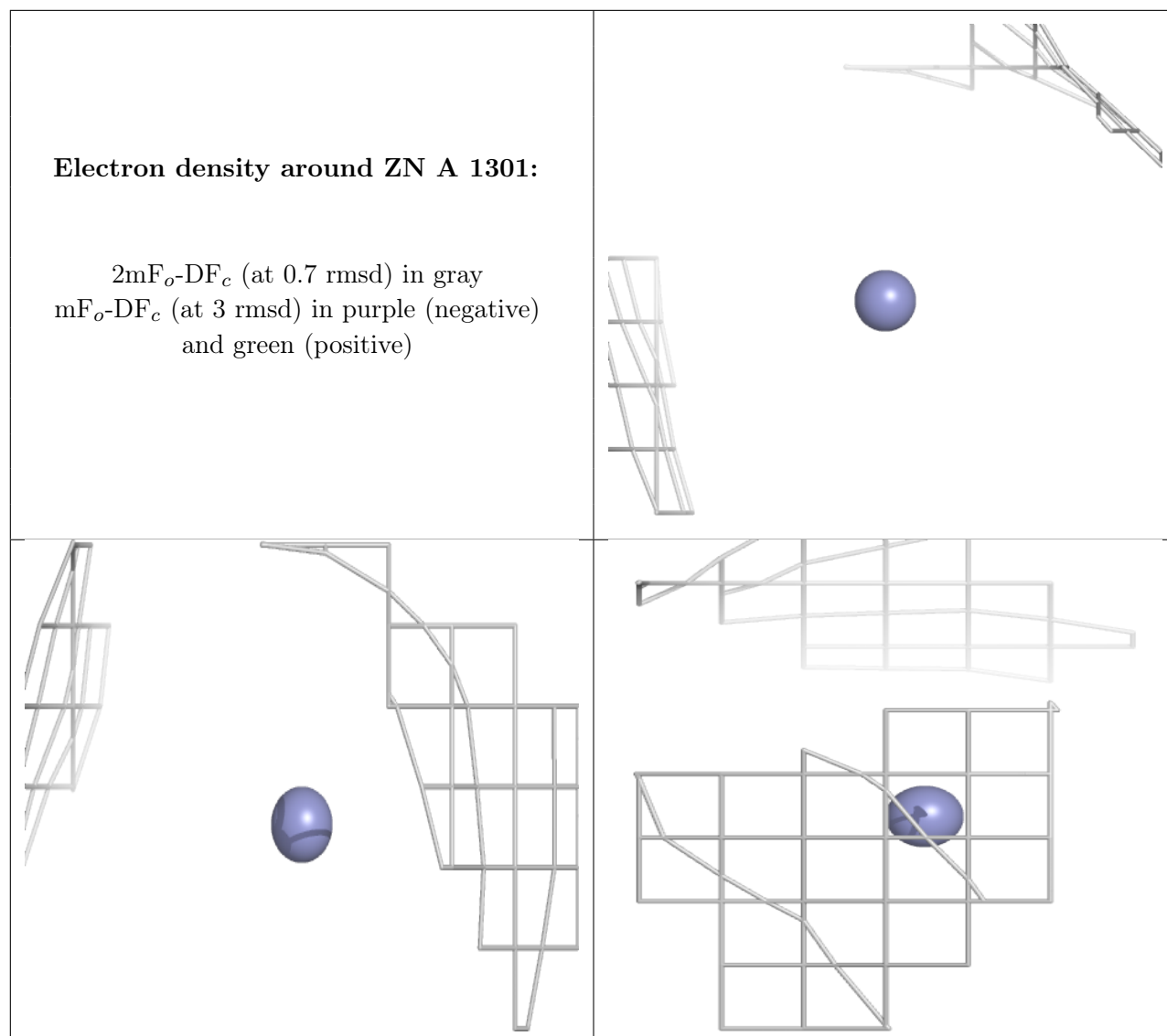
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN H 1301:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.