



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 26, 2020 – 05:28 PM BST

PDB ID : 4V44
Title : E. COLI (lacZ) BETA-GALACTOSIDASE IN COMPLEX WITH 2-F-LACTOSE
Authors : Juers, D.H.; McCarter, J.D.; Withers, S.G.; Matthews, B.W.
Deposited on : 2001-09-13
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

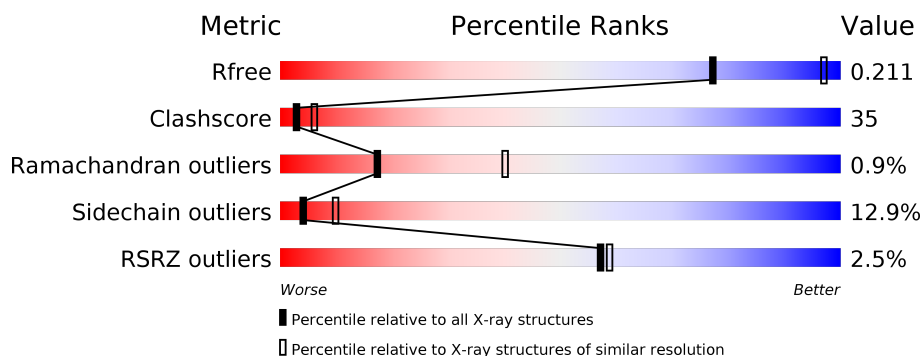
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1023	% <div> <div></div> <div>43%</div> <div>42%</div> <div>13%</div> <div>.</div> </div>
1	B	1023	% <div> <div></div> <div>43%</div> <div>42%</div> <div>13%</div> <div>.</div> </div>
1	C	1023	% <div> <div></div> <div>43%</div> <div>41%</div> <div>13%</div> <div>.</div> </div>
1	D	1023	% <div> <div></div> <div>43%</div> <div>42%</div> <div>13%</div> <div>.</div> </div>
1	E	1023	3% <div> <div></div> <div>43%</div> <div>42%</div> <div>13%</div> <div>.</div> </div>
1	F	1023	% <div> <div></div> <div>43%</div> <div>42%</div> <div>13%</div> <div>.</div> </div>


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Mol	Chain	Length	Quality of chain
1	G	1023	
1	H	1023	
1	I	1023	
1	J	1023	
1	K	1023	
1	L	1023	
1	M	1023	
1	N	1023	
1	O	1023	
1	P	1023	
2	Q	2	
2	R	2	
2	S	2	
2	T	2	
2	U	2	
2	V	2	
2	W	2	
2	X	2	
2	Y	2	
2	Z	2	
2	a	2	
2	b	2	
2	c	2	
2	d	2	
2	e	2	

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Mol	Chain	Length	Quality of chain
2	f	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
1	CME	A	1021	-	-	X	-
1	CME	B	1021	-	-	X	-
1	CME	C	1021	-	-	X	-
1	CME	D	1021	-	-	X	-
1	CME	E	1021	-	-	X	-
1	CME	F	1021	-	-	X	-
1	CME	G	1021	-	-	X	-
1	CME	H	1021	-	-	X	-
1	CME	I	1021	-	-	X	-
1	CME	J	1021	-	-	X	-
1	CME	K	1021	-	-	X	-
1	CME	L	1021	-	-	X	-
1	CME	M	1021	-	-	X	-
1	CME	N	1021	-	-	X	-
1	CME	O	1021	-	-	X	-
1	CME	P	1021	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 134528 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 Beta-Galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	B	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	C	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	D	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	E	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	F	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	G	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	H	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	I	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	J	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	K	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	L	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	M	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	N	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	O	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	P	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	748	CME	CYS	modified residue	UNP P00722
A	914	CME	CYS	modified residue	UNP P00722
A	1021	CME	CYS	modified residue	UNP P00722
B	748	CME	CYS	modified residue	UNP P00722
B	914	CME	CYS	modified residue	UNP P00722
B	1021	CME	CYS	modified residue	UNP P00722
C	748	CME	CYS	modified residue	UNP P00722
C	914	CME	CYS	modified residue	UNP P00722
C	1021	CME	CYS	modified residue	UNP P00722
D	748	CME	CYS	modified residue	UNP P00722
D	914	CME	CYS	modified residue	UNP P00722
D	1021	CME	CYS	modified residue	UNP P00722
E	748	CME	CYS	modified residue	UNP P00722
E	914	CME	CYS	modified residue	UNP P00722
E	1021	CME	CYS	modified residue	UNP P00722
F	748	CME	CYS	modified residue	UNP P00722
F	914	CME	CYS	modified residue	UNP P00722
F	1021	CME	CYS	modified residue	UNP P00722
G	748	CME	CYS	modified residue	UNP P00722
G	914	CME	CYS	modified residue	UNP P00722
G	1021	CME	CYS	modified residue	UNP P00722
H	748	CME	CYS	modified residue	UNP P00722
H	914	CME	CYS	modified residue	UNP P00722
H	1021	CME	CYS	modified residue	UNP P00722
I	748	CME	CYS	modified residue	UNP P00722
I	914	CME	CYS	modified residue	UNP P00722
I	1021	CME	CYS	modified residue	UNP P00722
J	748	CME	CYS	modified residue	UNP P00722
J	914	CME	CYS	modified residue	UNP P00722
J	1021	CME	CYS	modified residue	UNP P00722
K	748	CME	CYS	modified residue	UNP P00722
K	914	CME	CYS	modified residue	UNP P00722
K	1021	CME	CYS	modified residue	UNP P00722
L	748	CME	CYS	modified residue	UNP P00722
L	914	CME	CYS	modified residue	UNP P00722
L	1021	CME	CYS	modified residue	UNP P00722
M	748	CME	CYS	modified residue	UNP P00722
M	914	CME	CYS	modified residue	UNP P00722
M	1021	CME	CYS	modified residue	UNP P00722
N	748	CME	CYS	modified residue	UNP P00722
N	914	CME	CYS	modified residue	UNP P00722
N	1021	CME	CYS	modified residue	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
O	748	CME	CYS	modified residue	UNP P00722
O	914	CME	CYS	modified residue	UNP P00722
O	1021	CME	CYS	modified residue	UNP P00722
P	748	CME	CYS	modified residue	UNP P00722
P	914	CME	CYS	modified residue	UNP P00722
P	1021	CME	CYS	modified residue	UNP P00722

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Q	2	Total 23	C 12	F 1	O 10	0	0	0
2	R	2	Total 23	C 12	F 1	O 10	0	0	0
2	S	2	Total 23	C 12	F 1	O 10	0	0	0
2	T	2	Total 23	C 12	F 1	O 10	0	0	0
2	U	2	Total 23	C 12	F 1	O 10	0	0	0
2	V	2	Total 23	C 12	F 1	O 10	0	0	0
2	W	2	Total 23	C 12	F 1	O 10	0	0	0
2	X	2	Total 23	C 12	F 1	O 10	0	0	0
2	Y	2	Total 23	C 12	F 1	O 10	0	0	0
2	Z	2	Total 23	C 12	F 1	O 10	0	0	0
2	a	2	Total 23	C 12	F 1	O 10	0	0	0
2	b	2	Total 23	C 12	F 1	O 10	0	0	0
2	c	2	Total 23	C 12	F 1	O 10	0	0	0
2	d	2	Total 23	C 12	F 1	O 10	0	0	0
2	e	2	Total 23	C 12	F 1	O 10	0	0	0
2	f	2	Total 23	C 12	F 1	O 10	0	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	2	Total 2	Mg 2	0	0
3	G	2	Total 2	Mg 2	0	0
3	J	2	Total 2	Mg 2	0	0
3	D	2	Total 2	Mg 2	0	0
3	K	2	Total 2	Mg 2	0	0
3	E	2	Total 2	Mg 2	0	0
3	H	2	Total 2	Mg 2	0	0
3	B	2	Total 2	Mg 2	0	0
3	I	2	Total 2	Mg 2	0	0
3	C	2	Total 2	Mg 2	0	0
3	A	2	Total 2	Mg 2	0	0
3	N	2	Total 2	Mg 2	0	0
3	O	2	Total 2	Mg 2	0	0
3	L	2	Total 2	Mg 2	0	0
3	F	2	Total 2	Mg 2	0	0
3	M	2	Total 2	Mg 2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	2	Total 2	Na 2	0	0
4	G	2	Total 2	Na 2	0	0
4	J	2	Total 2	Na 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total 2	Na 2	0	0
4	K	2	Total 2	Na 2	0	0
4	E	2	Total 2	Na 2	0	0
4	H	2	Total 2	Na 2	0	0
4	B	2	Total 2	Na 2	0	0
4	I	2	Total 2	Na 2	0	0
4	C	2	Total 2	Na 2	0	0
4	A	2	Total 2	Na 2	0	0
4	N	2	Total 2	Na 2	0	0
4	O	2	Total 2	Na 2	0	0
4	L	2	Total 2	Na 2	0	0
4	F	2	Total 2	Na 2	0	0
4	M	2	Total 2	Na 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	160	Total 160	O 160	0	0
5	B	163	Total 163	O 163	0	0
5	C	162	Total 162	O 162	0	0
5	D	163	Total 163	O 163	0	0
5	E	162	Total 162	O 162	0	0
5	F	162	Total 162	O 162	0	0

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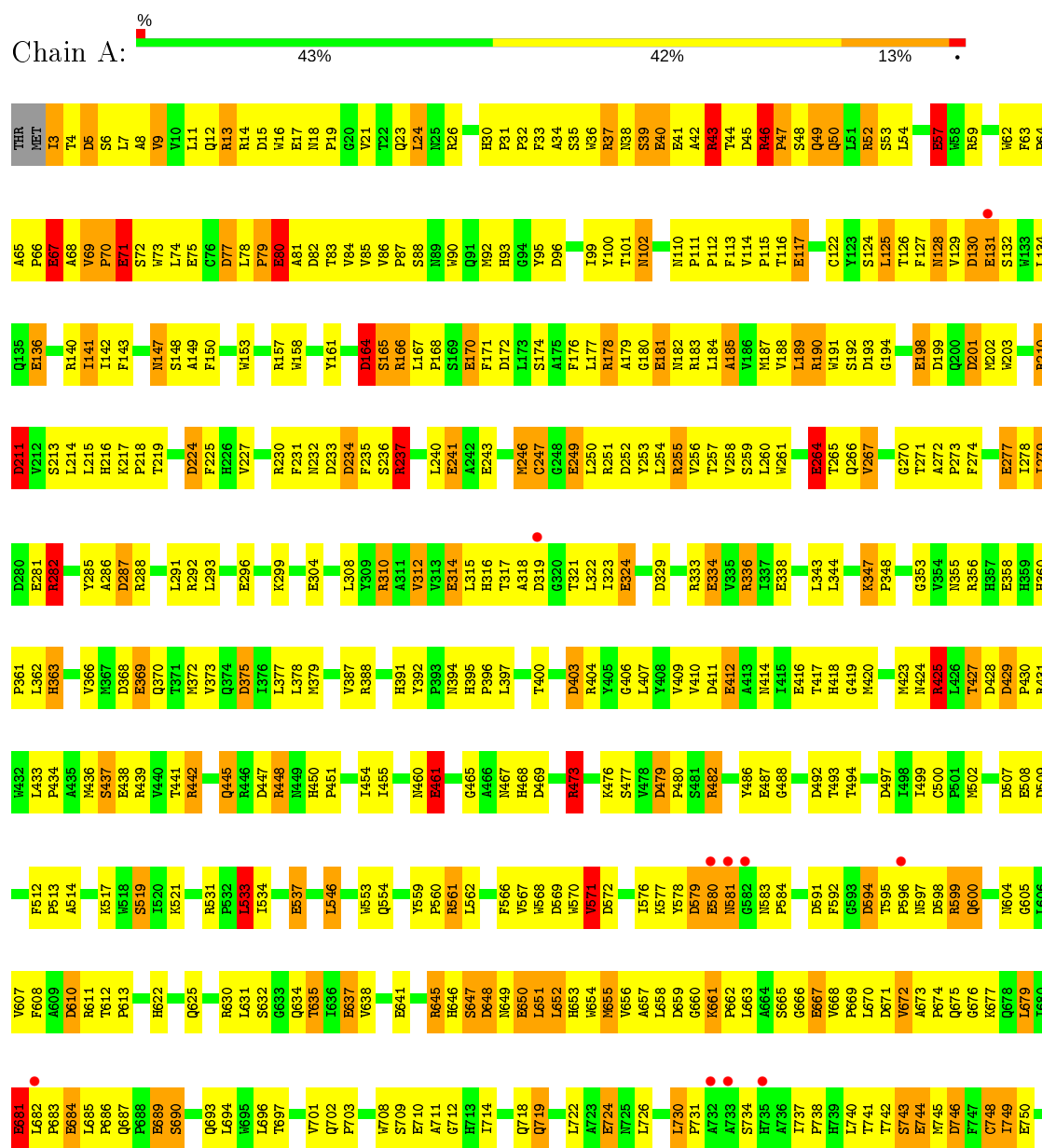
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	162	Total 162	O 162	0	0
5	H	162	Total 162	O 162	0	0
5	I	162	Total 162	O 162	0	0
5	J	162	Total 162	O 162	0	0
5	K	162	Total 162	O 162	0	0
5	L	162	Total 162	O 162	0	0
5	M	161	Total 161	O 161	0	0
5	N	163	Total 163	O 163	0	0
5	O	161	Total 161	O 161	0	0
5	P	163	Total 163	O 163	0	0

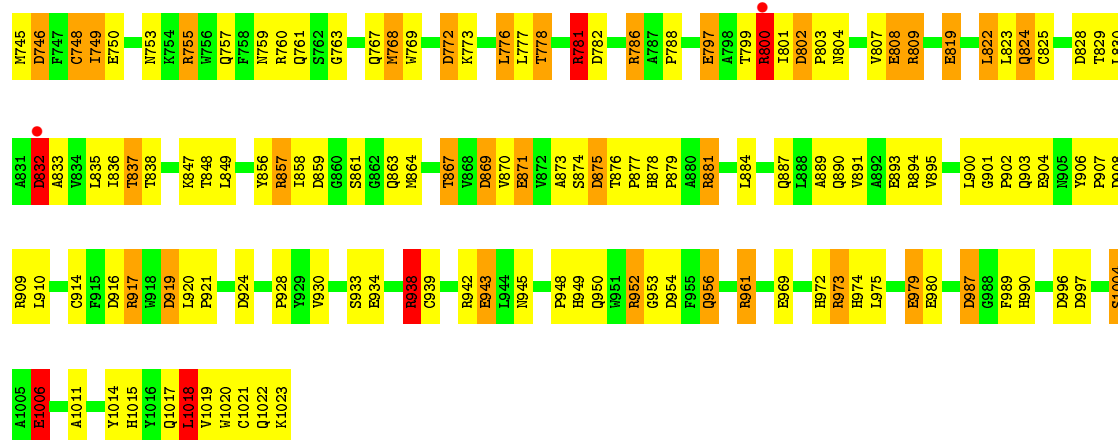
3 Residue-property plots

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.

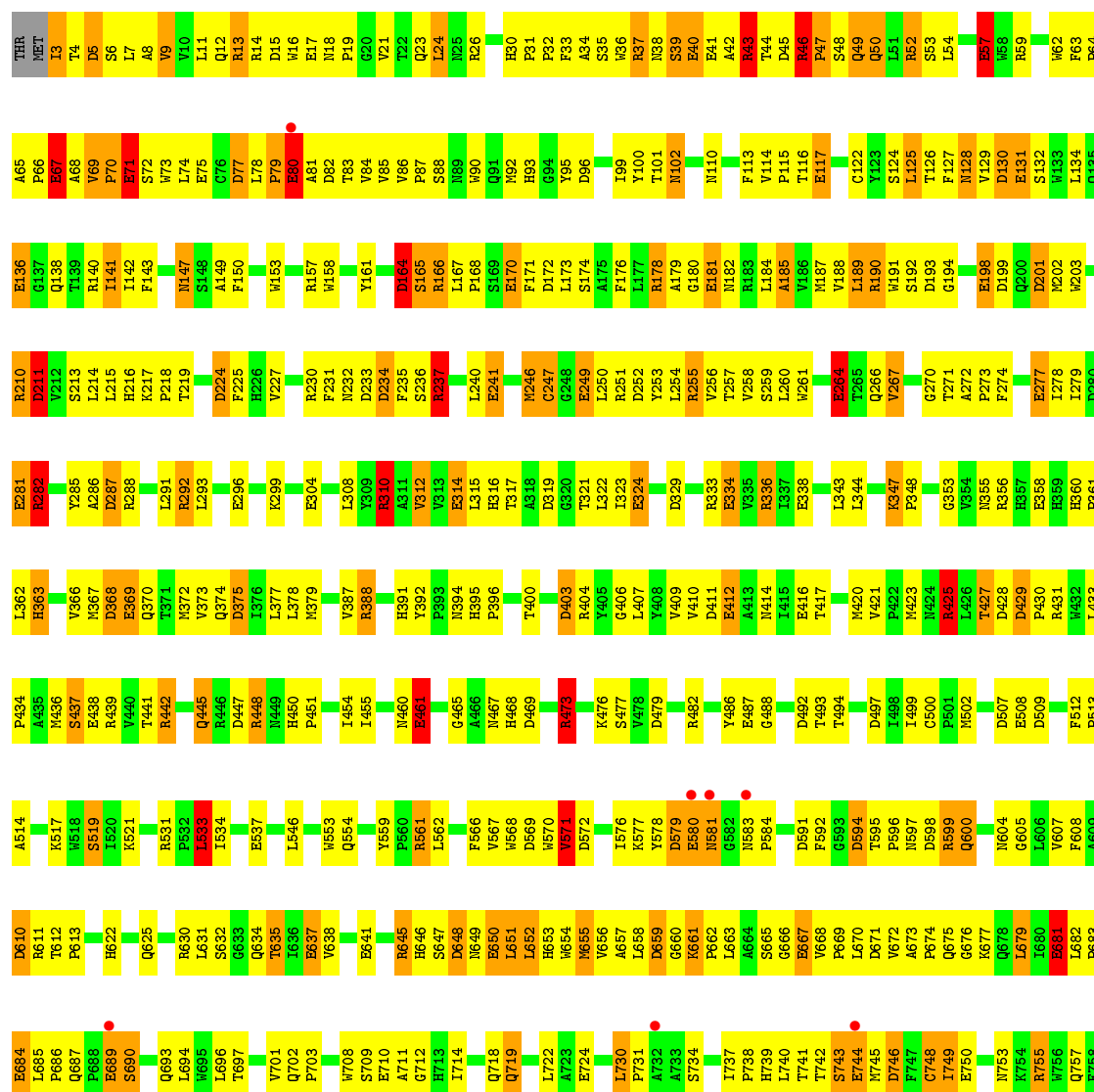
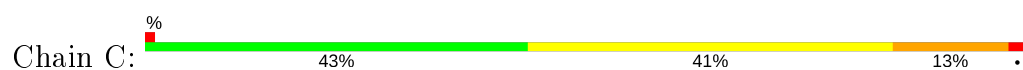
• Molecule 1: Beta-Galactosidase



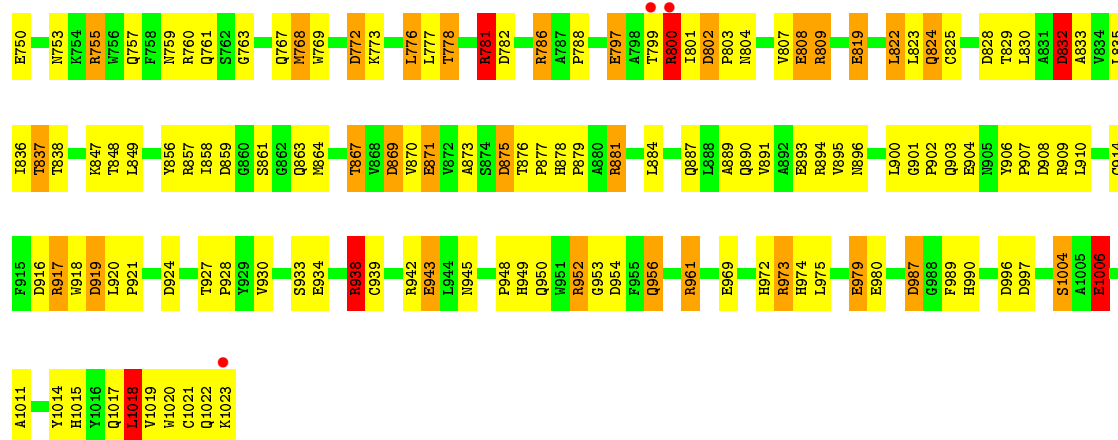




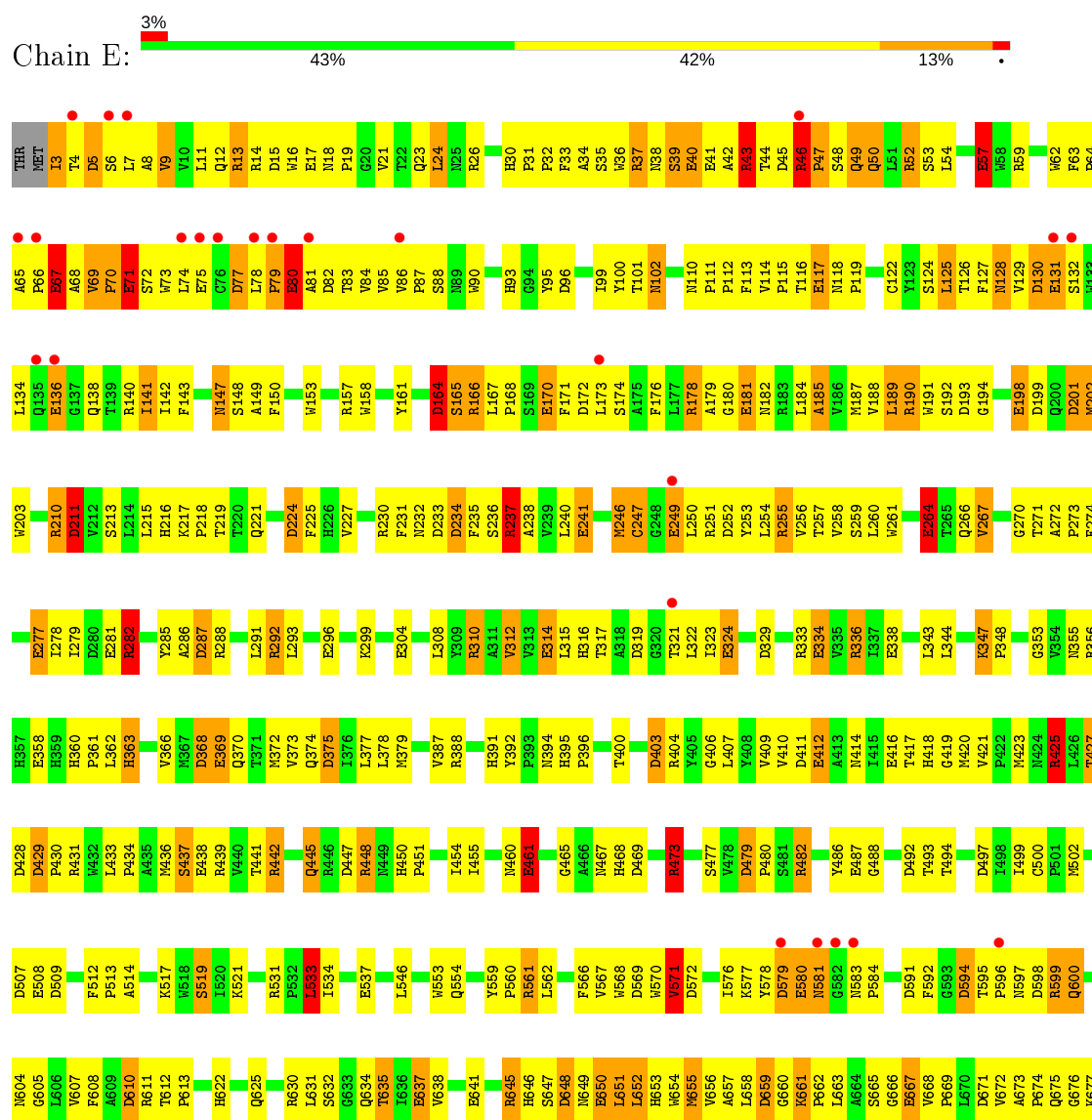
• Molecule 1: Beta-Galactosidase

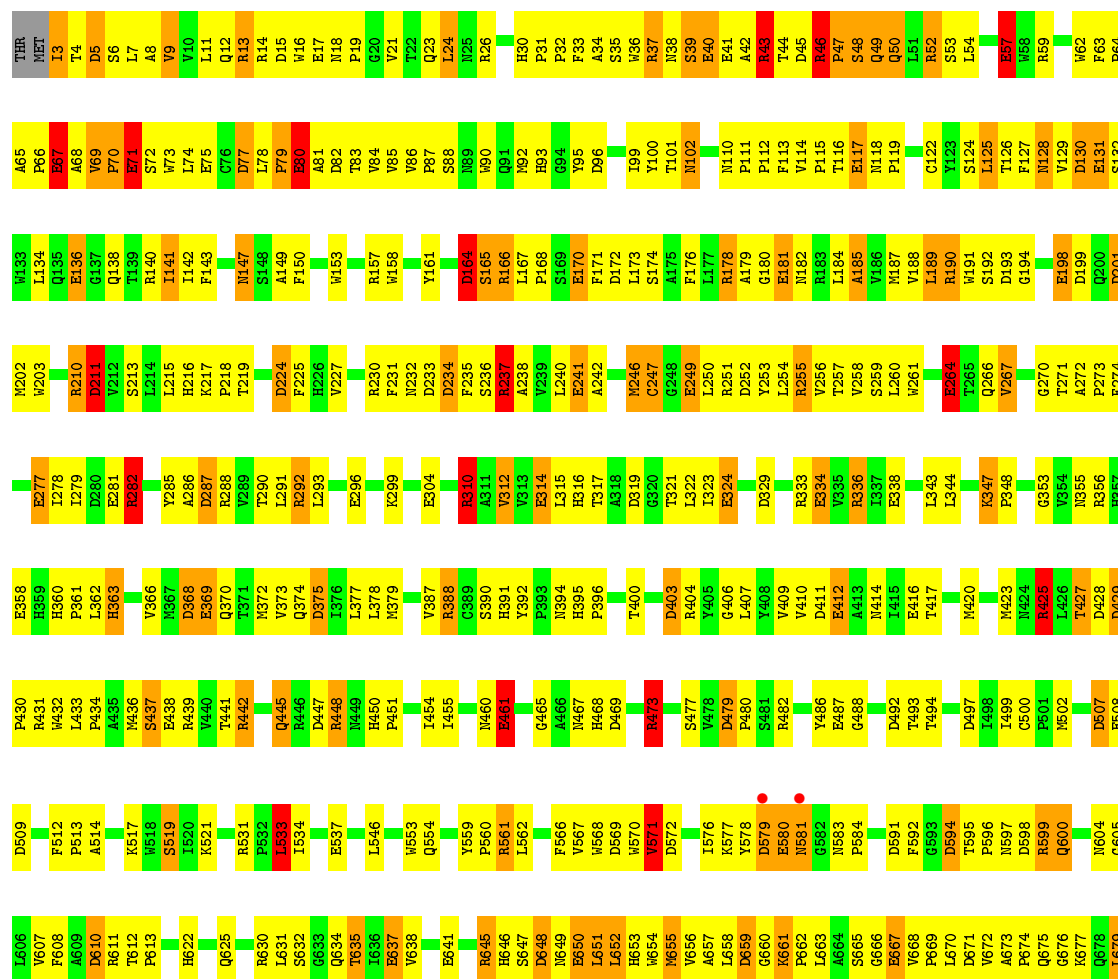


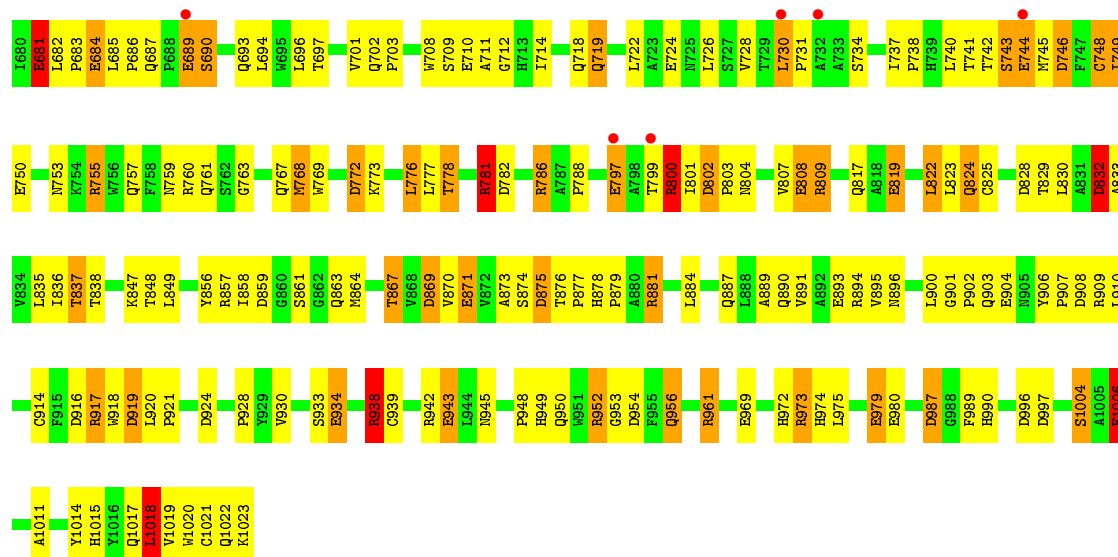




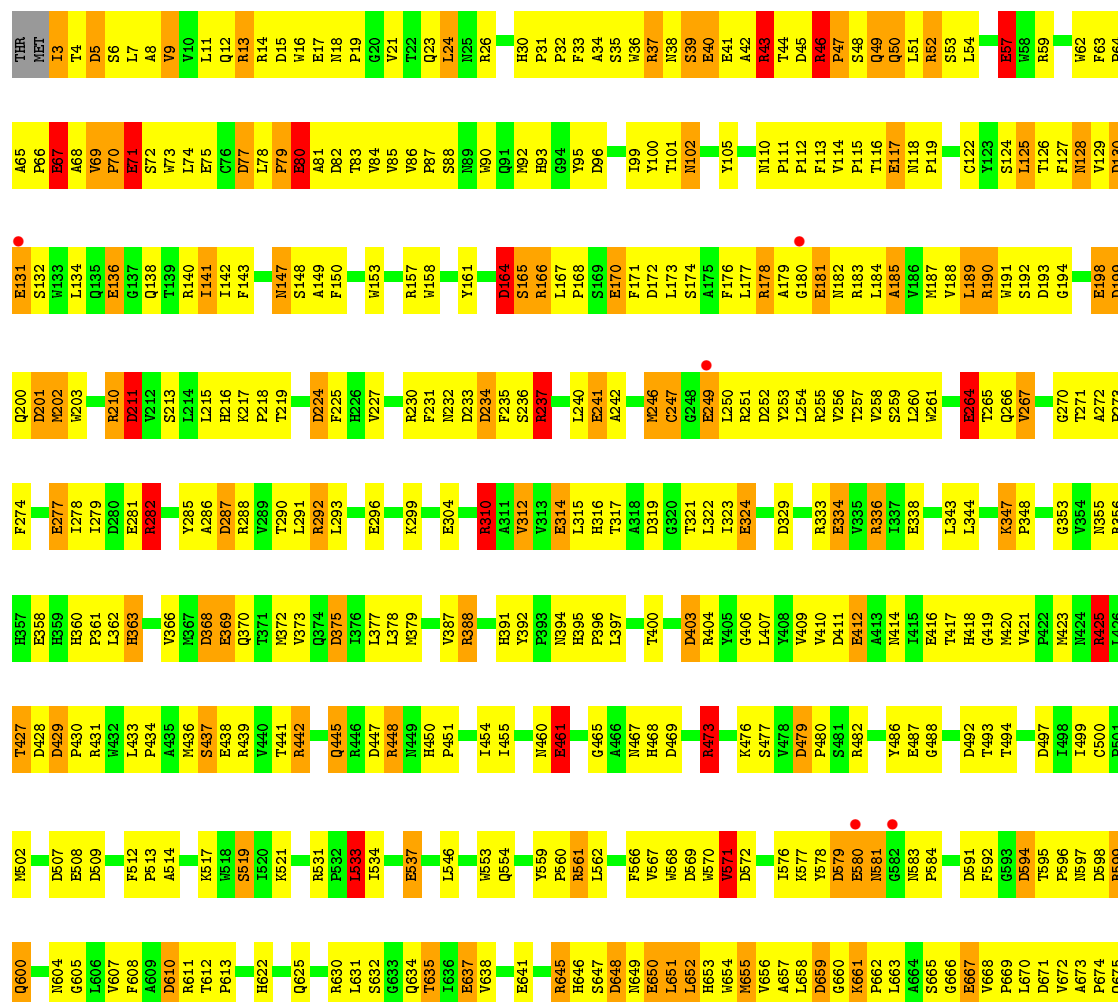
• Molecule 1: Beta-Galactosidase

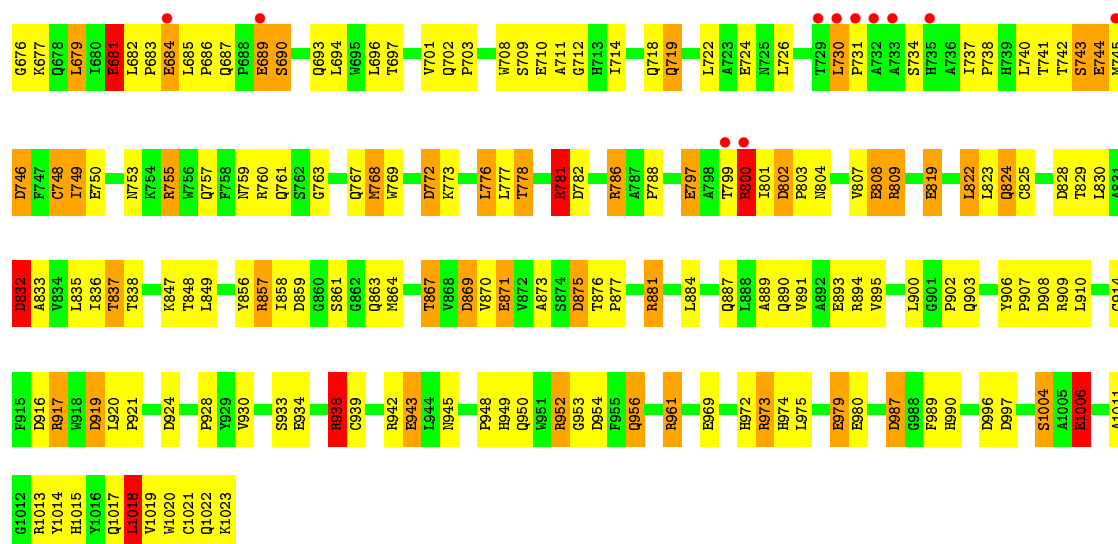




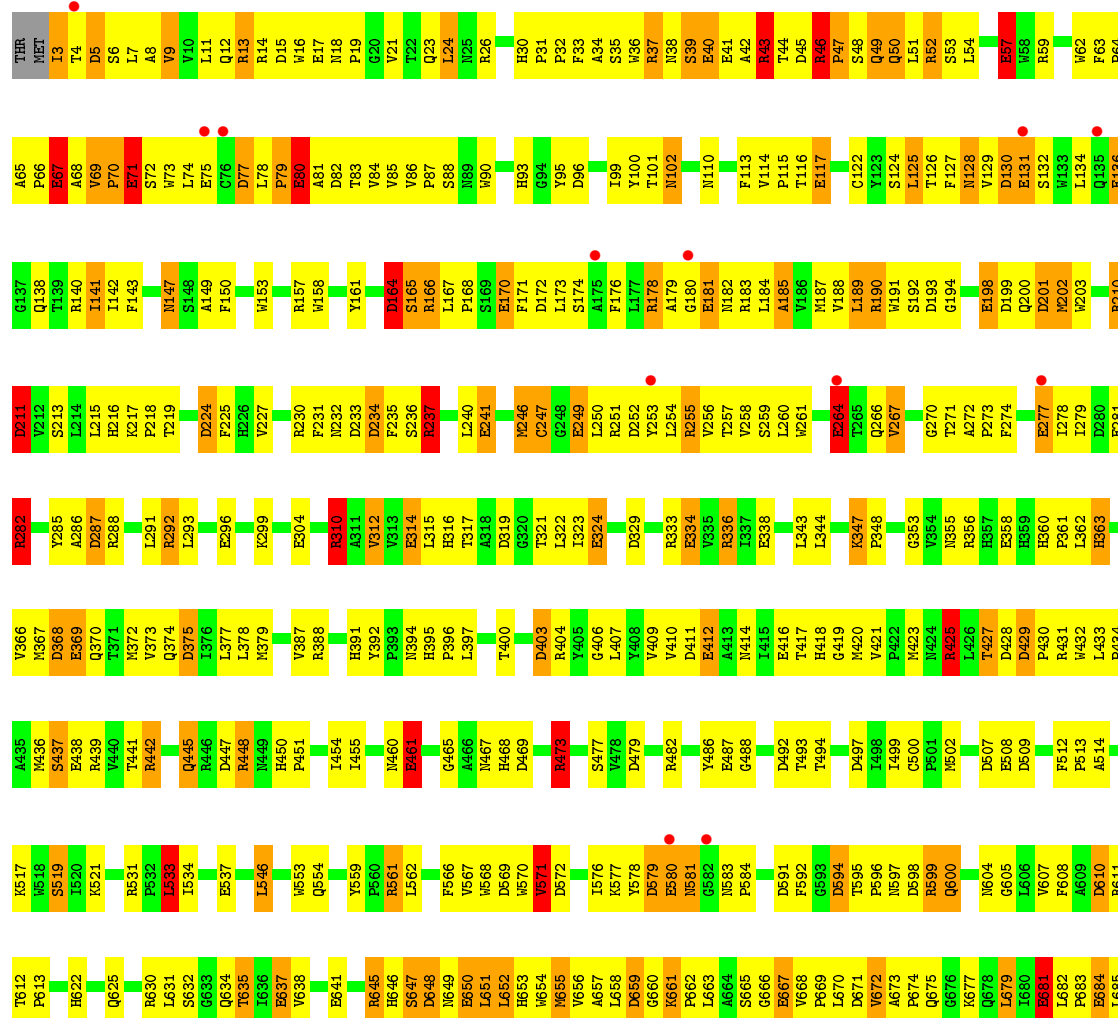
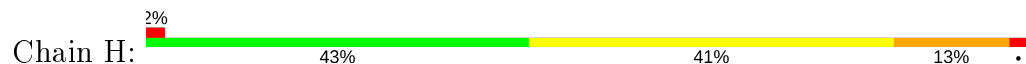


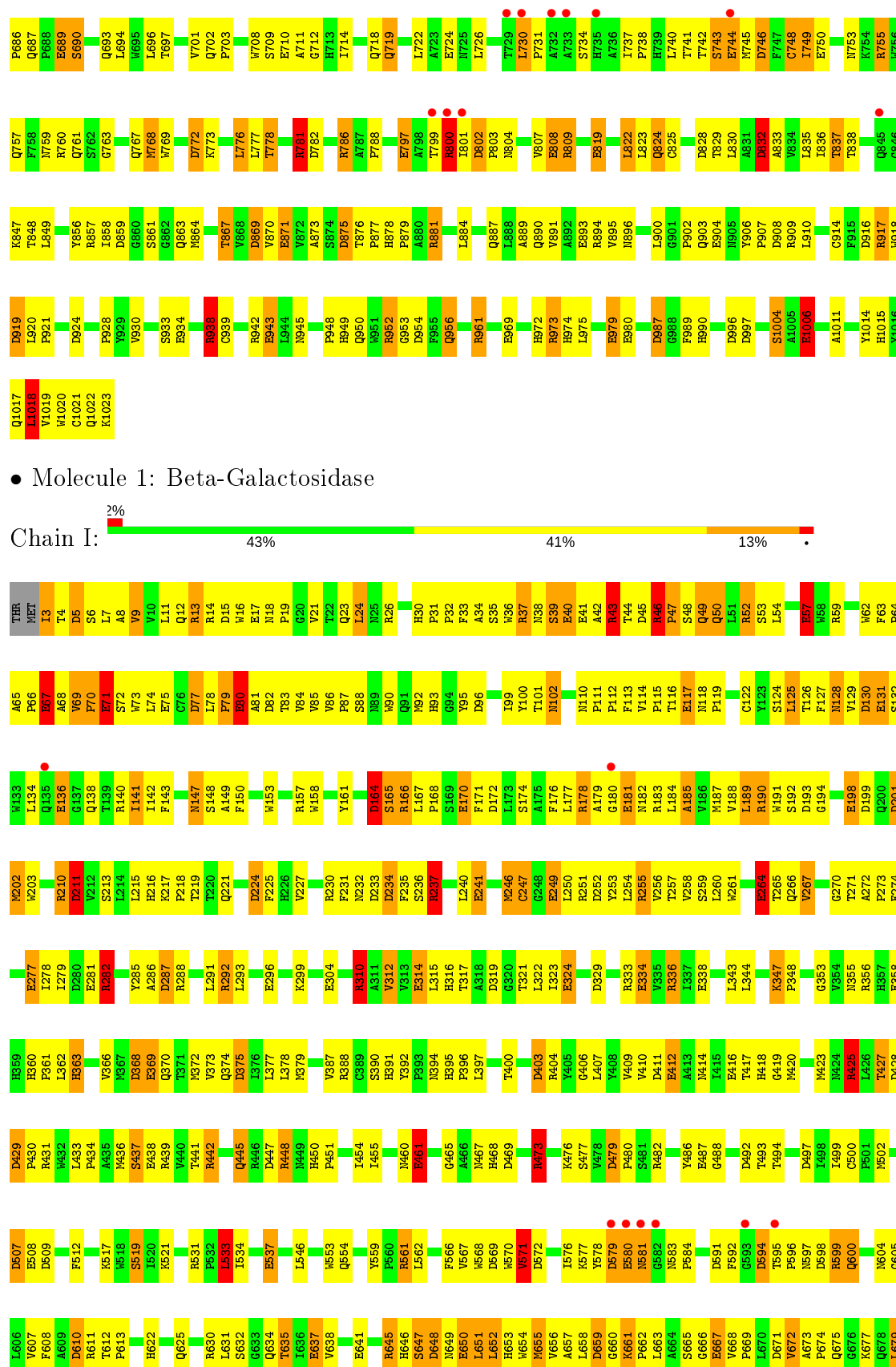
Molecule 1: Beta-Galactosidase

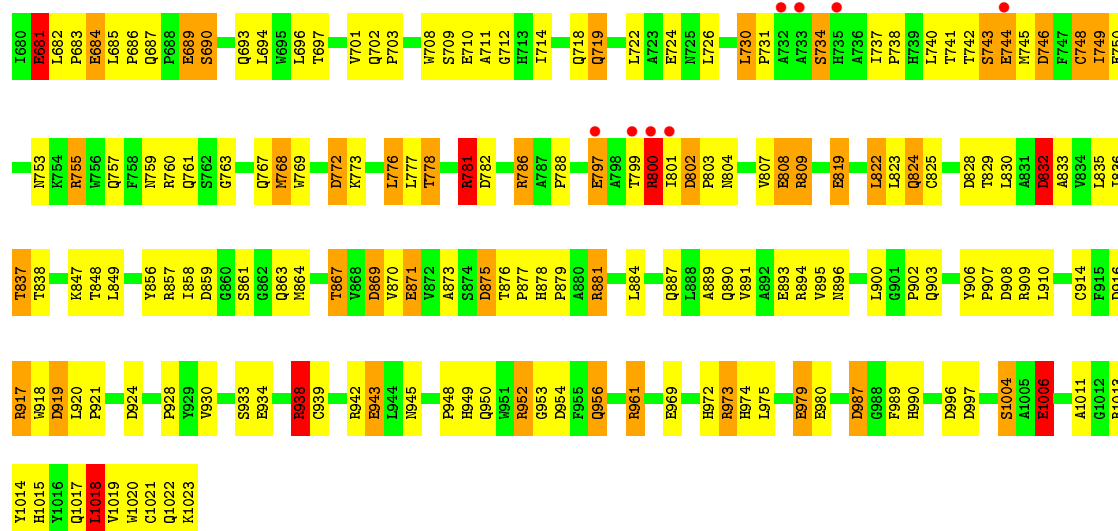




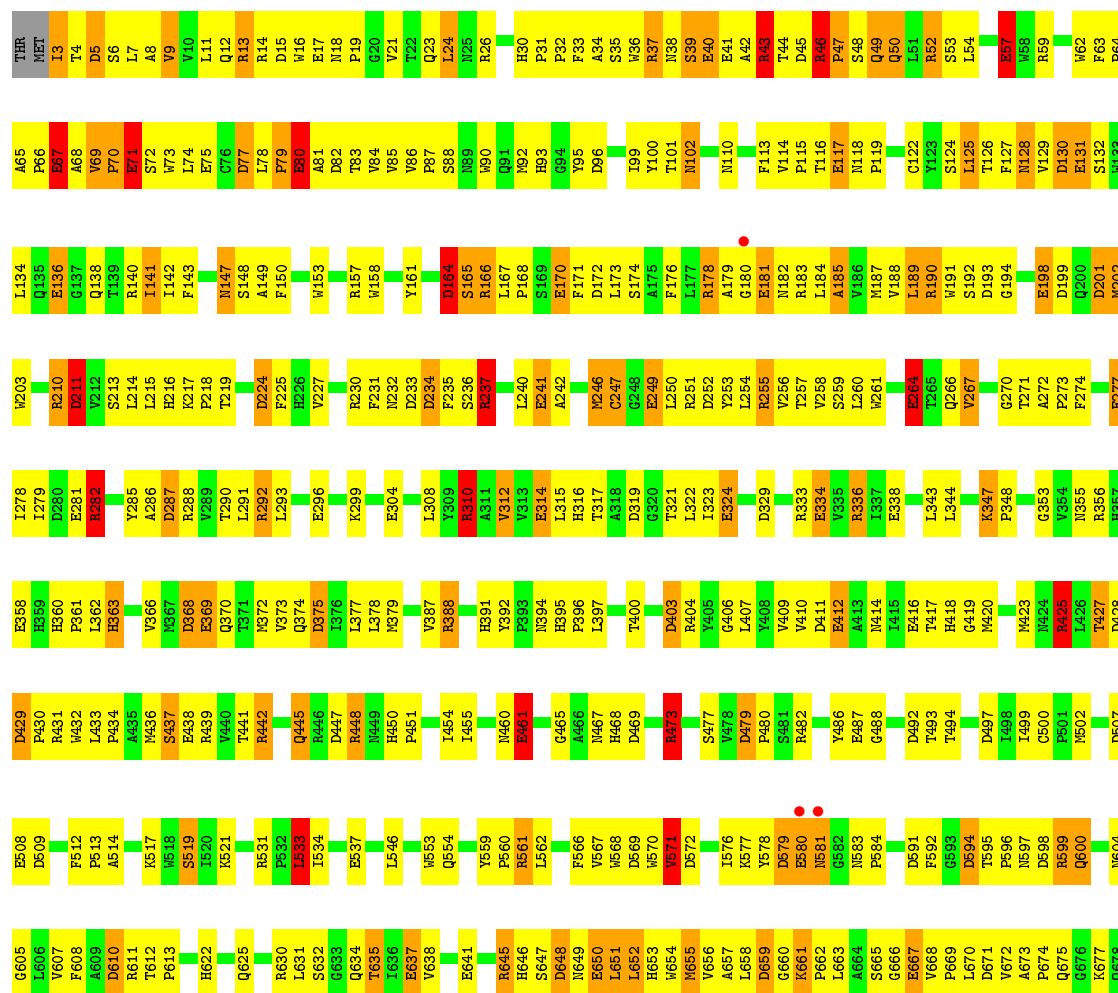
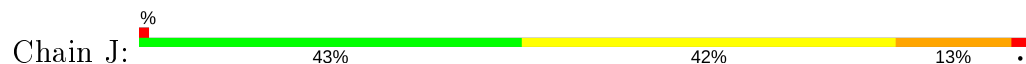
• Molecule 1: Beta-Galactosidase

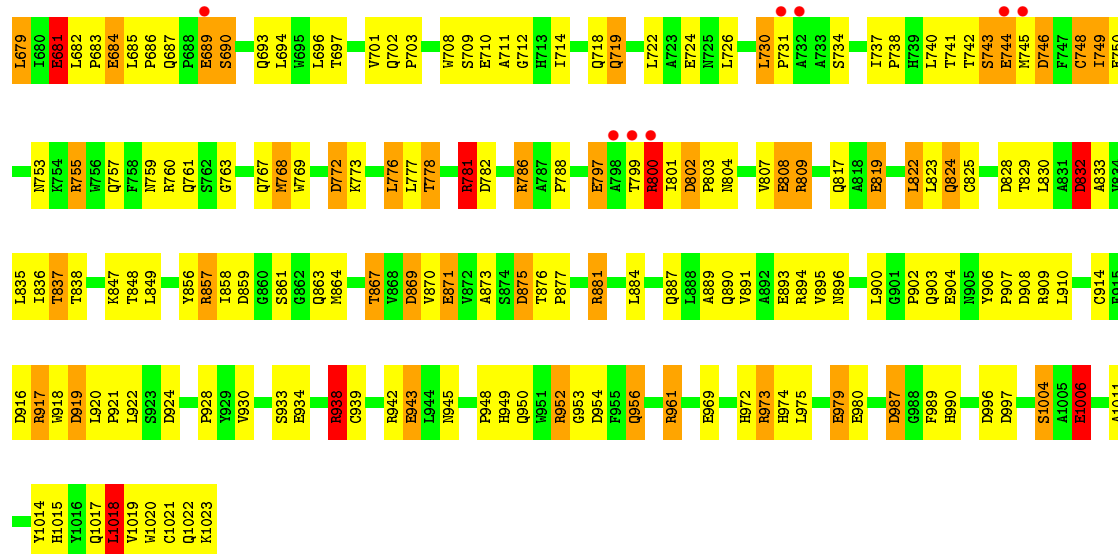




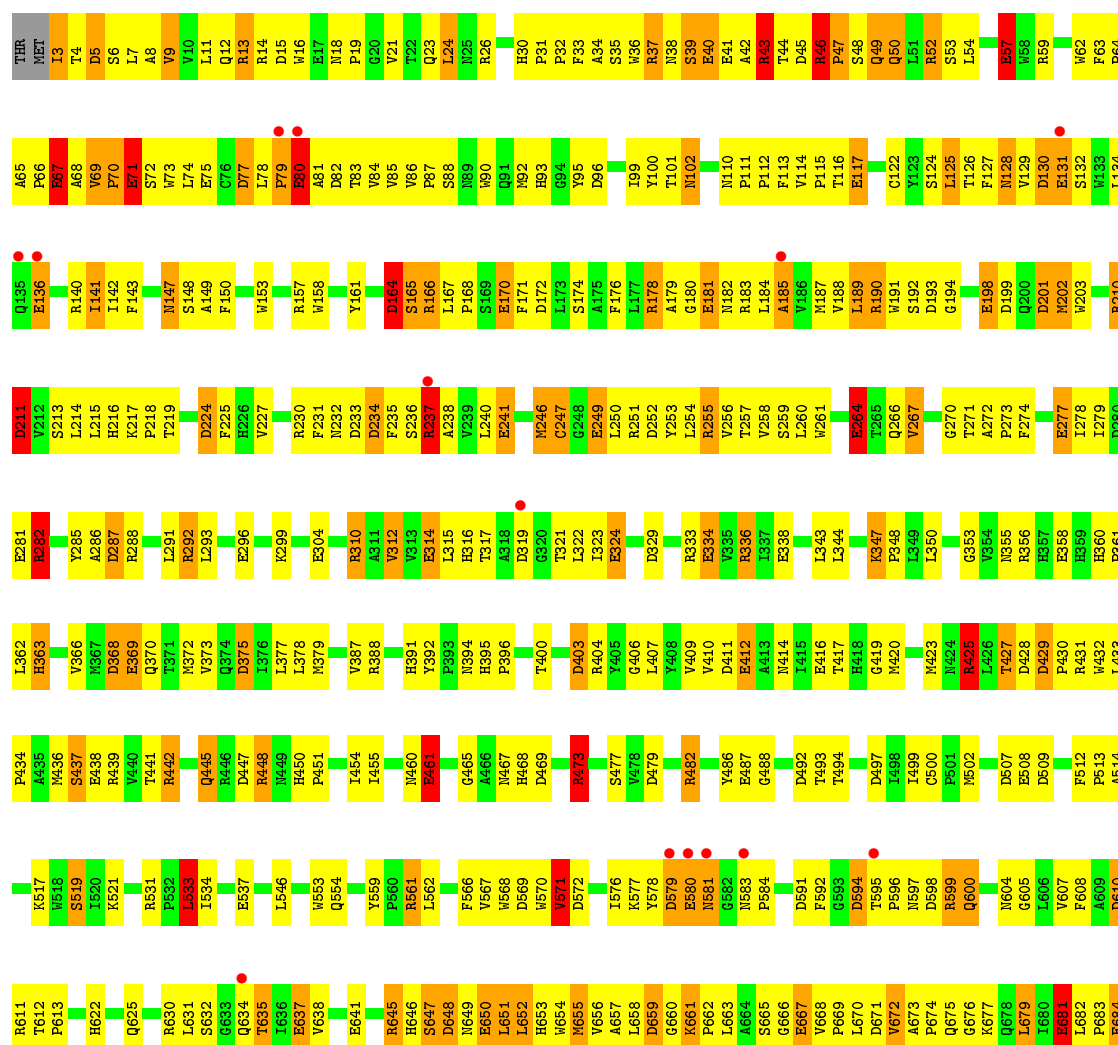
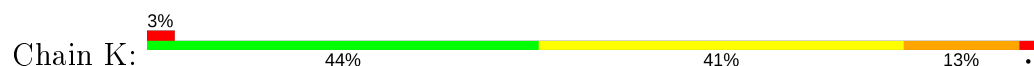


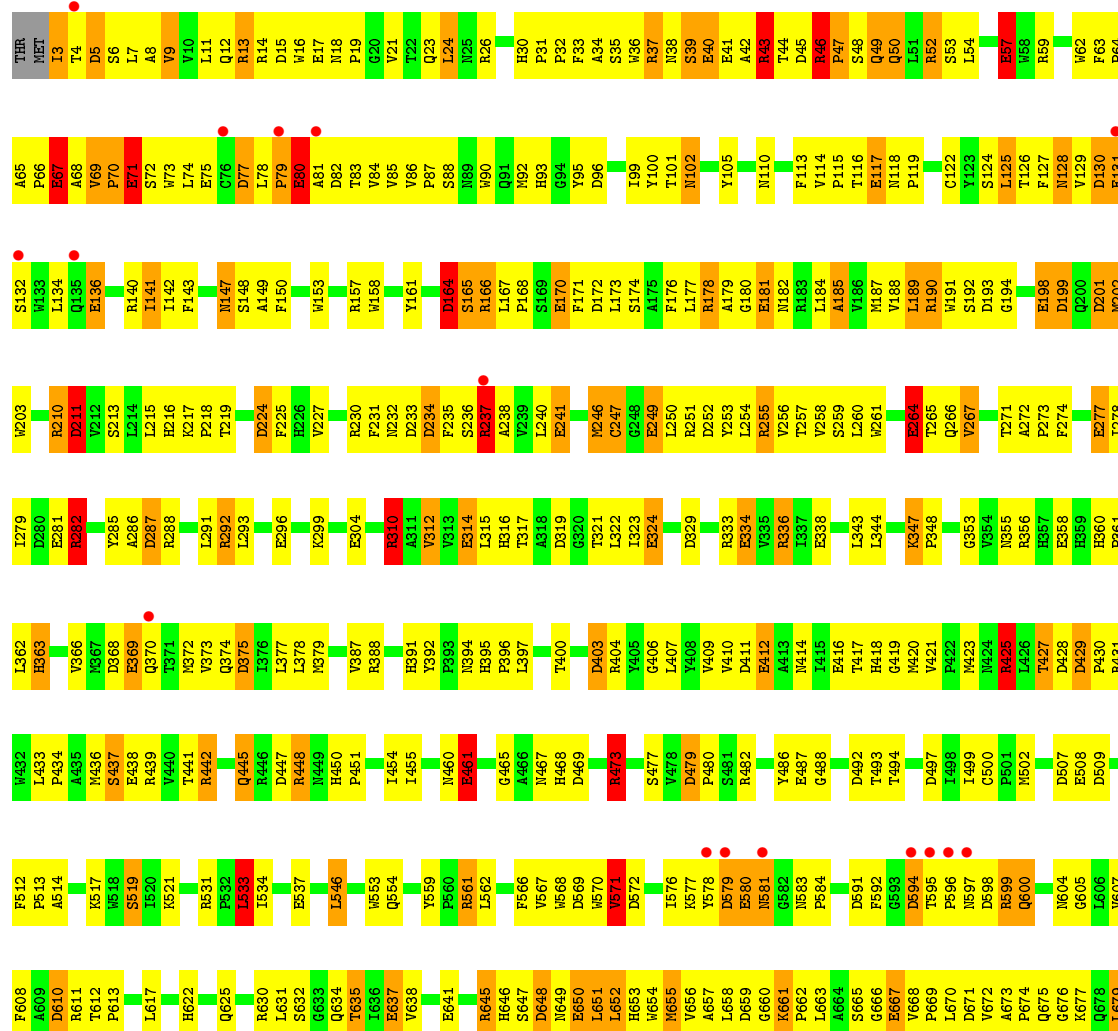
• Molecule 1: Beta-Galactosidase

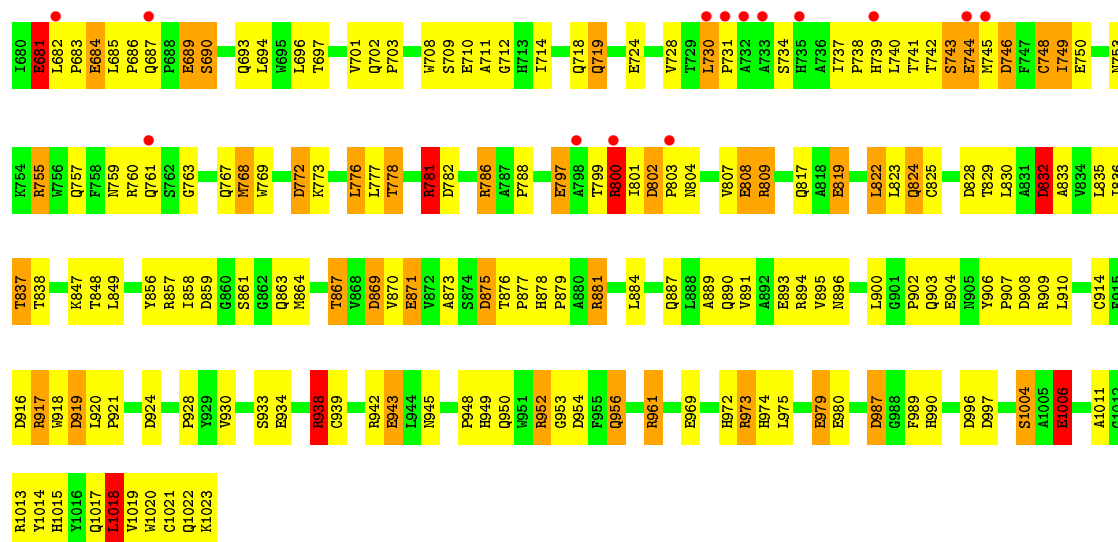




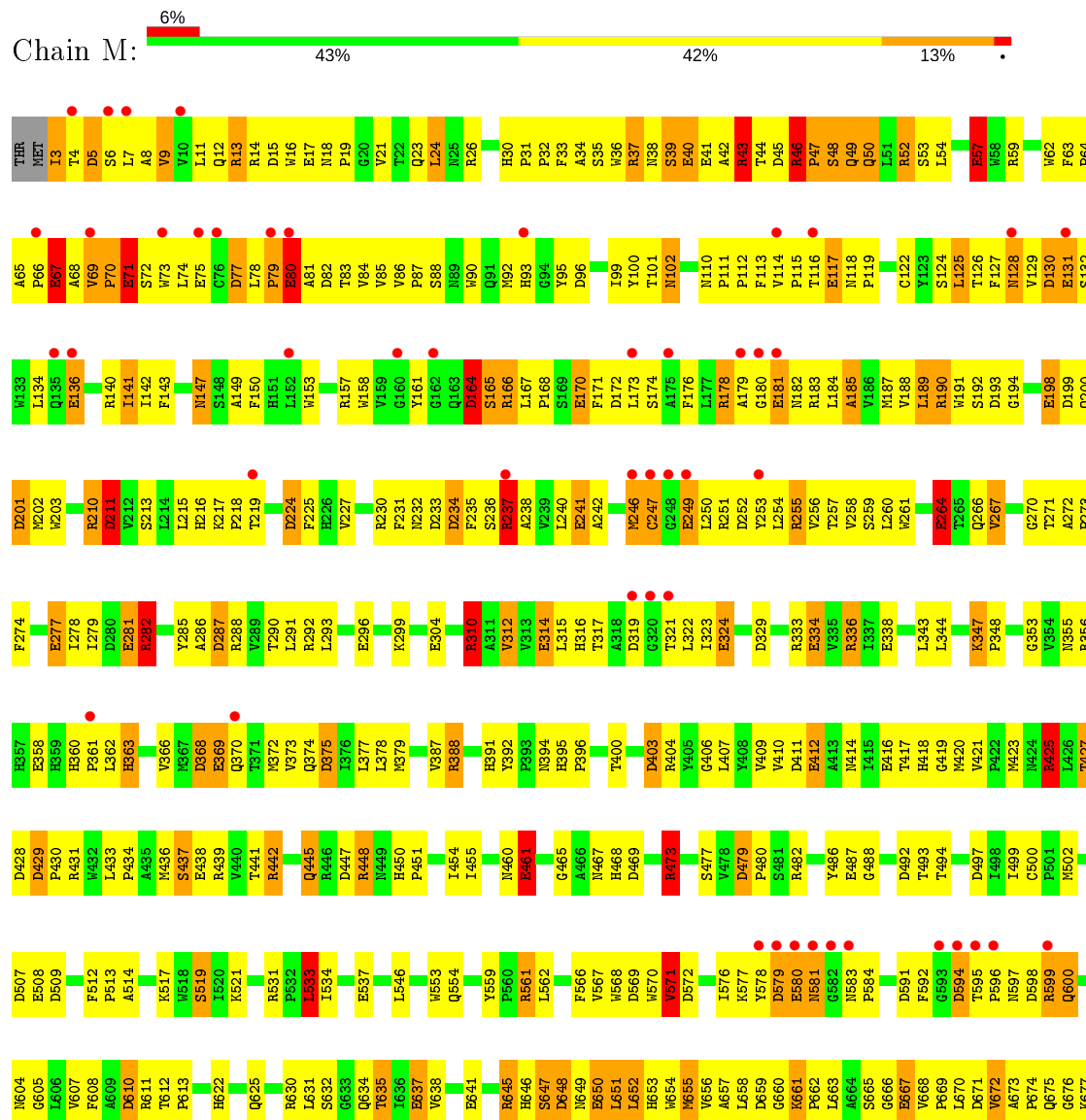
● Molecule 1: Beta-Galactosidase

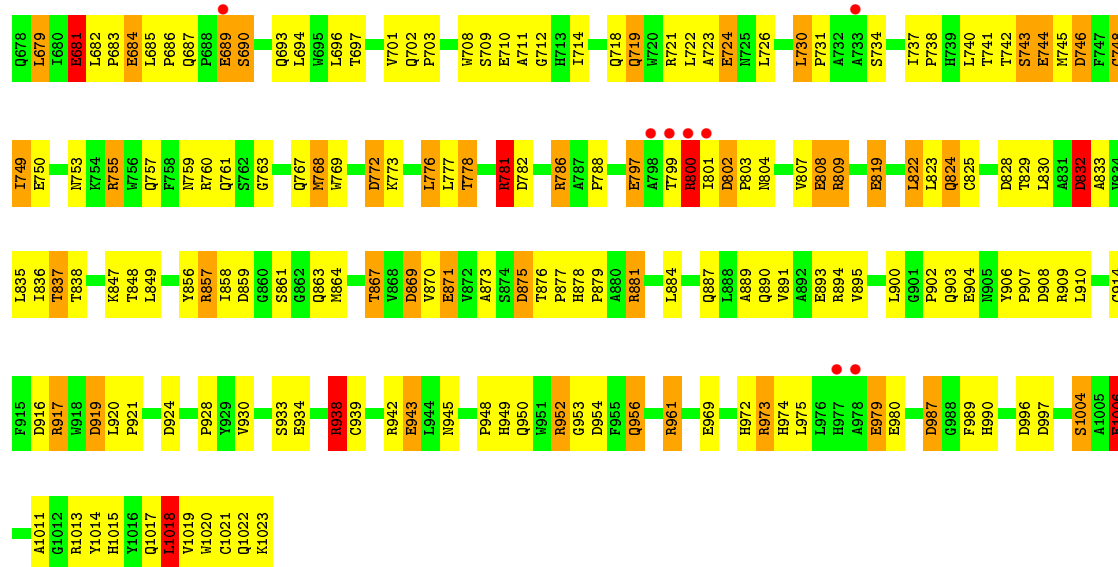




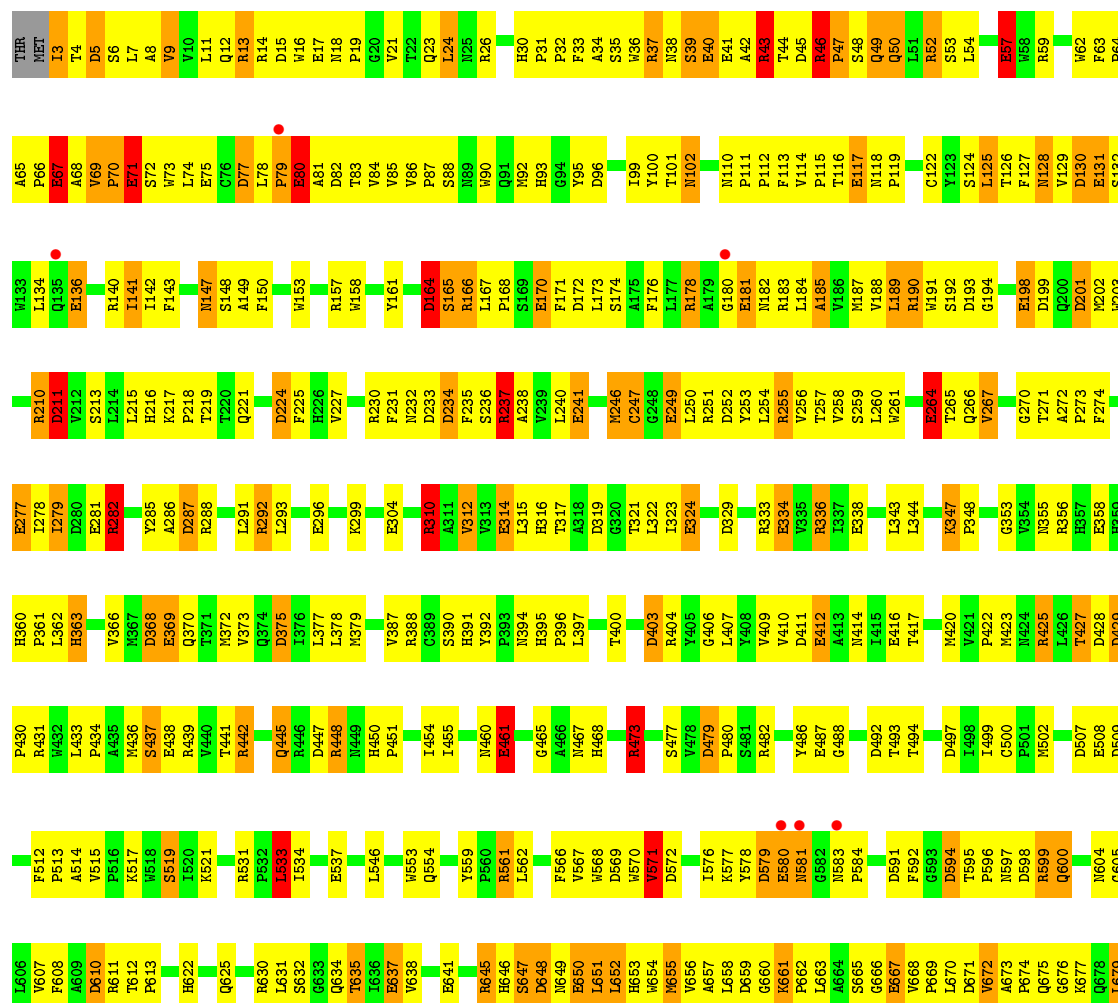


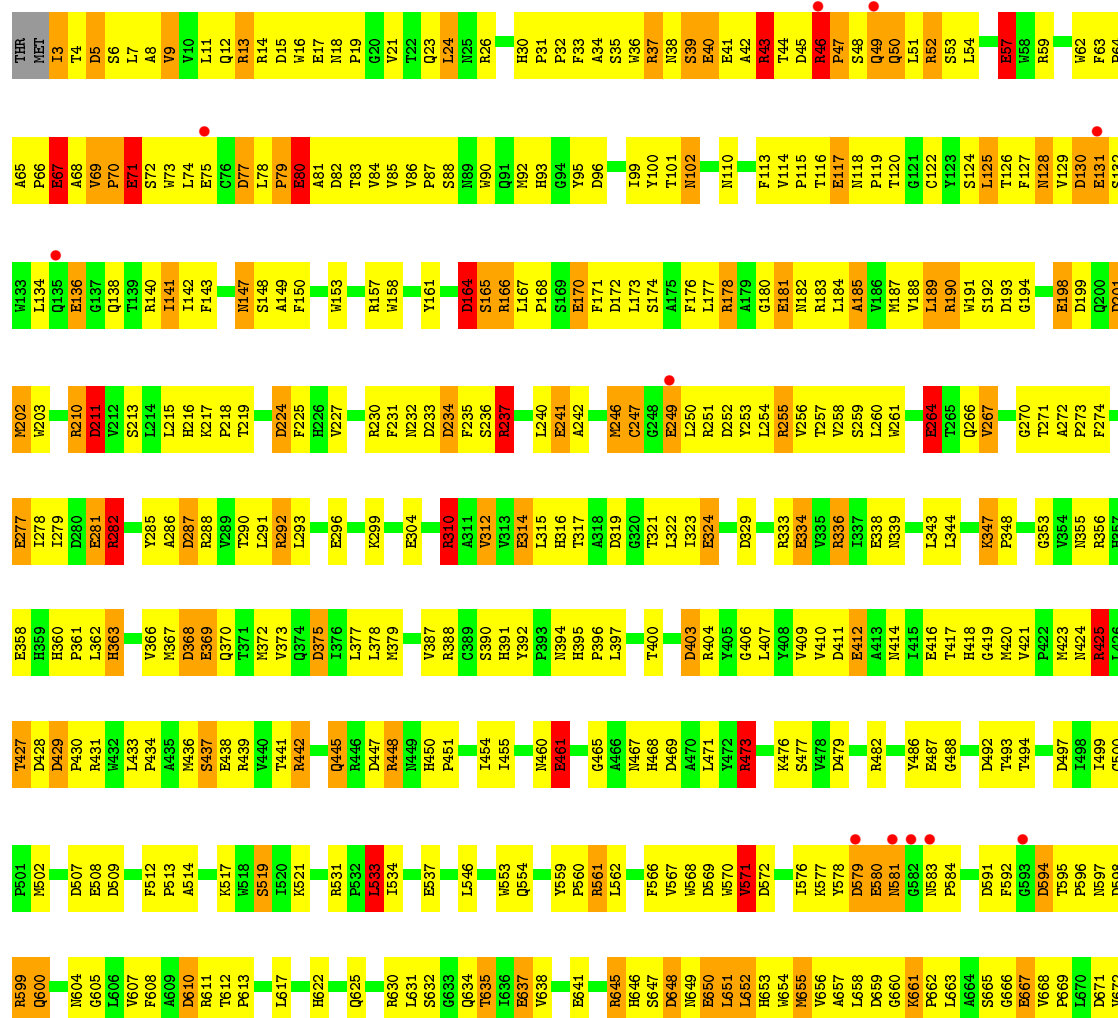
• Molecule 1: Beta-Galactosidase

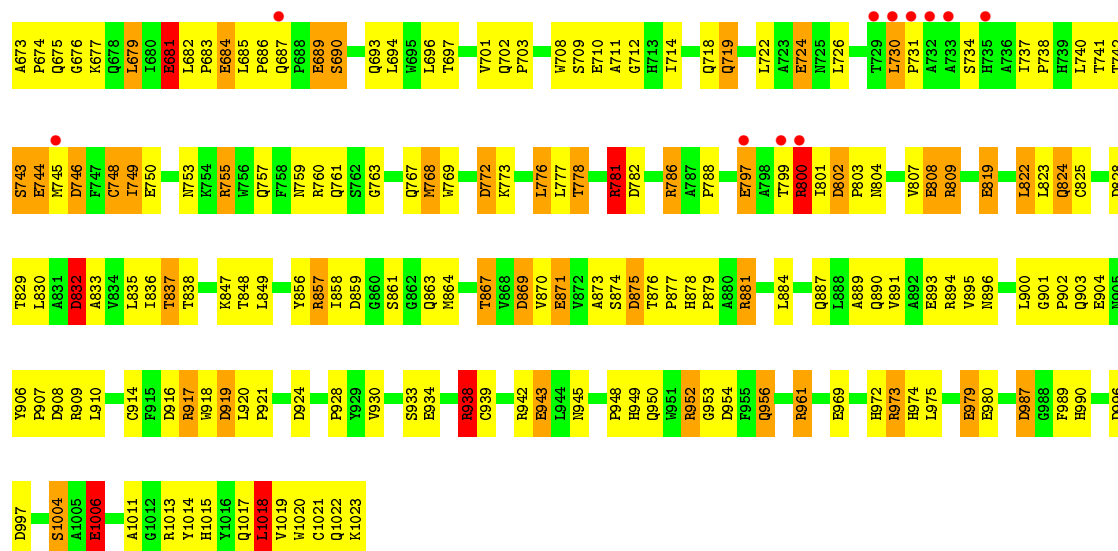




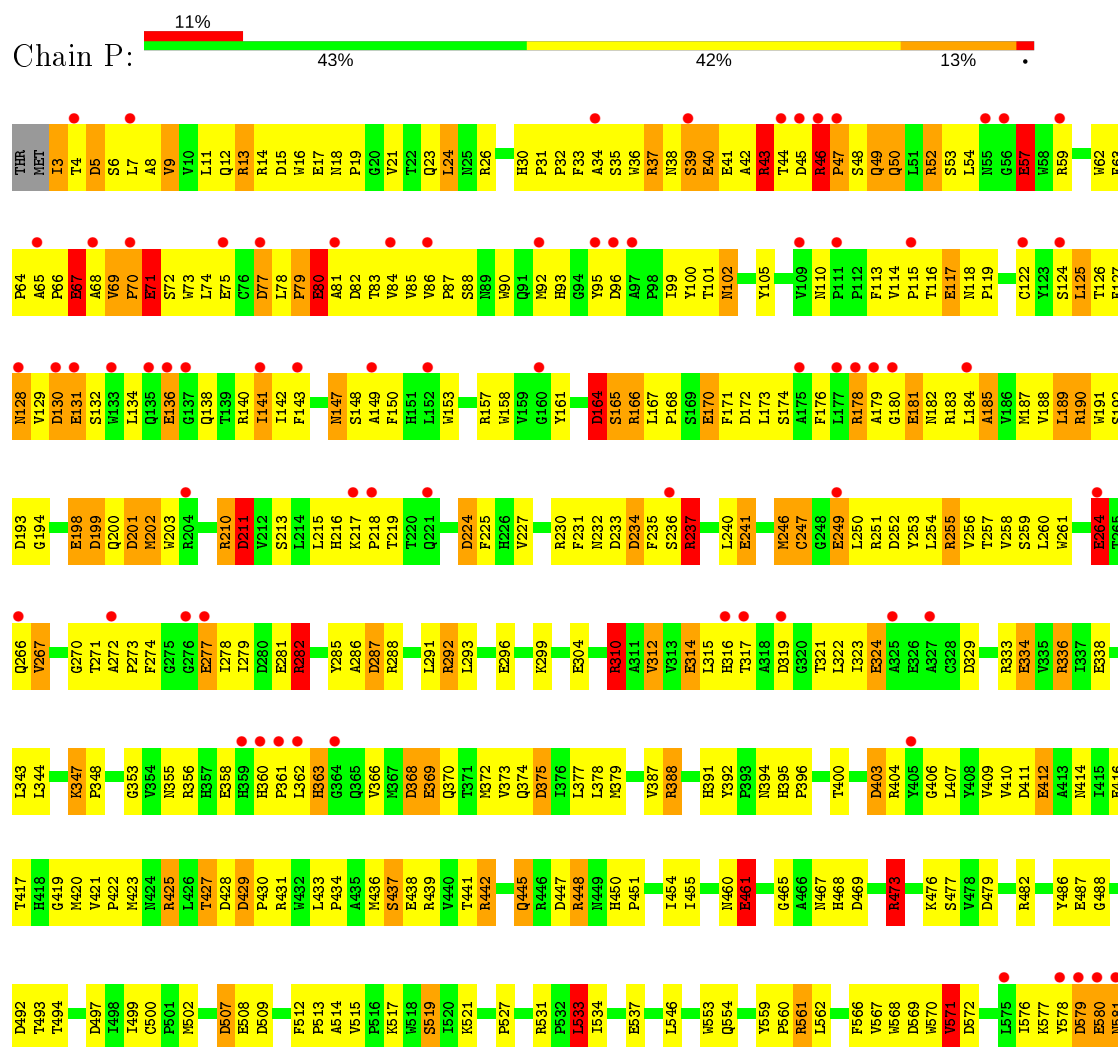
• Molecule 1: Beta-Galactosidase

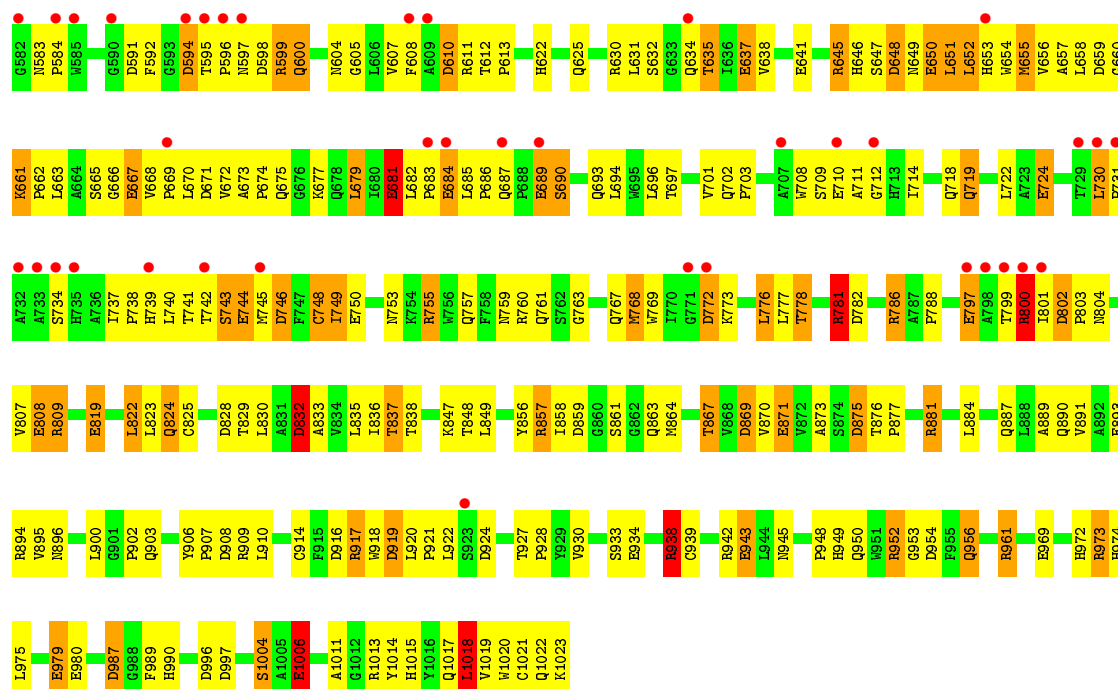






• Molecule 1: Beta-Galactosidase





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

Chain Q: 100%



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

Chain R: 100%



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

Chain S: 100%



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

Chain T: 100%



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

Chain U:  100%

B0C1
2FG2

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

Chain V:  100%

B0C1
2FG2

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

Chain W:  100%

B0C1
2FG2

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

Chain X:  100%

B0C1
2FG2

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

Chain Y:  100%

B0C1
2FG2

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

Chain Z:  100%

B0C1
2FG2

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

Chain a:  100%

B0C1
2FG2

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

Chain b:  100%

BCC1
2FG2

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

Chain c:  100%

BCC1
2FG2

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

Chain d:  100%

BCC1
2FG2

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

Chain e:  100%

BCC1
2FG2

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

Chain f:  100%

BCC1
2FG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.60Å 207.30Å 510.30Å 90.00° 95.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	66.0 (20.00-2.70) 66.0 (20.00-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.71Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.234 , (Not available) 0.211 , 0.211	Depositor DCC
R_{free} test set	1909 reflections (0.47%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 79.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	134528	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.52% 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: NA, MG, BGC, 2FG, CME

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	1.11	57/8439 (0.7%)	1.47	139/11510 (1.2%)
1	B	1.11	55/8439 (0.7%)	1.47	137/11510 (1.2%)
1	C	1.11	56/8439 (0.7%)	1.47	142/11510 (1.2%)
1	D	1.11	56/8439 (0.7%)	1.47	140/11510 (1.2%)
1	E	1.11	55/8439 (0.7%)	1.47	138/11510 (1.2%)
1	F	1.11	56/8439 (0.7%)	1.47	142/11510 (1.2%)
1	G	1.11	56/8439 (0.7%)	1.47	139/11510 (1.2%)
1	H	1.11	56/8439 (0.7%)	1.47	139/11510 (1.2%)
1	I	1.11	56/8439 (0.7%)	1.47	141/11510 (1.2%)
1	J	1.11	56/8439 (0.7%)	1.47	139/11510 (1.2%)
1	K	1.11	55/8439 (0.7%)	1.47	139/11510 (1.2%)
1	L	1.11	56/8439 (0.7%)	1.47	139/11510 (1.2%)
1	M	1.11	56/8439 (0.7%)	1.47	141/11510 (1.2%)
1	N	1.11	56/8439 (0.7%)	1.47	141/11510 (1.2%)
1	O	1.11	56/8439 (0.7%)	1.47	140/11510 (1.2%)
1	P	1.11	55/8439 (0.7%)	1.47	143/11510 (1.2%)
All	All	1.11	893/135024 (0.7%)	1.47	2239/184160 (1.2%)

The worst 5 of 893 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	710	GLU	CD-OE2	7.97	1.34	1.25
1	N	710	GLU	CD-OE2	7.97	1.34	1.25
1	A	710	GLU	CD-OE2	7.95	1.34	1.25
1	F	710	GLU	CD-OE2	7.95	1.34	1.25
1	P	710	GLU	CD-OE2	7.94	1.34	1.25

The worst 5 of 2239 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	561	ARG	NE-CZ-NH1	10.76	125.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	561	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	I	561	ARG	NE-CZ-NH1	10.71	125.65	120.30
1	C	561	ARG	NE-CZ-NH1	10.71	125.65	120.30
1	D	561	ARG	NE-CZ-NH1	10.68	125.64	120.30

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	8219	0	7811	586	3
1	B	8219	0	7811	563	5
1	C	8219	0	7811	548	1
1	D	8219	0	7811	584	0
1	E	8219	0	7811	568	0
1	F	8219	0	7811	557	1
1	G	8219	0	7811	571	1
1	H	8219	0	7811	564	0
1	I	8219	0	7811	573	1
1	J	8219	0	7811	566	0
1	K	8219	0	7811	561	0
1	L	8219	0	7811	574	1
1	M	8219	0	7811	566	0
1	N	8219	0	7811	566	0
1	O	8219	0	7811	575	0
1	P	8219	0	7811	576	2
2	Q	23	0	20	0	0
2	R	23	0	20	0	0
2	S	23	0	20	0	0
2	T	23	0	20	0	0
2	U	23	0	20	0	0
2	V	23	0	20	0	0
2	W	23	0	20	0	0
2	X	23	0	20	0	0
2	Y	23	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Z	23	0	20	0	0
2	a	23	0	20	0	0
2	b	23	0	20	0	0
2	c	23	0	20	0	0
2	d	23	0	20	0	0
2	e	23	0	20	0	0
2	f	23	0	20	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
3	M	2	0	0	0	0
3	N	2	0	0	0	0
3	O	2	0	0	0	0
3	P	2	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	2	0	0	0	0
4	M	2	0	0	0	0
4	N	2	0	0	0	0
4	O	2	0	0	0	0
4	P	2	0	0	0	0
5	A	160	0	0	6	0
5	B	163	0	0	6	0
5	C	162	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	163	0	0	6	0
5	E	162	0	0	6	0
5	F	162	0	0	6	0
5	G	162	0	0	6	0
5	H	162	0	0	6	0
5	I	162	0	0	6	1
5	J	162	0	0	6	0
5	K	162	0	0	6	0
5	L	162	0	0	6	0
5	M	161	0	0	6	0
5	N	163	0	0	6	0
5	O	161	0	0	6	0
5	P	163	0	0	6	0
All	All	134528	0	125296	8965	8

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 35.

The worst 5 of 8965 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:J:43:ARG:HH11	1:J:43:ARG:HG2	1.20	1.07
1:H:43:ARG:HG2	1:H:43:ARG:HH11	1.20	1.07
1:I:43:ARG:HH11	1:I:43:ARG:HG2	1.20	1.07
1:A:43:ARG:HH11	1:A:43:ARG:HG2	1.20	1.07
1:M:43:ARG:HH11	1:M:43:ARG:HG2	1.20	1.06

The worst 5 of 8 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:GLU:O	1:B:578:TYR:CG[2_555]	1.57	0.63
1:A:580:GLU:O	1:B:578:TYR:CB[2_555]	1.68	0.52
1:G:740:LEU:O	1:L:739:HIS:CD2[1_455]	1.94	0.26
1:A:580:GLU:O	1:B:578:TYR:CD1[2_555]	1.97	0.23
1:B:740:LEU:O	1:P:739:HIS:CD2[1_354]	2.09	0.11

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	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	17	40
1	B	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	17	40
1	C	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	17	40
1	D	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	17	40
1	E	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	17	40
1	F	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	17	40
1	G	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	17	40
1	H	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	17	40
1	I	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	17	40
1	J	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	17	40
1	K	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	17	40
1	L	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	17	40
1	M	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	17	40
1	N	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	17	40
1	O	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	17	40
1	P	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	17	40
All	All	16288/16368 (100%)	15296 (94%)	848 (5%)	144 (1%)	17	40

5 of 144 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	SER
1	B	174	SER
1	C	174	SER
1	D	174	SER
1	E	174	SER

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	872/872 (100%)	759 (87%)	113 (13%)	4	10
1	B	872/872 (100%)	759 (87%)	113 (13%)	4	10
1	C	872/872 (100%)	759 (87%)	113 (13%)	4	10
1	D	872/872 (100%)	759 (87%)	113 (13%)	4	10
1	E	872/872 (100%)	759 (87%)	113 (13%)	4	10
1	F	872/872 (100%)	759 (87%)	113 (13%)	4	10
1	G	872/872 (100%)	759 (87%)	113 (13%)	4	10
1	H	872/872 (100%)	759 (87%)	113 (13%)	4	10
1	I	872/872 (100%)	759 (87%)	113 (13%)	4	10
1	J	872/872 (100%)	759 (87%)	113 (13%)	4	10
1	K	872/872 (100%)	759 (87%)	113 (13%)	4	10
1	L	872/872 (100%)	759 (87%)	113 (13%)	4	10
1	M	872/872 (100%)	759 (87%)	113 (13%)	4	10
1	N	872/872 (100%)	759 (87%)	113 (13%)	4	10
1	O	872/872 (100%)	759 (87%)	113 (13%)	4	10
1	P	872/872 (100%)	759 (87%)	113 (13%)	4	10
All	All	13952/13952 (100%)	12144 (87%)	1808 (13%)	4	10

5 of 1808 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	165	SER
1	I	938	ARG
1	O	768	MET
1	H	347	LYS
1	I	71	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 317 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	316	HIS
1	I	1017	GLN
1	O	761	GLN
1	H	467	ASN
1	I	128	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

48 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CME	H	914	1	8,9,10	0.89	0	5,9,11	1.69	1 (20%)
1	CME	H	748	1	8,9,10	0.90	0	5,9,11	1.57	1 (20%)
1	CME	E	1021	1	8,9,10	0.67	0	5,9,11	1.20	0
1	CME	J	914	1	8,9,10	0.89	0	5,9,11	1.69	1 (20%)
1	CME	L	914	1	8,9,10	0.90	0	5,9,11	1.69	1 (20%)
1	CME	C	1021	1	8,9,10	0.66	0	5,9,11	1.20	0
1	CME	K	914	1	8,9,10	0.89	0	5,9,11	1.70	1 (20%)
1	CME	K	748	1	8,9,10	0.91	0	5,9,11	1.57	1 (20%)
1	CME	A	1021	1	8,9,10	0.66	0	5,9,11	1.20	0
1	CME	F	1021	1	8,9,10	0.68	0	5,9,11	1.20	0
1	CME	P	914	1	8,9,10	0.90	0	5,9,11	1.70	1 (20%)
1	CME	J	1021	1	8,9,10	0.67	0	5,9,11	1.20	0
1	CME	C	748	1	8,9,10	0.90	0	5,9,11	1.57	1 (20%)
1	CME	A	748	1	8,9,10	0.90	0	5,9,11	1.57	1 (20%)
1	CME	J	748	1	8,9,10	0.91	0	5,9,11	1.57	1 (20%)
1	CME	B	748	1	8,9,10	0.90	0	5,9,11	1.57	1 (20%)
1	CME	E	914	1	8,9,10	0.90	0	5,9,11	1.70	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CME	I	748	1	8,9,10	0.91	0	5,9,11	1.57	1 (20%)
1	CME	D	1021	1	8,9,10	0.68	0	5,9,11	1.19	0
1	CME	K	1021	1	8,9,10	0.67	0	5,9,11	1.20	0
1	CME	H	1021	1	8,9,10	0.67	0	5,9,11	1.20	0
1	CME	L	748	1	8,9,10	0.90	0	5,9,11	1.57	1 (20%)
1	CME	E	748	1	8,9,10	0.90	0	5,9,11	1.57	1 (20%)
1	CME	N	1021	1	8,9,10	0.67	0	5,9,11	1.20	0
1	CME	M	914	1	8,9,10	0.90	0	5,9,11	1.70	1 (20%)
1	CME	F	748	1	8,9,10	0.91	0	5,9,11	1.57	1 (20%)
1	CME	O	914	1	8,9,10	0.90	0	5,9,11	1.69	1 (20%)
1	CME	I	914	1	8,9,10	0.89	0	5,9,11	1.70	1 (20%)
1	CME	O	748	1	8,9,10	0.91	0	5,9,11	1.57	1 (20%)
1	CME	B	1021	1	8,9,10	0.66	0	5,9,11	1.20	0
1	CME	B	914	1	8,9,10	0.89	0	5,9,11	1.70	1 (20%)
1	CME	A	914	1	8,9,10	0.90	0	5,9,11	1.69	1 (20%)
1	CME	F	914	1	8,9,10	0.89	0	5,9,11	1.70	1 (20%)
1	CME	O	1021	1	8,9,10	0.67	0	5,9,11	1.20	0
1	CME	P	1021	1	8,9,10	0.67	0	5,9,11	1.20	0
1	CME	N	748	1	8,9,10	0.91	0	5,9,11	1.57	1 (20%)
1	CME	L	1021	1	8,9,10	0.67	0	5,9,11	1.20	0
1	CME	N	914	1	8,9,10	0.89	0	5,9,11	1.69	1 (20%)
1	CME	G	914	1	8,9,10	0.89	0	5,9,11	1.70	1 (20%)
1	CME	I	1021	1	8,9,10	0.67	0	5,9,11	1.20	0
1	CME	D	748	1	8,9,10	0.91	0	5,9,11	1.57	1 (20%)
1	CME	G	1021	1	8,9,10	0.67	0	5,9,11	1.20	0
1	CME	M	1021	1	8,9,10	0.67	0	5,9,11	1.20	0
1	CME	D	914	1	8,9,10	0.89	0	5,9,11	1.69	1 (20%)
1	CME	G	748	1	8,9,10	0.90	0	5,9,11	1.56	1 (20%)
1	CME	M	748	1	8,9,10	0.90	0	5,9,11	1.57	1 (20%)
1	CME	P	748	1	8,9,10	0.91	0	5,9,11	1.57	1 (20%)
1	CME	C	914	1	8,9,10	0.90	0	5,9,11	1.69	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CME	H	914	1	-	3/5/8/10	-
1	CME	H	748	1	-	4/5/8/10	-
1	CME	E	1021	1	-	4/5/8/10	-
1	CME	J	914	1	-	3/5/8/10	-
1	CME	L	914	1	-	2/5/8/10	-
1	CME	C	1021	1	-	4/5/8/10	-
1	CME	K	914	1	-	3/5/8/10	-
1	CME	K	748	1	-	4/5/8/10	-
1	CME	A	1021	1	-	4/5/8/10	-
1	CME	F	1021	1	-	4/5/8/10	-
1	CME	P	914	1	-	3/5/8/10	-
1	CME	J	1021	1	-	4/5/8/10	-
1	CME	C	748	1	-	4/5/8/10	-
1	CME	A	748	1	-	4/5/8/10	-
1	CME	J	748	1	-	4/5/8/10	-
1	CME	B	748	1	-	4/5/8/10	-
1	CME	E	914	1	-	2/5/8/10	-
1	CME	I	748	1	-	4/5/8/10	-
1	CME	D	1021	1	-	4/5/8/10	-
1	CME	K	1021	1	-	4/5/8/10	-
1	CME	H	1021	1	-	4/5/8/10	-
1	CME	L	748	1	-	4/5/8/10	-
1	CME	E	748	1	-	4/5/8/10	-
1	CME	N	1021	1	-	4/5/8/10	-
1	CME	M	914	1	-	3/5/8/10	-
1	CME	F	748	1	-	4/5/8/10	-
1	CME	O	914	1	-	3/5/8/10	-
1	CME	I	914	1	-	3/5/8/10	-
1	CME	O	748	1	-	4/5/8/10	-
1	CME	B	1021	1	-	4/5/8/10	-
1	CME	B	914	1	-	3/5/8/10	-
1	CME	A	914	1	-	3/5/8/10	-
1	CME	F	914	1	-	2/5/8/10	-
1	CME	O	1021	1	-	4/5/8/10	-
1	CME	P	1021	1	-	4/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CME	N	748	1	-	4/5/8/10	-
1	CME	L	1021	1	-	4/5/8/10	-
1	CME	N	914	1	-	3/5/8/10	-
1	CME	G	914	1	-	3/5/8/10	-
1	CME	I	1021	1	-	4/5/8/10	-
1	CME	D	748	1	-	4/5/8/10	-
1	CME	G	1021	1	-	4/5/8/10	-
1	CME	M	1021	1	-	4/5/8/10	-
1	CME	D	914	1	-	3/5/8/10	-
1	CME	G	748	1	-	4/5/8/10	-
1	CME	M	748	1	-	4/5/8/10	-
1	CME	P	748	1	-	4/5/8/10	-
1	CME	C	914	1	-	3/5/8/10	-

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	914	CME	CB-SG-SD	-3.43	94.94	103.82
1	I	914	CME	CB-SG-SD	-3.42	94.95	103.82
1	E	914	CME	CB-SG-SD	-3.42	94.95	103.82
1	K	914	CME	CB-SG-SD	-3.42	94.95	103.82
1	F	914	CME	CB-SG-SD	-3.42	94.95	103.82

There are no chirality outliers.

5 of 173 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	H	748	CME	SD-CE-CZ-OH
1	E	1021	CME	N-CA-CB-SG
1	E	1021	CME	SD-CE-CZ-OH
1	C	1021	CME	N-CA-CB-SG
1	C	1021	CME	SD-CE-CZ-OH

There are no ring outliers.

32 monomers are involved in 136 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	748	CME	2	0
1	E	1021	CME	7	0
1	C	1021	CME	6	0
1	K	748	CME	2	0
1	A	1021	CME	7	0
1	F	1021	CME	6	0
1	J	1021	CME	7	0
1	C	748	CME	2	0
1	A	748	CME	2	0
1	J	748	CME	2	0
1	B	748	CME	2	0
1	I	748	CME	2	0
1	D	1021	CME	6	0
1	K	1021	CME	6	0
1	H	1021	CME	6	0
1	L	748	CME	2	0
1	E	748	CME	2	0
1	N	1021	CME	7	0
1	F	748	CME	2	0
1	O	748	CME	2	0
1	B	1021	CME	7	0
1	O	1021	CME	7	0
1	P	1021	CME	6	0
1	N	748	CME	2	0
1	L	1021	CME	6	0
1	I	1021	CME	7	0
1	D	748	CME	2	0
1	G	1021	CME	7	0
1	M	1021	CME	6	0
1	G	748	CME	2	0
1	M	748	CME	2	0
1	P	748	CME	2	0

5.5 Carbohydrates

32 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	Q	1	2	12,12,12	0.68	0	17,17,17	0.72	0
2	2FG	Q	2	2,4	11,11,12	0.90	0	10,15,17	0.80	0
2	BGC	R	1	2	12,12,12	0.67	0	17,17,17	0.72	0
2	2FG	R	2	2,4	11,11,12	0.90	0	10,15,17	0.80	0
2	BGC	S	1	2	12,12,12	0.68	0	17,17,17	0.72	0
2	2FG	S	2	2,4	11,11,12	0.90	0	10,15,17	0.80	0
2	BGC	T	1	2	12,12,12	0.68	0	17,17,17	0.73	0
2	2FG	T	2	2,4	11,11,12	0.89	0	10,15,17	0.79	0
2	BGC	U	1	2	12,12,12	0.69	0	17,17,17	0.73	0
2	2FG	U	2	2,4	11,11,12	0.90	0	10,15,17	0.79	0
2	BGC	V	1	2	12,12,12	0.69	0	17,17,17	0.73	0
2	2FG	V	2	2,4	11,11,12	0.91	0	10,15,17	0.79	0
2	BGC	W	1	2	12,12,12	0.69	0	17,17,17	0.73	0
2	2FG	W	2	2,4	11,11,12	0.92	0	10,15,17	0.78	0
2	BGC	X	1	2	12,12,12	0.68	0	17,17,17	0.73	0
2	2FG	X	2	2,4	11,11,12	0.90	0	10,15,17	0.79	0
2	BGC	Y	1	2	12,12,12	0.69	0	17,17,17	0.73	0
2	2FG	Y	2	2,4	11,11,12	0.89	0	10,15,17	0.79	0
2	BGC	Z	1	2	12,12,12	0.69	0	17,17,17	0.72	0
2	2FG	Z	2	2,4	11,11,12	0.91	0	10,15,17	0.79	0
2	BGC	a	1	2	12,12,12	0.68	0	17,17,17	0.72	0
2	2FG	a	2	2,4	11,11,12	0.89	0	10,15,17	0.79	0
2	BGC	b	1	2	12,12,12	0.69	0	17,17,17	0.73	0
2	2FG	b	2	2,4	11,11,12	0.90	0	10,15,17	0.78	0
2	BGC	c	1	2	12,12,12	0.68	0	17,17,17	0.73	0
2	2FG	c	2	2,4	11,11,12	0.90	0	10,15,17	0.80	0
2	BGC	d	1	2	12,12,12	0.68	0	17,17,17	0.73	0
2	2FG	d	2	2,4	11,11,12	0.90	0	10,15,17	0.78	0
2	BGC	e	1	2	12,12,12	0.68	0	17,17,17	0.72	0
2	2FG	e	2	2,4	11,11,12	0.89	0	10,15,17	0.79	0
2	BGC	f	1	2	12,12,12	0.69	0	17,17,17	0.73	0
2	2FG	f	2	2,4	11,11,12	0.90	0	10,15,17	0.79	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
2	BGC	Q	1	2	-	2/2/22/22	0/1/1/1
2	2FG	Q	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	R	1	2	-	2/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2FG	R	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	S	1	2	-	2/2/22/22	0/1/1/1
2	2FG	S	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	T	1	2	-	2/2/22/22	0/1/1/1
2	2FG	T	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	U	1	2	-	2/2/22/22	0/1/1/1
2	2FG	U	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	V	1	2	-	2/2/22/22	0/1/1/1
2	2FG	V	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	W	1	2	-	2/2/22/22	0/1/1/1
2	2FG	W	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	X	1	2	-	2/2/22/22	0/1/1/1
2	2FG	X	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	Y	1	2	-	2/2/22/22	0/1/1/1
2	2FG	Y	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	Z	1	2	-	2/2/22/22	0/1/1/1
2	2FG	Z	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	a	1	2	-	2/2/22/22	0/1/1/1
2	2FG	a	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	b	1	2	-	2/2/22/22	0/1/1/1
2	2FG	b	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	c	1	2	-	2/2/22/22	0/1/1/1
2	2FG	c	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	d	1	2	-	2/2/22/22	0/1/1/1
2	2FG	d	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	e	1	2	-	2/2/22/22	0/1/1/1
2	2FG	e	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	f	1	2	-	2/2/22/22	0/1/1/1
2	2FG	f	2	2,4	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	1	BGC	O5-C5-C6-O6
2	b	1	BGC	O5-C5-C6-O6

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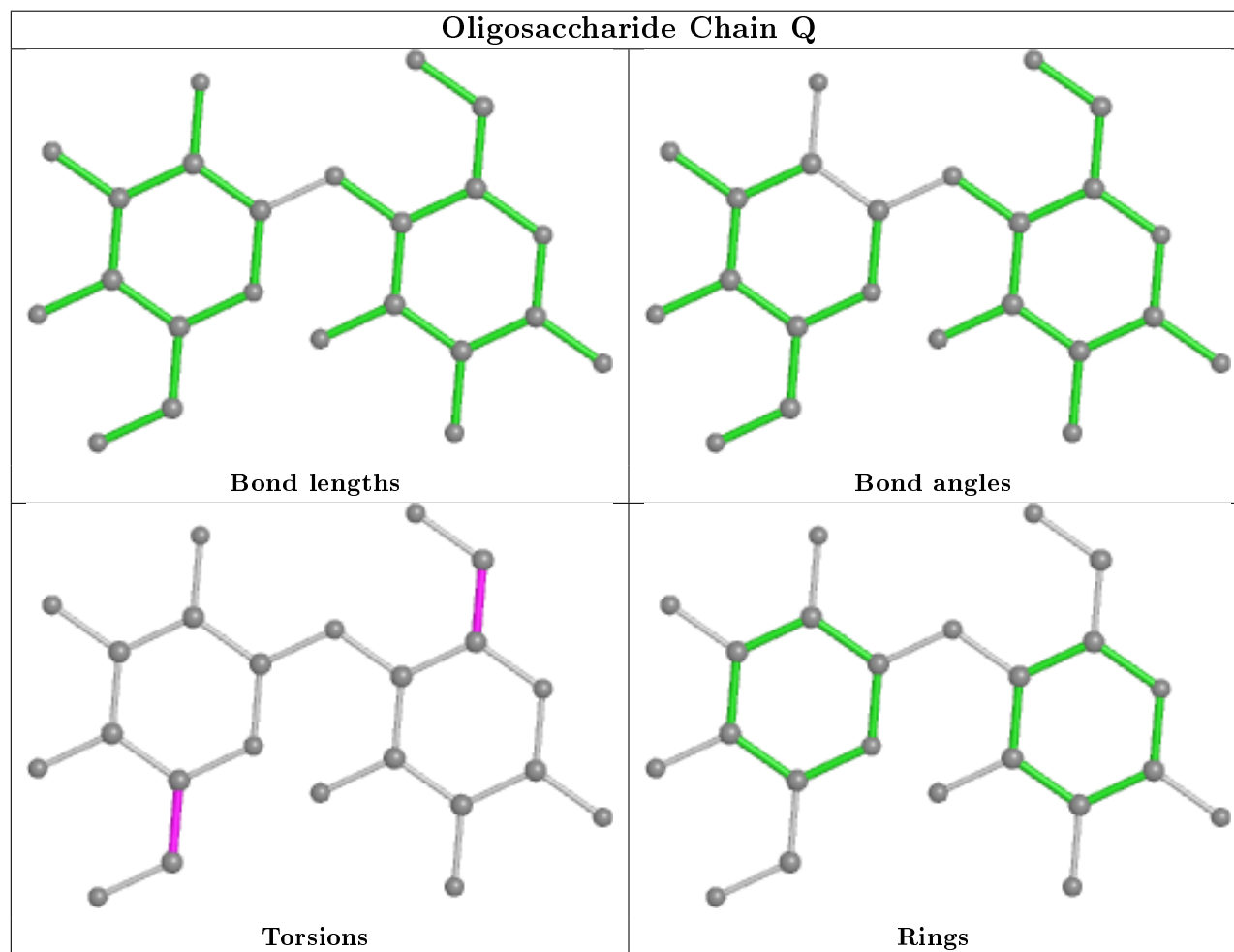
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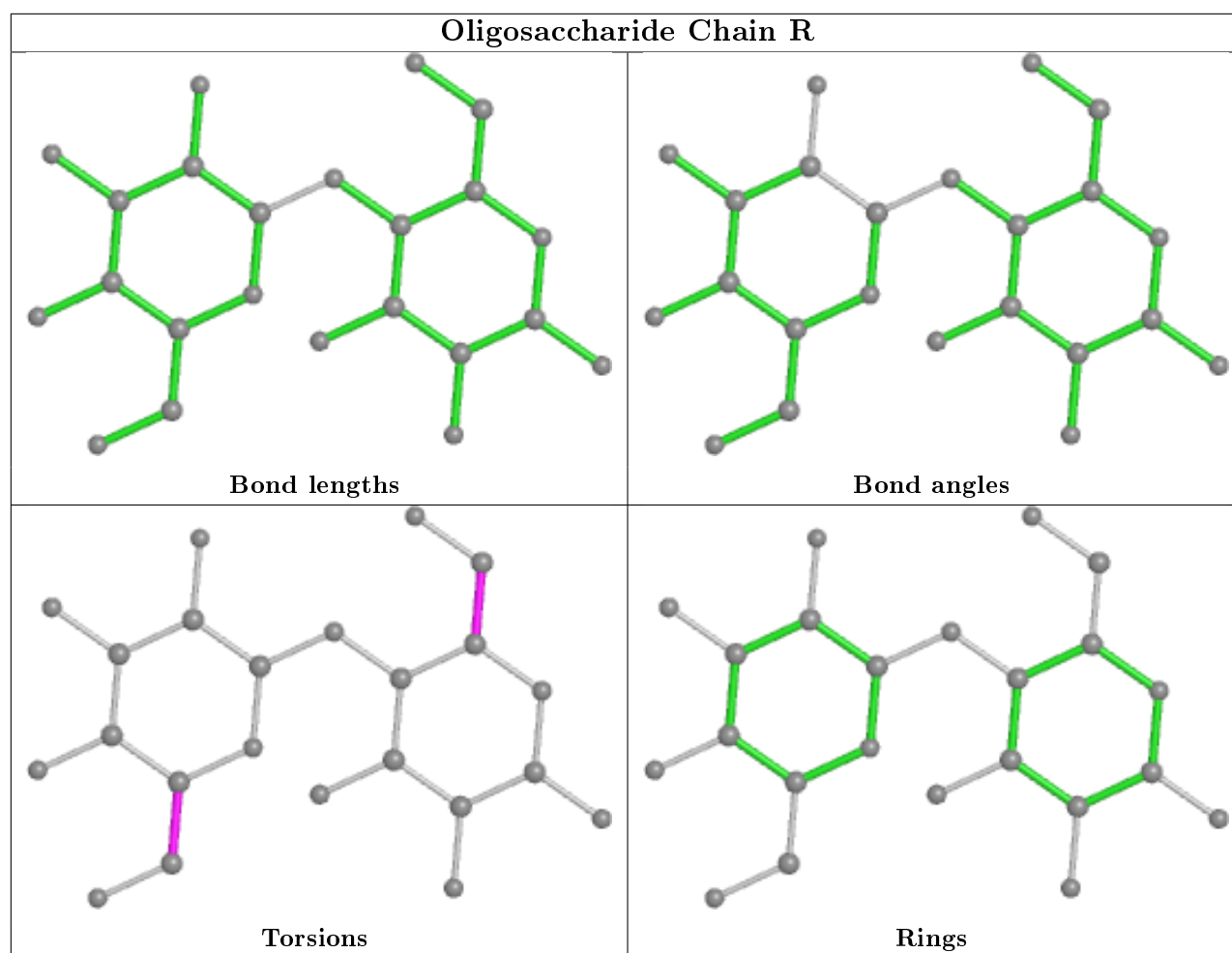
Mol	Chain	Res	Type	Atoms
2	R	1	BGC	O5-C5-C6-O6
2	Q	1	BGC	O5-C5-C6-O6
2	f	1	BGC	O5-C5-C6-O6

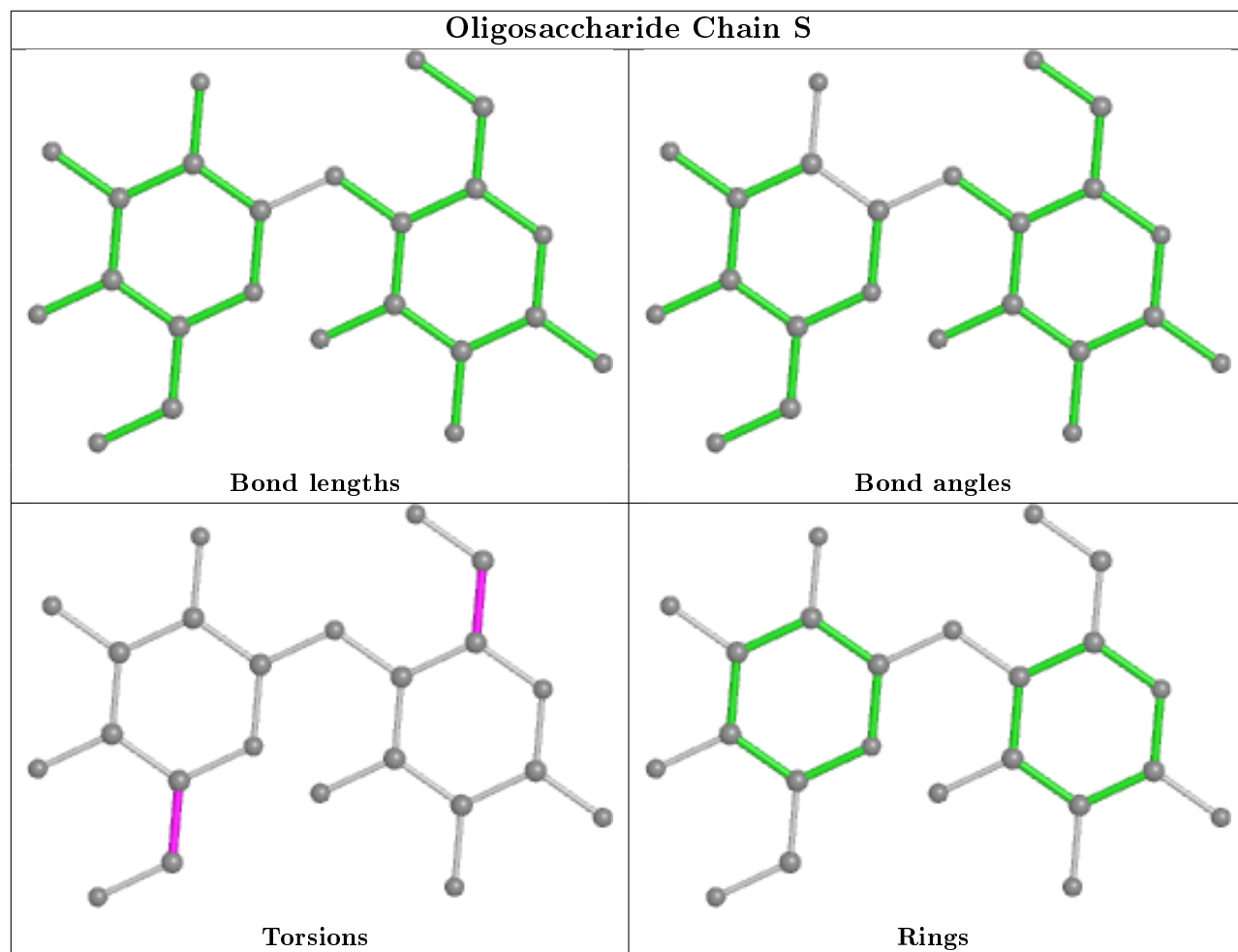
There are no ring outliers.

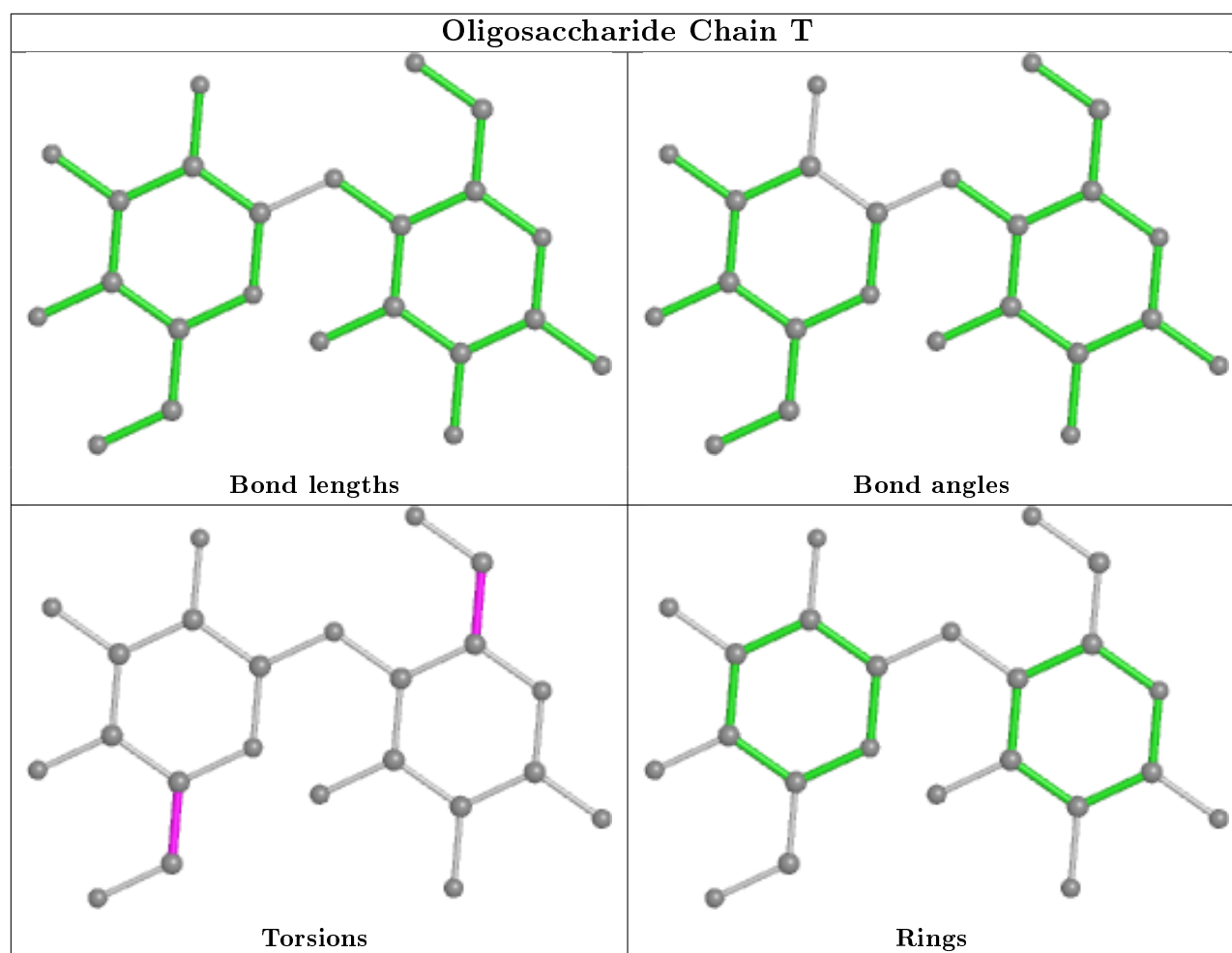
No monomer is involved in short contacts.

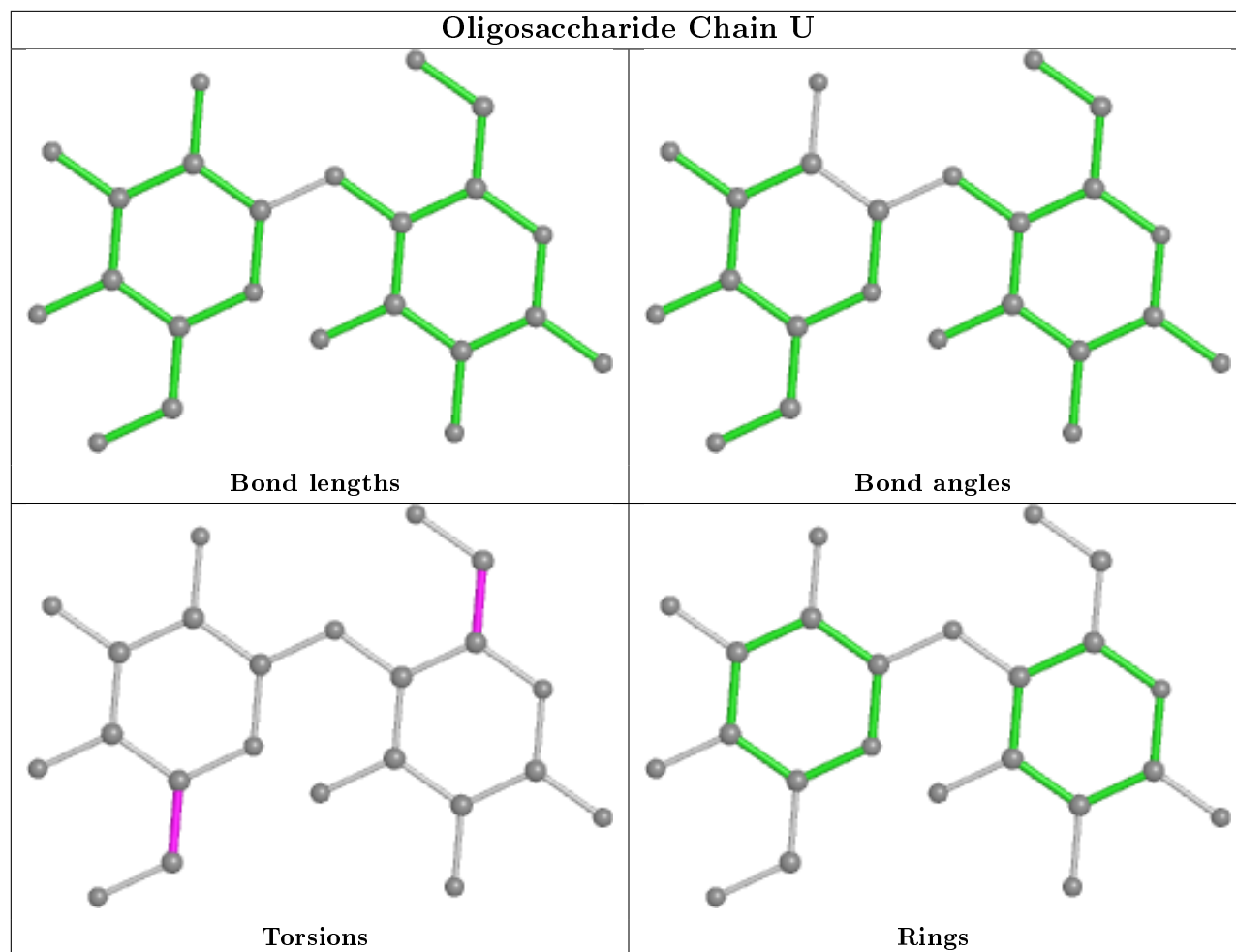
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

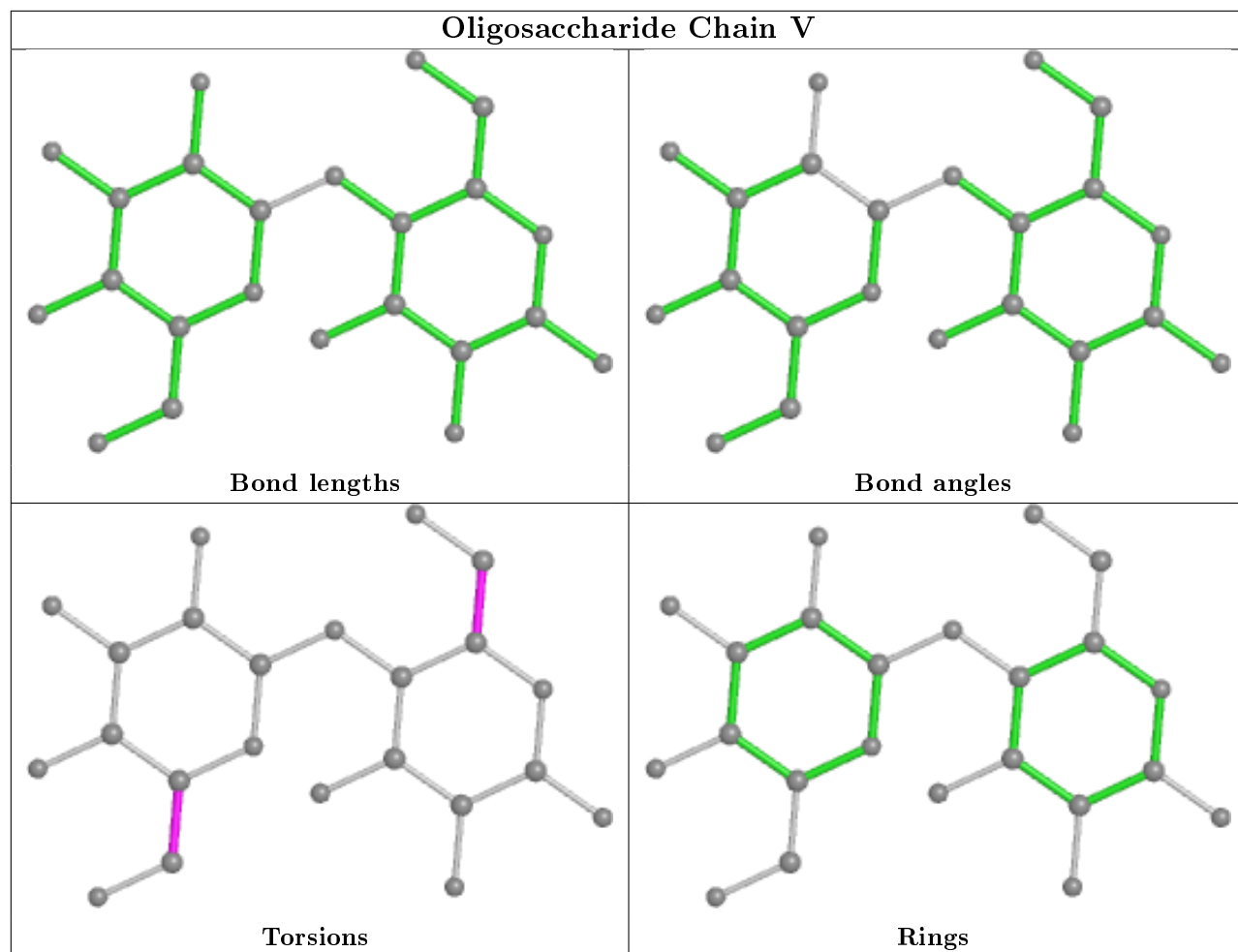


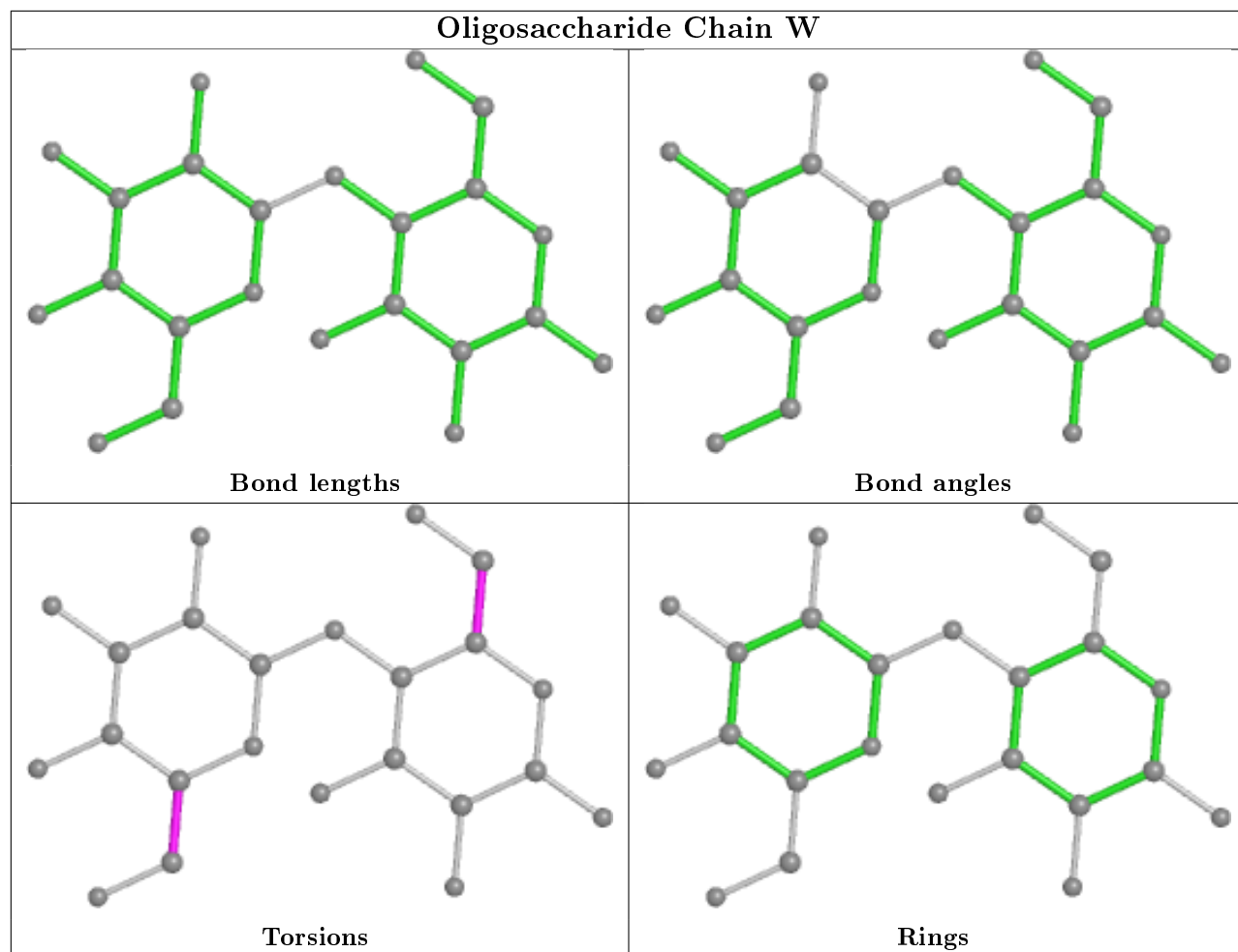


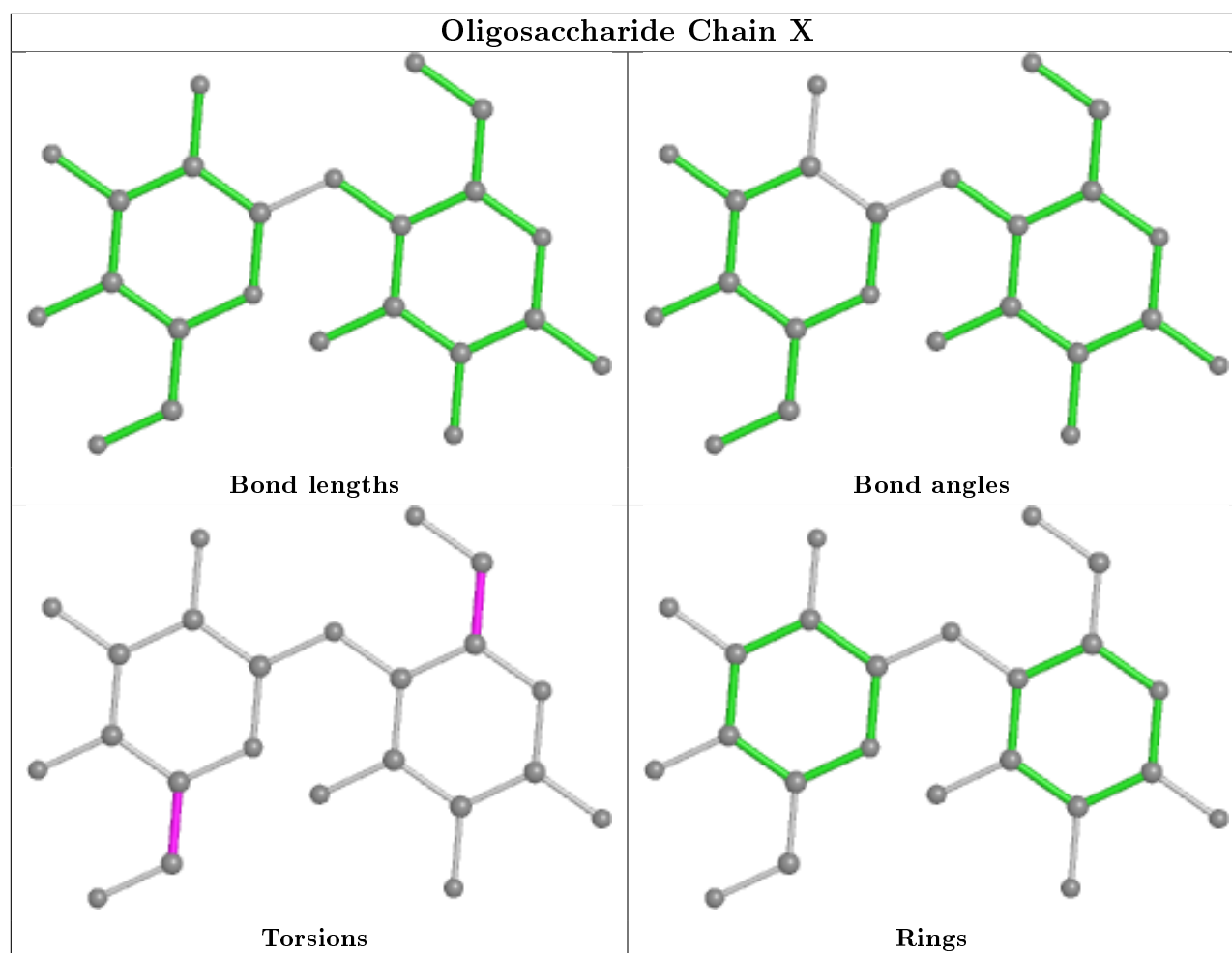


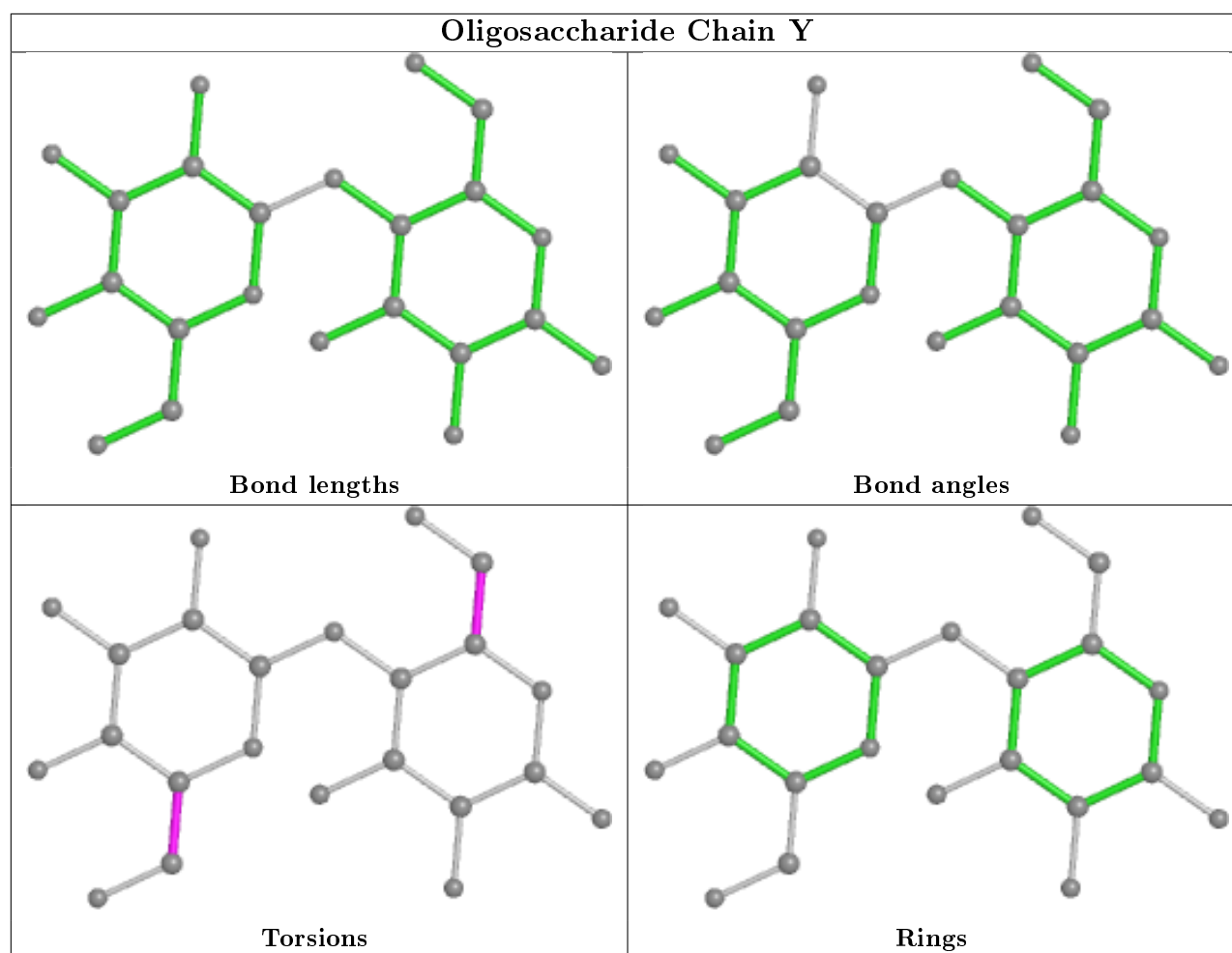


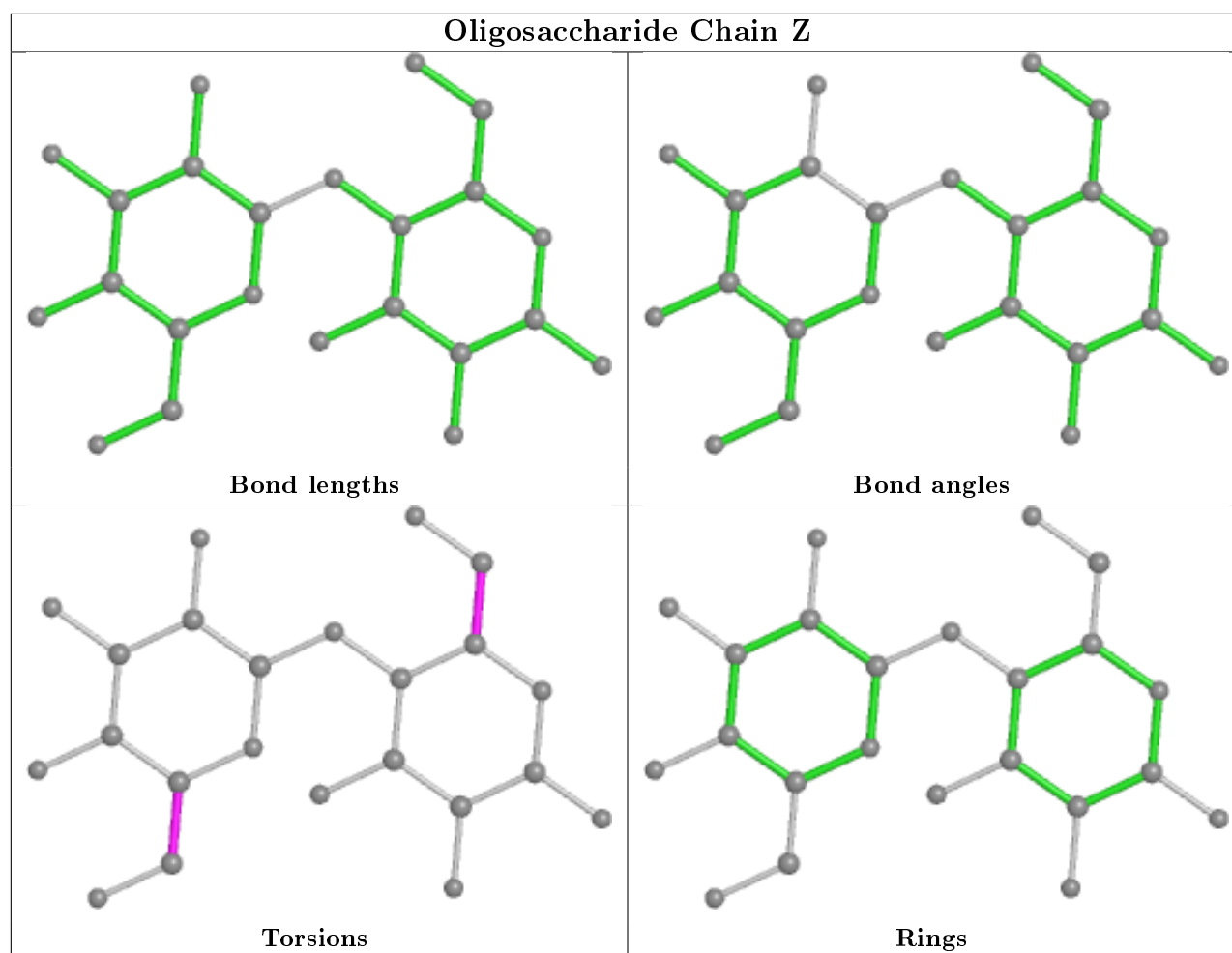












5.6 Ligand geometry [i](#)

Of 64 ligands modelled in this entry, 64 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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	1018/1023 (99%)	-0.63	12 (1%) 79 80	2, 23, 63, 99	0
1	B	1018/1023 (99%)	-0.64	10 (0%) 82 83	1, 21, 61, 98	0
1	C	1018/1023 (99%)	-0.65	9 (0%) 84 85	1, 21, 61, 98	0
1	D	1018/1023 (99%)	-0.42	11 (1%) 80 82	10, 31, 69, 100	0
1	E	1018/1023 (99%)	0.10	34 (3%) 46 46	27, 48, 83, 100	0
1	F	1018/1023 (99%)	-0.55	8 (0%) 86 87	8, 28, 67, 100	0
1	G	1018/1023 (99%)	-0.49	16 (1%) 72 74	8, 28, 68, 100	0
1	H	1018/1023 (99%)	-0.17	22 (2%) 62 63	18, 38, 75, 100	0
1	I	1018/1023 (99%)	-0.38	16 (1%) 72 74	11, 32, 70, 100	0
1	J	1018/1023 (99%)	-0.53	11 (1%) 80 82	10, 30, 69, 100	0
1	K	1018/1023 (99%)	-0.15	31 (3%) 50 51	24, 45, 81, 100	0
1	L	1018/1023 (99%)	-0.11	30 (2%) 51 52	25, 45, 81, 100	0
1	M	1018/1023 (99%)	0.31	57 (5%) 24 23	27, 48, 83, 100	0
1	N	1018/1023 (99%)	-0.36	11 (1%) 80 82	16, 36, 74, 100	0
1	O	1018/1023 (99%)	-0.24	22 (2%) 62 63	21, 42, 78, 100	0
1	P	1018/1023 (99%)	0.76	111 (10%) 5 4	39, 60, 91, 100	0
All	All	16288/16368 (99%)	-0.26	411 (2%) 57 59	1, 37, 76, 100	0

The worst 5 of 411 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	735	HIS	6.3
1	P	799	THR	6.3
1	F	581	ASN	6.0
1	G	732	ALA	5.8
1	K	735	HIS	5.8

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

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
1	CME	P	1021	10/11	0.81	0.32	72,87,100,100	0
1	CME	P	914	10/11	0.84	0.22	54,62,98,100	0
1	CME	P	748	10/11	0.84	0.25	68,80,100,100	0
1	CME	O	748	10/11	0.86	0.33	50,62,95,100	0
1	CME	J	1021	10/11	0.87	0.22	42,58,93,100	0
1	CME	B	1021	10/11	0.87	0.25	33,49,84,97	0
1	CME	H	1021	10/11	0.87	0.20	50,66,100,100	0
1	CME	L	1021	10/11	0.87	0.16	57,73,100,100	0
1	CME	N	1021	10/11	0.87	0.18	48,64,99,100	0
1	CME	E	1021	10/11	0.88	0.20	60,76,100,100	0
1	CME	F	1021	10/11	0.89	0.17	40,56,91,100	0
1	CME	M	748	10/11	0.89	0.26	56,68,100,100	0
1	CME	A	1021	10/11	0.89	0.19	35,50,85,99	0
1	CME	K	1021	10/11	0.90	0.21	57,73,100,100	0
1	CME	M	1021	10/11	0.90	0.17	60,75,100,100	0
1	CME	L	748	10/11	0.90	0.20	53,65,99,100	0
1	CME	N	748	10/11	0.90	0.24	44,56,90,100	0
1	CME	D	1021	10/11	0.91	0.19	43,58,93,100	0
1	CME	M	914	10/11	0.91	0.16	42,50,86,92	0
1	CME	C	1021	10/11	0.91	0.15	33,49,84,97	0
1	CME	G	748	10/11	0.91	0.18	37,48,82,93	0
1	CME	K	748	10/11	0.91	0.19	53,65,98,100	0
1	CME	H	748	10/11	0.91	0.21	46,58,92,100	0
1	CME	E	914	10/11	0.92	0.19	42,50,87,92	0
1	CME	I	748	10/11	0.92	0.17	40,52,85,97	0
1	CME	C	748	10/11	0.92	0.19	29,41,74,86	0
1	CME	D	748	10/11	0.92	0.20	39,51,84,95	0
1	CME	F	748	10/11	0.92	0.19	36,48,81,93	0
1	CME	J	748	10/11	0.92	0.16	38,50,84,95	0
1	CME	B	748	10/11	0.92	0.17	29,41,75,86	0
1	CME	O	1021	10/11	0.92	0.20	54,69,100,100	0
1	CME	L	914	10/11	0.93	0.15	40,47,84,89	0
1	CME	A	748	10/11	0.93	0.19	31,43,76,87	0
1	CME	G	1021	10/11	0.93	0.17	41,56,91,100	0
1	CME	E	748	10/11	0.93	0.25	56,68,100,100	0
1	CME	A	914	10/11	0.94	0.17	17,25,61,67	0
1	CME	K	914	10/11	0.94	0.12	40,47,84,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	CME	I	1021	10/11	0.94	0.15	44,60,94,100	0
1	CME	H	914	10/11	0.95	0.15	33,40,77,82	0
1	CME	O	914	10/11	0.95	0.13	36,44,80,86	0
1	CME	I	914	10/11	0.95	0.13	26,34,70,76	0
1	CME	G	914	10/11	0.96	0.10	23,31,67,73	0
1	CME	B	914	10/11	0.96	0.12	16,23,60,66	0
1	CME	J	914	10/11	0.96	0.14	25,32,69,75	0
1	CME	F	914	10/11	0.96	0.13	23,30,67,72	0
1	CME	D	914	10/11	0.96	0.14	25,33,69,75	0
1	CME	N	914	10/11	0.97	0.13	31,38,75,81	0
1	CME	C	914	10/11	0.97	0.10	16,23,60,65	0

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.

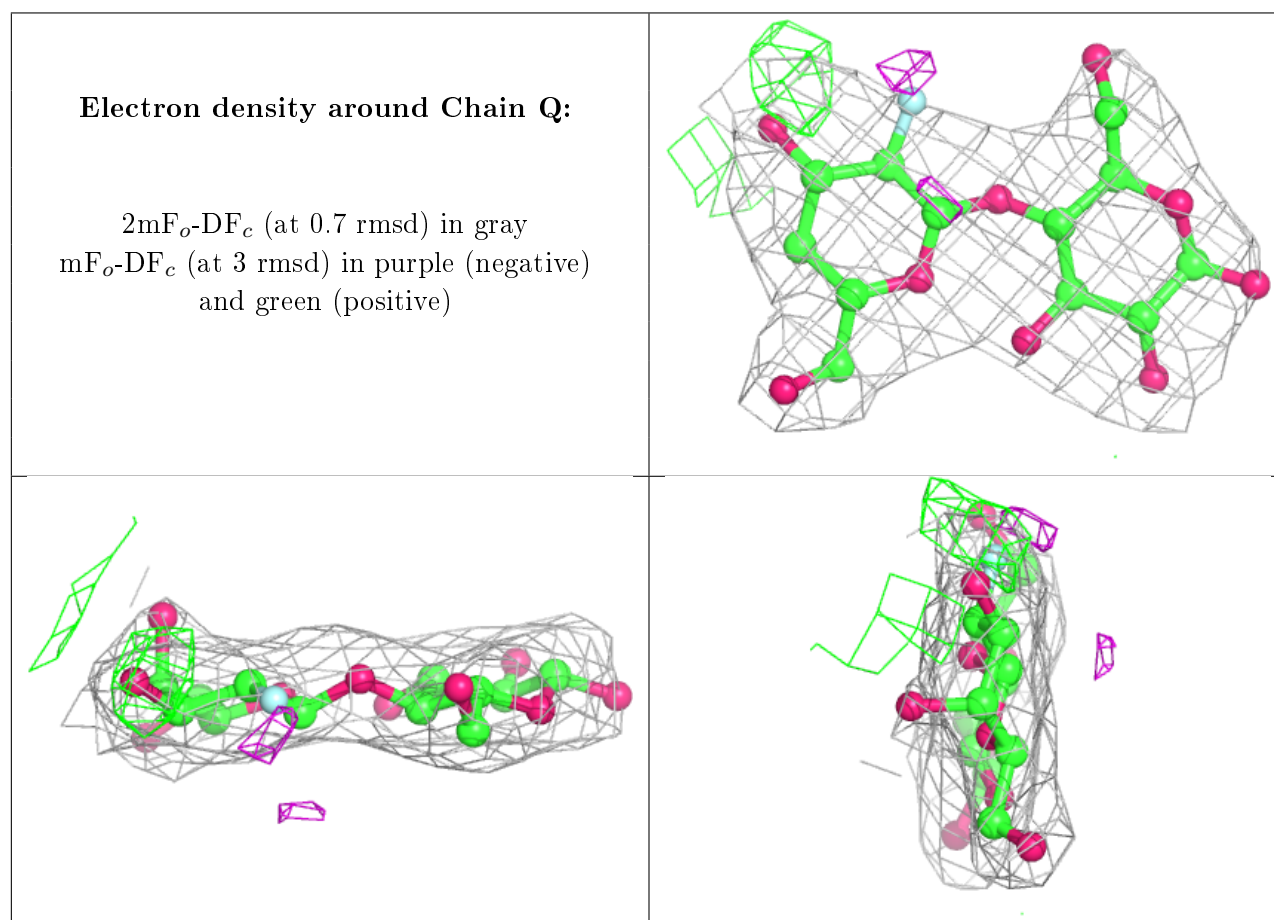
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	2FG	X	2	11/12	0.79	0.34	56,61,72,78	0
2	BGC	a	1	12/12	0.83	0.28	65,80,97,100	0
2	2FG	b	2	11/12	0.84	0.30	63,68,79,85	0
2	BGC	b	1	12/12	0.85	0.28	65,80,97,100	0
2	2FG	f	2	11/12	0.85	0.28	77,83,94,100	0
2	2FG	e	2	11/12	0.86	0.23	59,65,76,82	0
2	BGC	f	1	12/12	0.86	0.21	79,94,100,100	0
2	BGC	Z	1	12/12	0.87	0.23	50,65,82,99	0
2	BGC	S	1	12/12	0.87	0.23	41,56,73,89	0
2	BGC	e	1	12/12	0.87	0.24	61,76,93,100	0
2	2FG	a	2	11/12	0.88	0.27	63,68,79,85	0
2	BGC	c	1	12/12	0.88	0.17	67,82,99,100	0
2	BGC	W	1	12/12	0.89	0.20	48,63,80,97	0
2	2FG	S	2	11/12	0.89	0.19	39,44,55,61	0
2	2FG	V	2	11/12	0.90	0.19	46,51,62,68	0
2	BGC	X	1	12/12	0.91	0.22	58,73,90,100	0
2	2FG	U	2	11/12	0.91	0.25	66,71,82,88	0
2	BGC	T	1	12/12	0.91	0.22	50,65,82,99	0
2	2FG	Q	2	11/12	0.91	0.18	40,46,57,63	0
2	BGC	V	1	12/12	0.91	0.18	48,63,80,96	0
2	2FG	c	2	11/12	0.91	0.21	65,71,82,88	0
2	BGC	U	1	12/12	0.92	0.17	67,83,100,100	0

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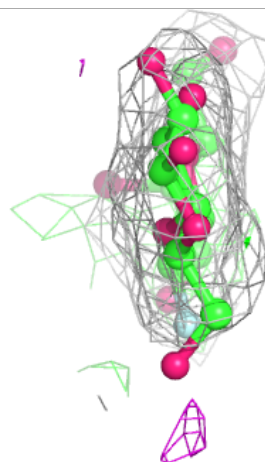
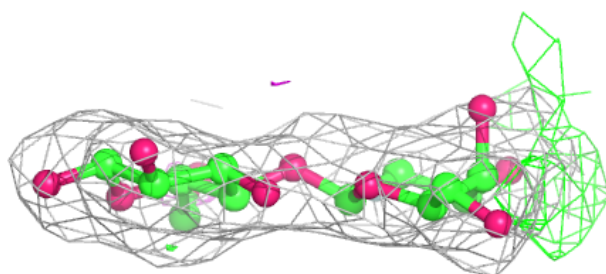
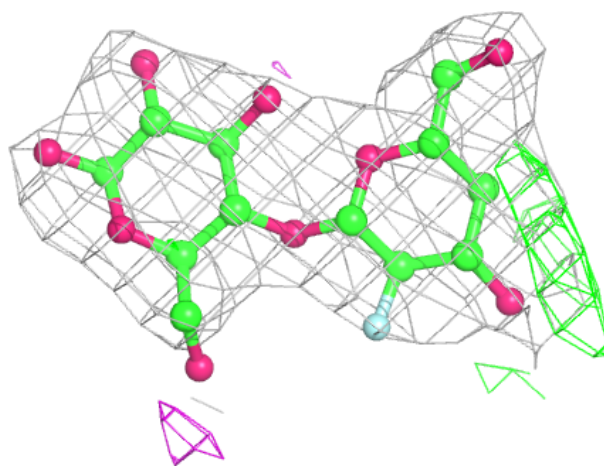
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	2FG	Y	2	11/12	0.92	0.18	49,55,66,72	0
2	BGC	d	1	12/12	0.92	0.18	56,71,88,100	0
2	2FG	R	2	11/12	0.92	0.17	39,44,55,61	0
2	2FG	Z	2	11/12	0.92	0.18	48,53,64,70	0
2	2FG	d	2	11/12	0.93	0.15	54,59,70,76	0
2	BGC	R	1	12/12	0.93	0.15	41,56,73,90	0
2	BGC	Y	1	12/12	0.93	0.14	51,67,84,100	0
2	2FG	W	2	11/12	0.93	0.16	46,51,63,68	0
2	BGC	Q	1	12/12	0.94	0.13	42,57,74,91	0
2	2FG	T	2	11/12	0.96	0.18	48,54,65,71	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.



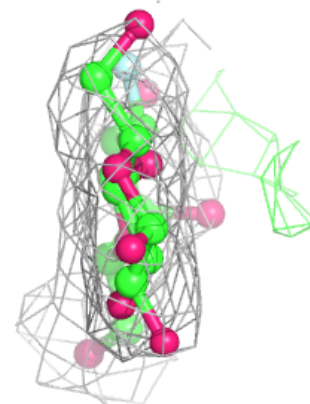
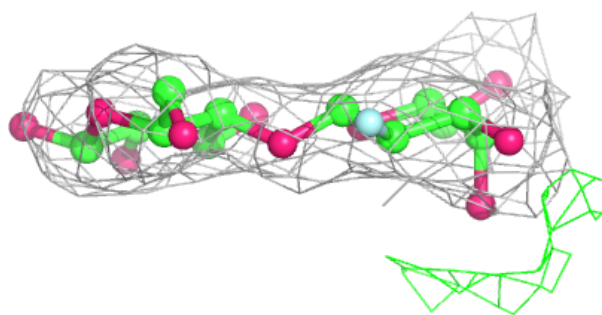
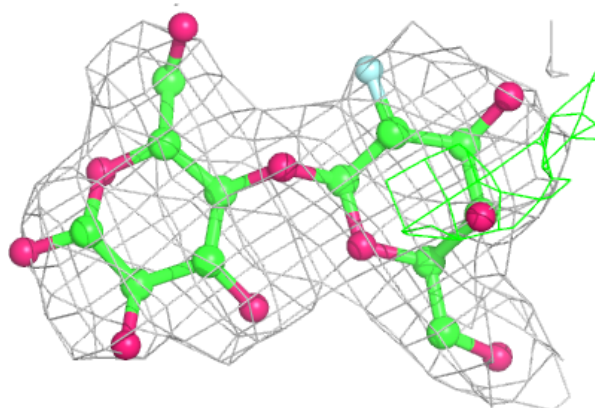
Electron density around Chain R:

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

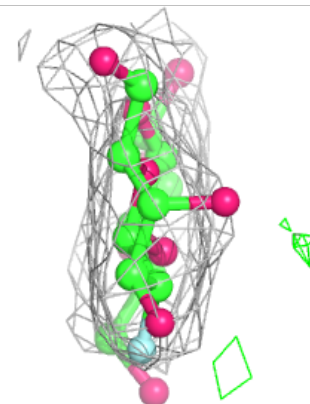
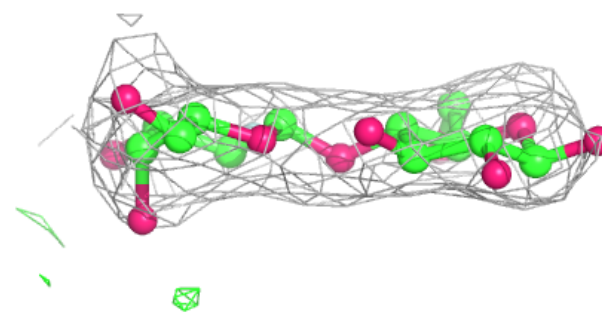
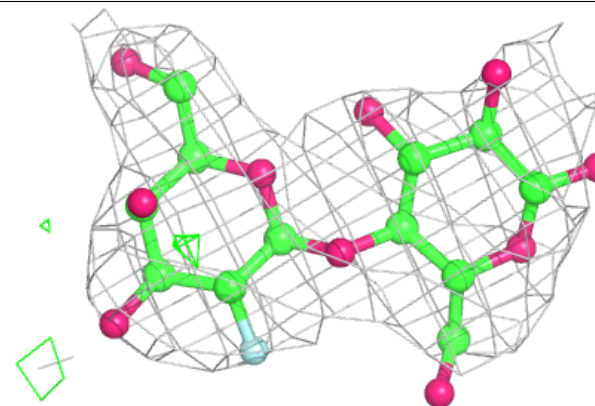


Electron density around Chain S:

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

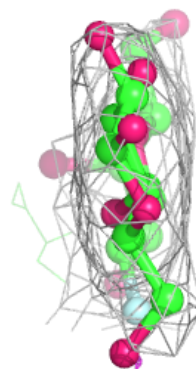
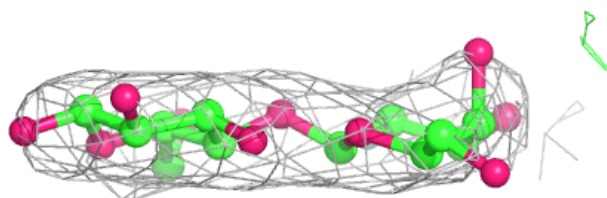
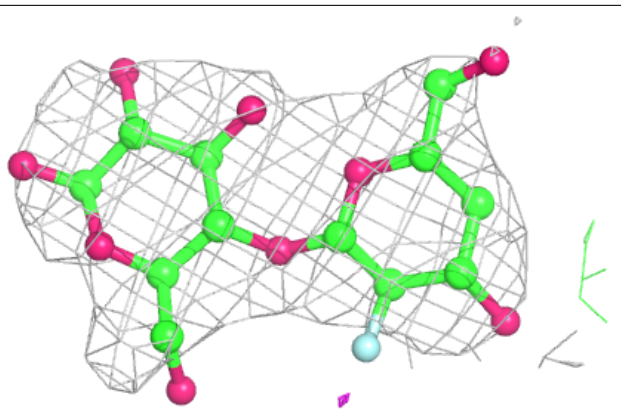
**Electron density around Chain T:**

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



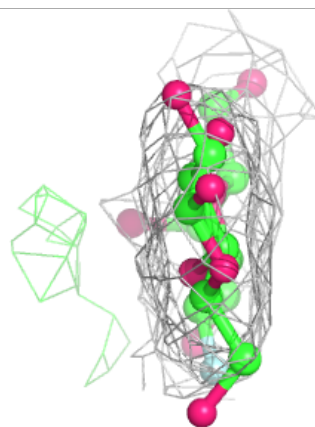
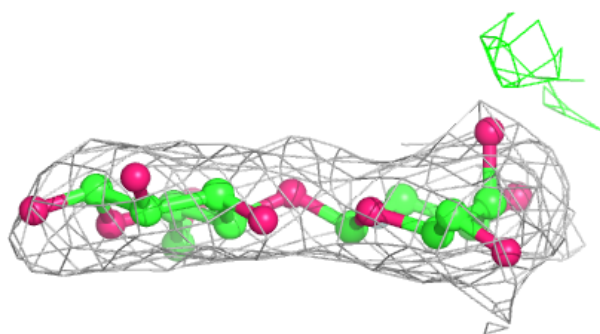
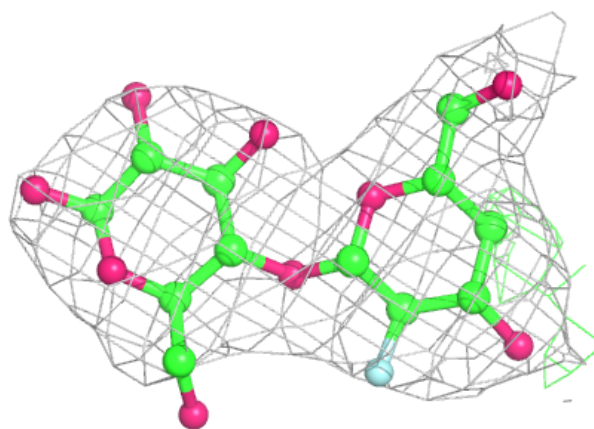
Electron density around Chain U:

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



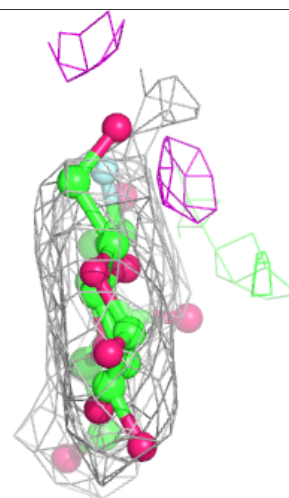
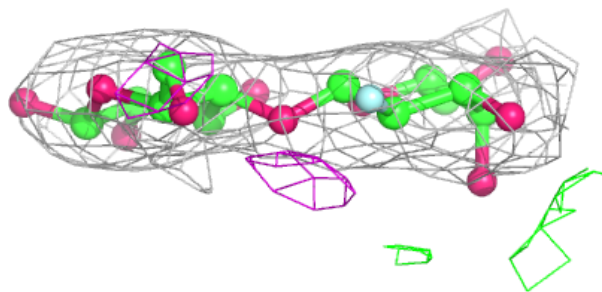
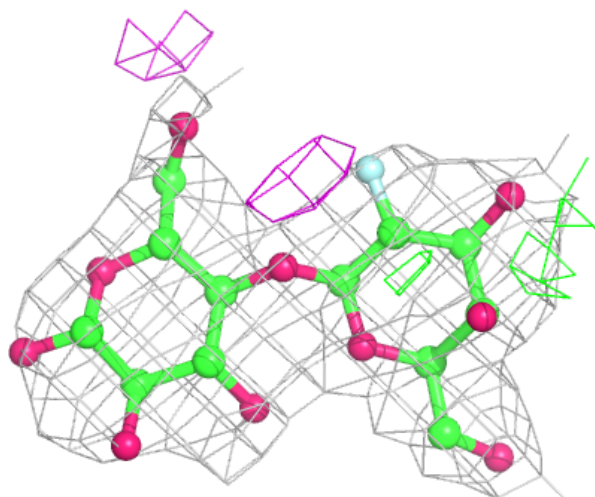
Electron density around Chain V:

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



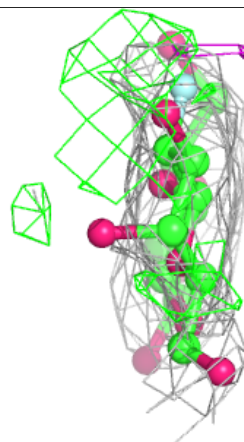
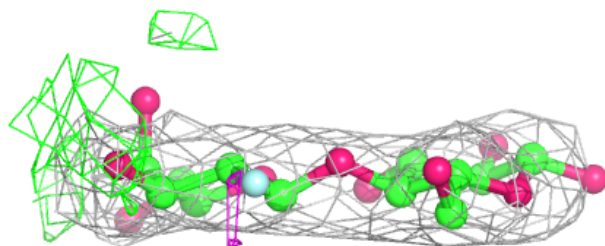
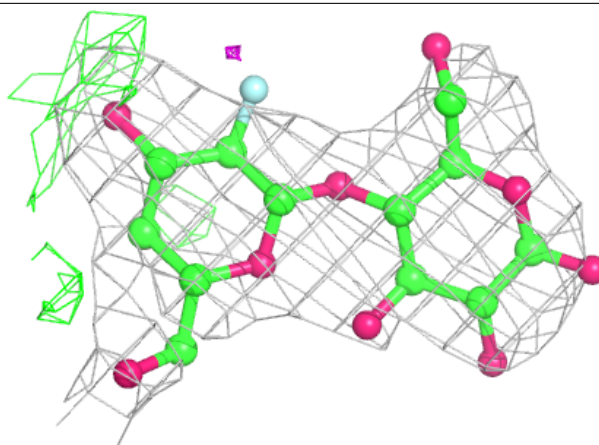
Electron density around Chain W:

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



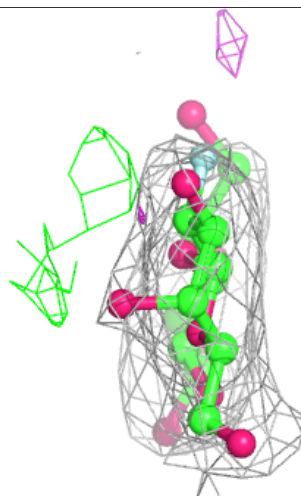
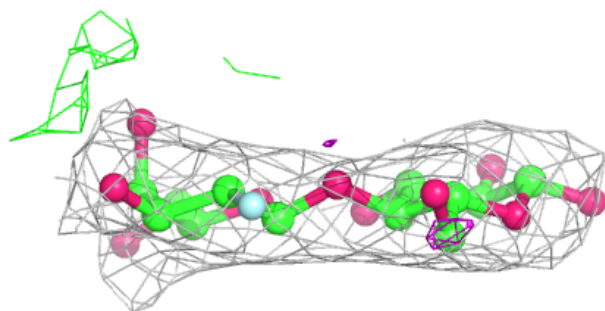
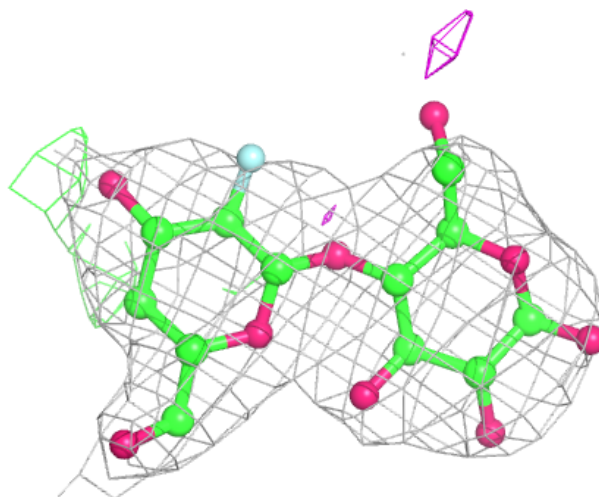
Electron density around Chain X:

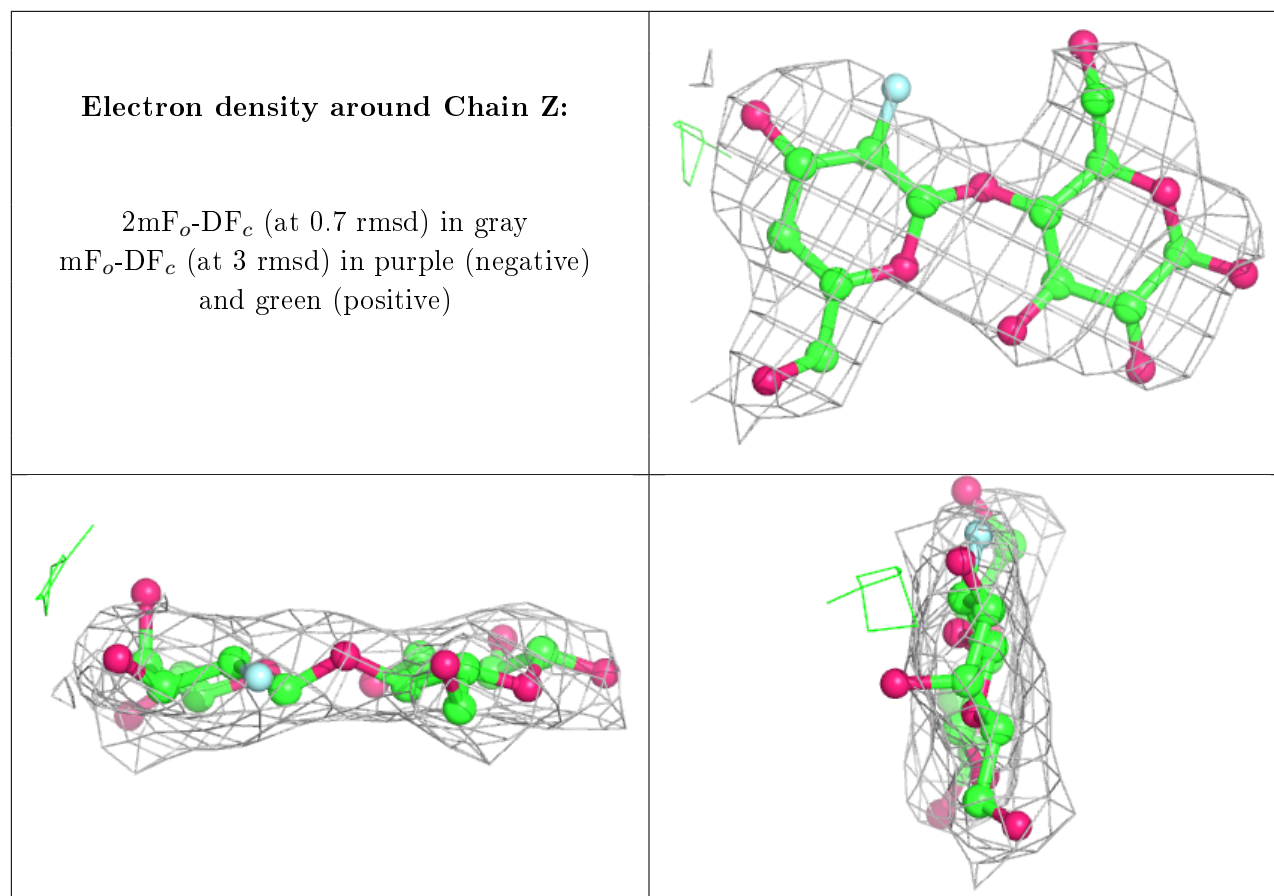
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain Y:

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





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	NA	P	2004	1/1	0.42	0.35	67,67,67,67	0
3	MG	P	2003	1/1	0.72	0.14	53,53,53,53	0
4	NA	M	2004	1/1	0.73	0.32	55,55,55,55	0
3	MG	N	2003	1/1	0.80	0.09	30,30,30,30	0
4	NA	P	2005	1/1	0.81	0.16	55,55,55,55	0
4	NA	A	2005	1/1	0.81	0.09	18,18,18,18	0
4	NA	L	2004	1/1	0.83	0.25	53,53,53,53	0
4	NA	E	2004	1/1	0.83	0.36	55,55,55,55	0
4	NA	D	2005	1/1	0.85	0.13	26,26,26,26	0
4	NA	J	2004	1/1	0.85	0.20	38,38,38,38	0
4	NA	O	2005	1/1	0.86	0.16	37,37,37,37	0
3	MG	E	2003	1/1	0.87	0.14	42,42,42,42	0
3	MG	J	2003	1/1	0.88	0.14	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	G	2003	1/1	0.88	0.11	22,22,22,22	0
4	NA	D	2004	1/1	0.88	0.14	38,38,38,38	0
4	NA	M	2005	1/1	0.88	0.11	43,43,43,43	0
3	MG	F	2003	1/1	0.89	0.11	22,22,22,22	0
4	NA	H	2004	1/1	0.89	0.18	46,46,46,46	0
4	NA	F	2005	1/1	0.89	0.13	23,23,23,23	0
4	NA	K	2004	1/1	0.90	0.21	53,53,53,53	0
3	MG	P	2002	1/1	0.91	0.24	60,60,60,60	0
4	NA	O	2004	1/1	0.91	0.17	49,49,49,49	0
4	NA	A	2004	1/1	0.92	0.10	30,30,30,30	0
4	NA	J	2005	1/1	0.92	0.17	25,25,25,25	0
4	NA	C	2005	1/1	0.92	0.08	16,16,16,16	0
3	MG	L	2003	1/1	0.93	0.11	39,39,39,39	0
3	MG	M	2002	1/1	0.93	0.15	48,48,48,48	0
4	NA	G	2005	1/1	0.93	0.11	24,24,24,24	0
4	NA	I	2005	1/1	0.93	0.13	27,27,27,27	0
3	MG	I	2003	1/1	0.94	0.14	26,26,26,26	0
3	MG	K	2003	1/1	0.94	0.13	39,39,39,39	0
3	MG	D	2003	1/1	0.94	0.07	24,24,24,24	0
4	NA	E	2005	1/1	0.94	0.18	43,43,43,43	0
4	NA	F	2004	1/1	0.94	0.12	36,36,36,36	0
3	MG	H	2003	1/1	0.94	0.09	32,32,32,32	0
3	MG	B	2003	1/1	0.94	0.09	15,15,15,15	0
3	MG	C	2003	1/1	0.94	0.09	15,15,15,15	0
3	MG	O	2003	1/1	0.94	0.14	35,35,35,35	0
4	NA	N	2004	1/1	0.94	0.13	44,44,44,44	0
4	NA	G	2004	1/1	0.95	0.13	36,36,36,36	0
4	NA	L	2005	1/1	0.95	0.16	40,40,40,40	0
4	NA	B	2005	1/1	0.95	0.12	16,16,16,16	0
3	MG	M	2003	1/1	0.95	0.22	41,41,41,41	0
3	MG	D	2002	1/1	0.95	0.18	31,31,31,31	0
3	MG	C	2002	1/1	0.95	0.22	22,22,22,22	0
3	MG	L	2002	1/1	0.95	0.20	46,46,46,46	0
3	MG	E	2002	1/1	0.96	0.20	48,48,48,48	0
4	NA	K	2005	1/1	0.96	0.08	40,40,40,40	0
3	MG	G	2002	1/1	0.96	0.27	29,29,29,29	0
4	NA	H	2005	1/1	0.96	0.13	33,33,33,33	0
4	NA	C	2004	1/1	0.97	0.14	29,29,29,29	0
4	NA	I	2004	1/1	0.97	0.09	39,39,39,39	0
3	MG	J	2002	1/1	0.97	0.10	31,31,31,31	0
3	MG	H	2002	1/1	0.97	0.26	39,39,39,39	0
3	MG	F	2002	1/1	0.98	0.22	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	O	2002	1/1	0.98	0.25	42,42,42,42	0
3	MG	N	2002	1/1	0.98	0.19	37,37,37,37	0
3	MG	K	2002	1/1	0.98	0.17	45,45,45,45	0
4	NA	N	2005	1/1	0.98	0.17	31,31,31,31	0
3	MG	A	2002	1/1	0.98	0.09	23,23,23,23	0
4	NA	B	2004	1/1	0.98	0.08	29,29,29,29	0
3	MG	A	2003	1/1	0.98	0.16	16,16,16,16	0
3	MG	I	2002	1/1	0.98	0.22	32,32,32,32	0
3	MG	B	2002	1/1	0.99	0.23	22,22,22,22	0

6.5 Other polymers ⓘ

There are no such residues in this entry.