



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 04:08 PM UTC

PDB ID : 4V44 / pdb_00004v44
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 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:

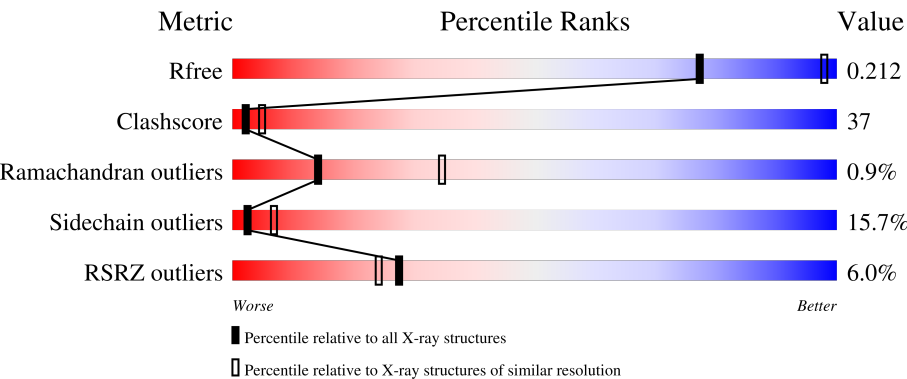
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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	1023	2% 43% 41% 14% .
1	B	1023	% 43% 41% 14% .
1	C	1023	2% 45% 40% 14% .
1	D	1023	4% 43% 42% 14% .
1	E	1023	12% 43% 41% 14% .

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Mol	Chain	Length	Quality of chain
1	F	1023	2% 44% 41% 14%
1	G	1023	% 43% 42% 13%
1	H	1023	5% 44% 41% 13%
1	I	1023	2% 44% 40% 14%
1	J	1023	2% 44% 41% 13%
1	K	1023	2% 44% 40% 14%
1	L	1023	4% 43% 41% 14%
1	M	1023	16% 43% 41% 14%
1	N	1023	3% 44% 40% 14%
1	O	1023	2% 43% 42% 14%
1	P	1023	35% 43% 42% 14%
2	Q	2	50% 50%
2	R	2	50% 50%
2	S	2	50% 50%
2	T	2	50% 50%
2	U	2	50% 50%
2	V	2	50% 50%
2	W	2	50% 50%
2	X	2	50% 50%
2	Y	2	50% 50%
2	Z	2	50% 50%
2	a	2	50% 50%
2	b	2	50% 50%
2	c	2	50% 50%
2	d	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	e	2	 50% 50%
2	f	2	 50% 50%

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 [i](#)

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 (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Na 2	0	0
4	B	2	Total 2	Na 2	0	0
4	C	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	E	2	Total 2	Na 2	0	0
4	F	2	Total 2	Na 2	0	0
4	G	2	Total 2	Na 2	0	0
4	H	2	Total 2	Na 2	0	0
4	I	2	Total 2	Na 2	0	0
4	J	2	Total 2	Na 2	0	0
4	K	2	Total 2	Na 2	0	0
4	L	2	Total 2	Na 2	0	0
4	M	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	P	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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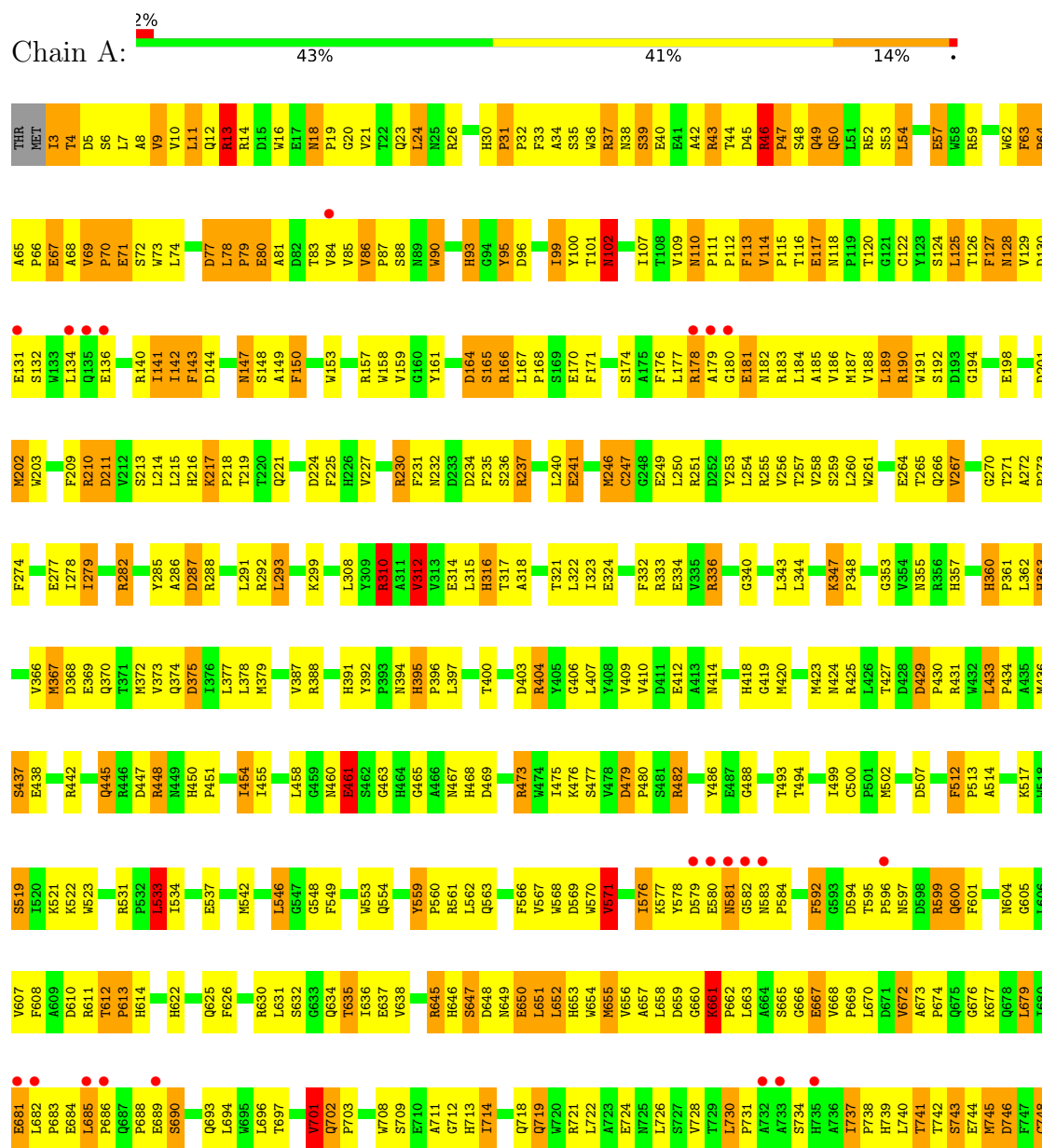
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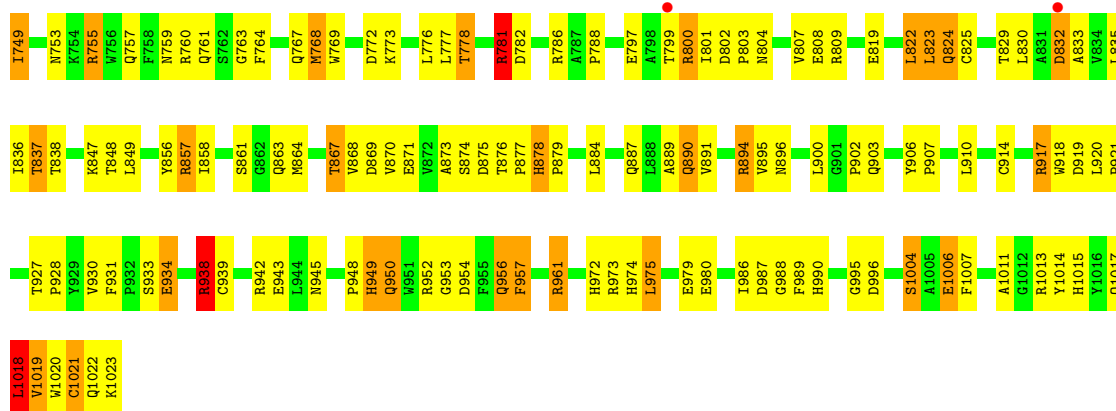
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	162	Total 162	O 162	0	0
5	H	162	Total 162	O 162	0	0
5	I	162	Total 162	O 162	0	0
5	J	162	Total 162	O 162	0	0
5	K	162	Total 162	O 162	0	0
5	L	162	Total 162	O 162	0	0
5	M	161	Total 161	O 161	0	0
5	N	163	Total 163	O 163	0	0
5	O	161	Total 161	O 161	0	0
5	P	163	Total 163	O 163	0	0

3 Residue-property plots

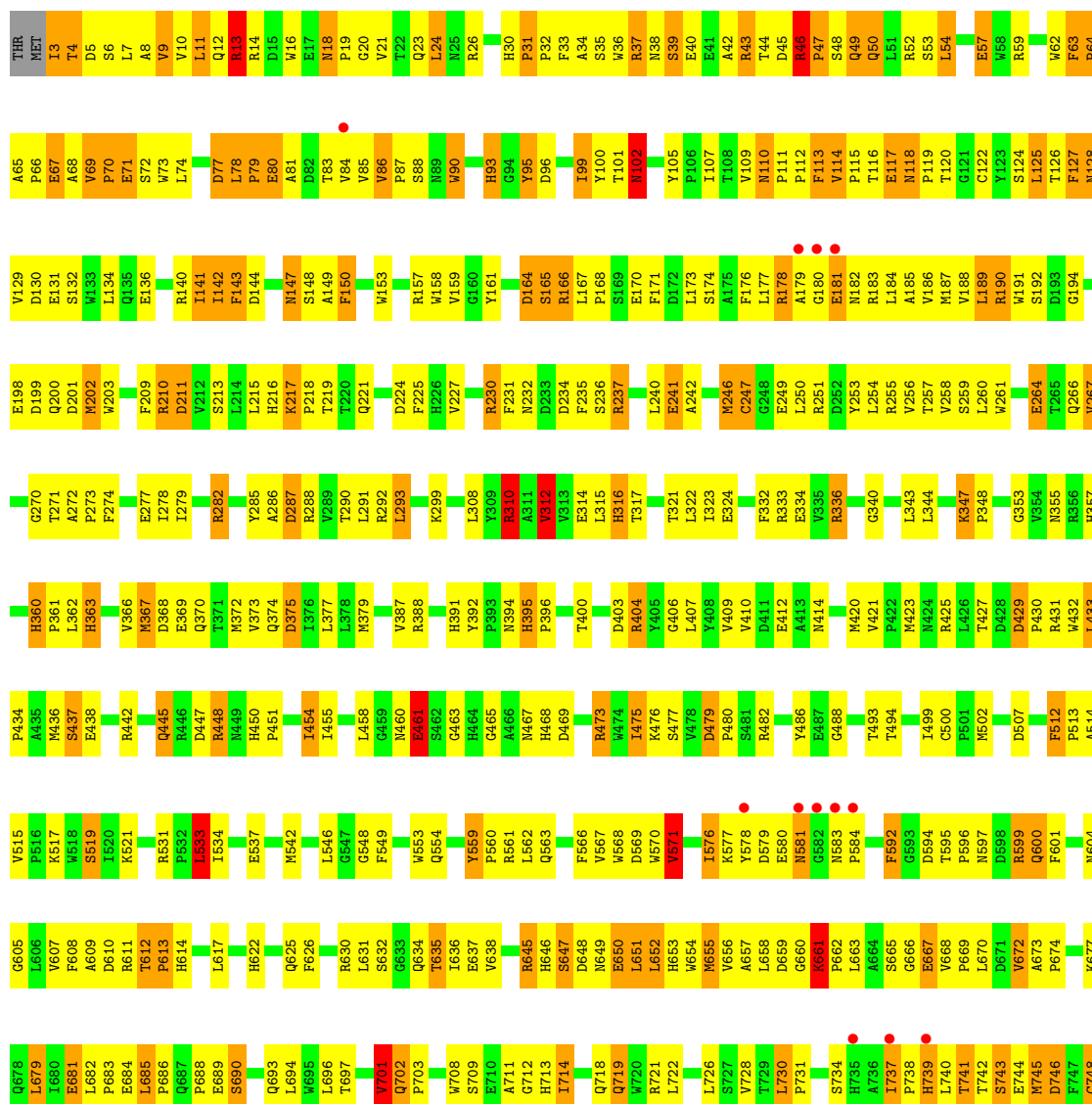
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

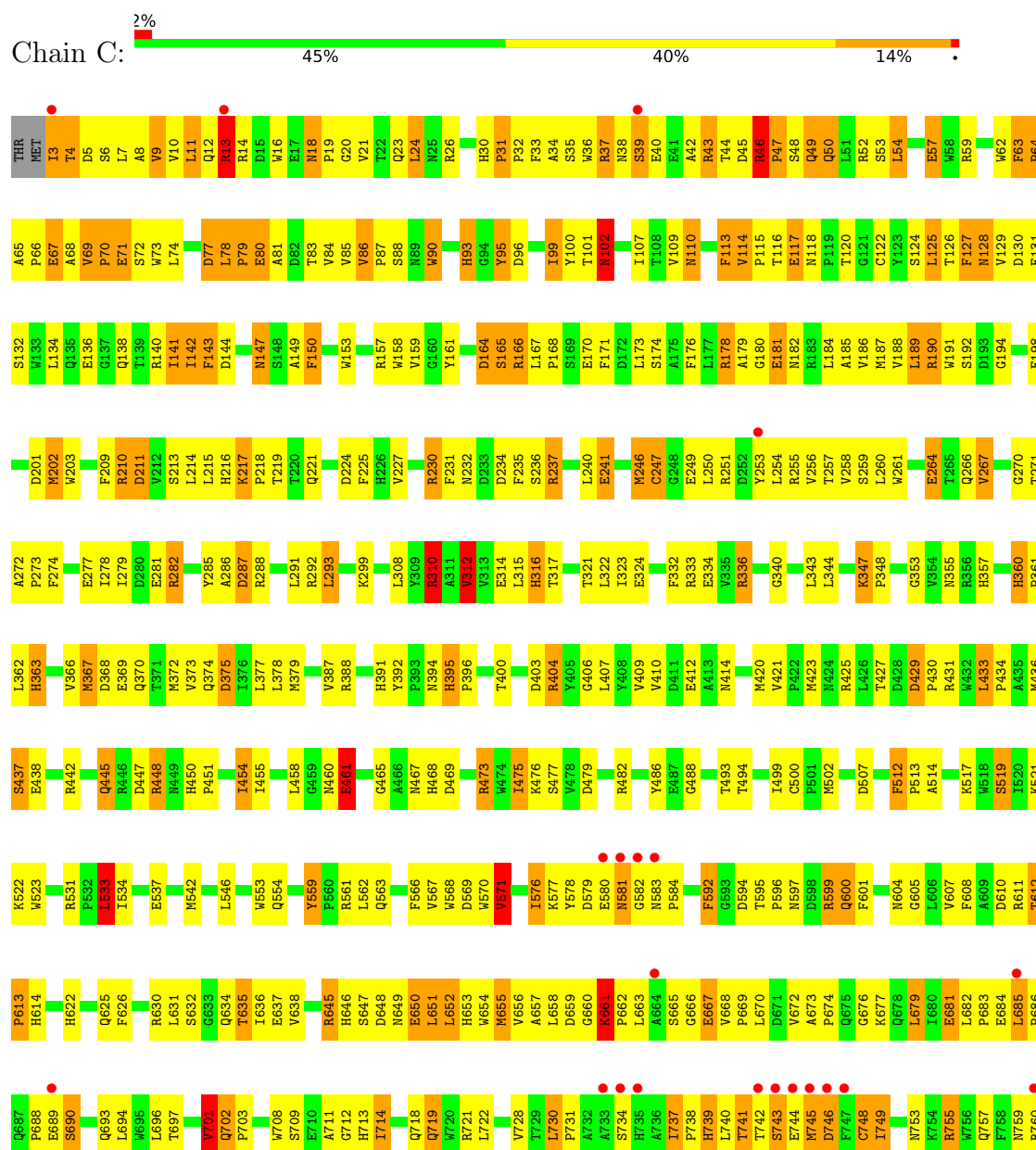


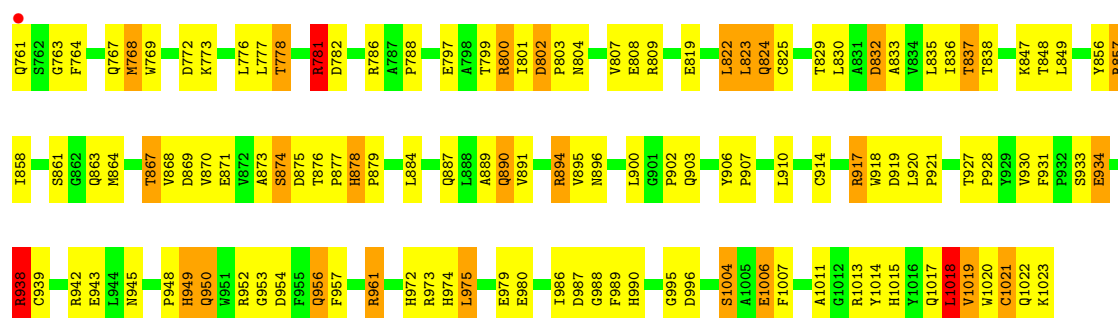


• Molecule 1: Beta-Galactosidase

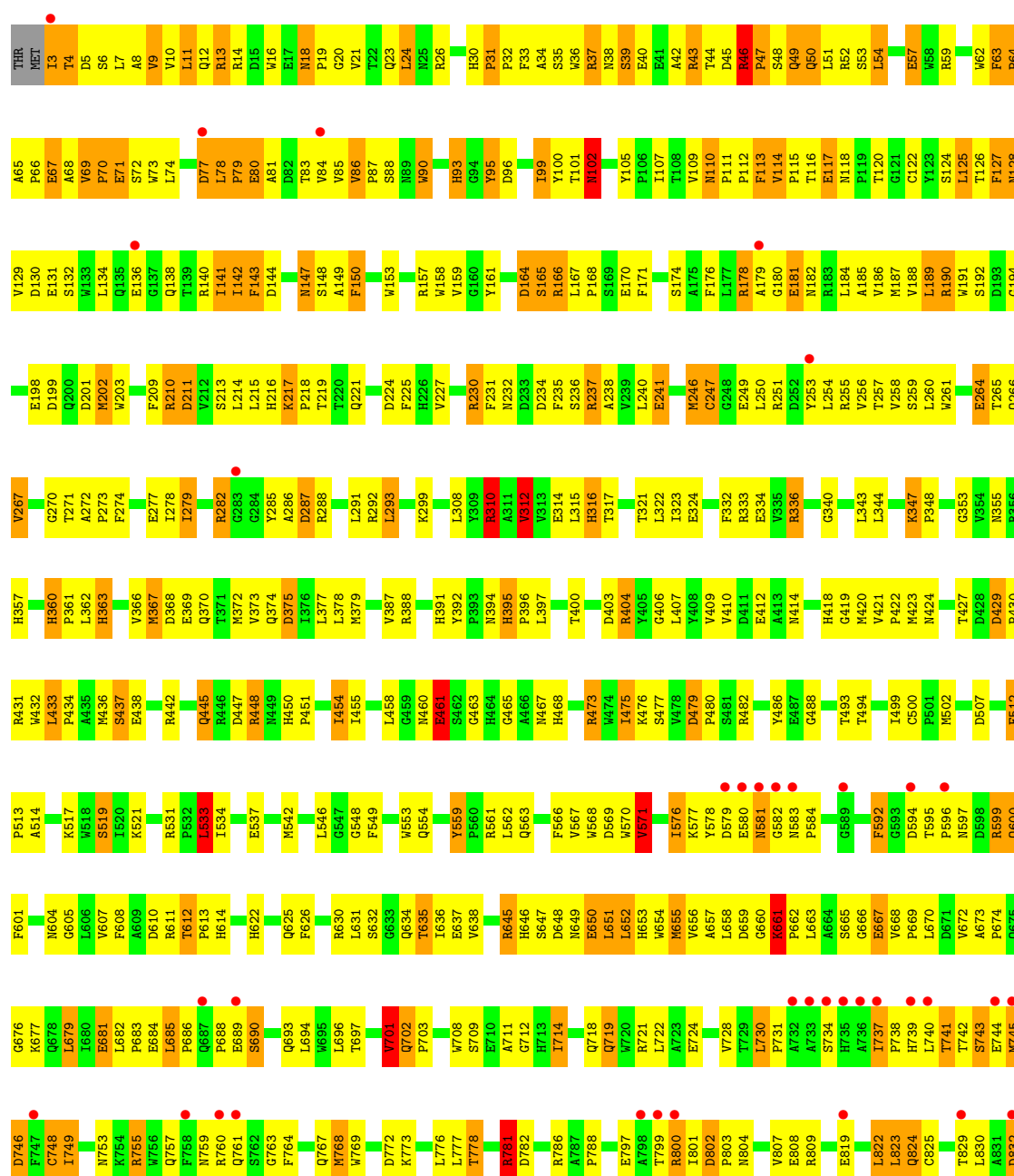
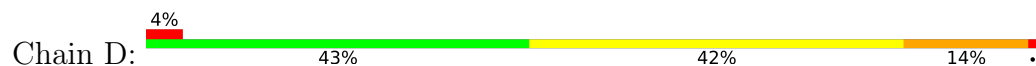


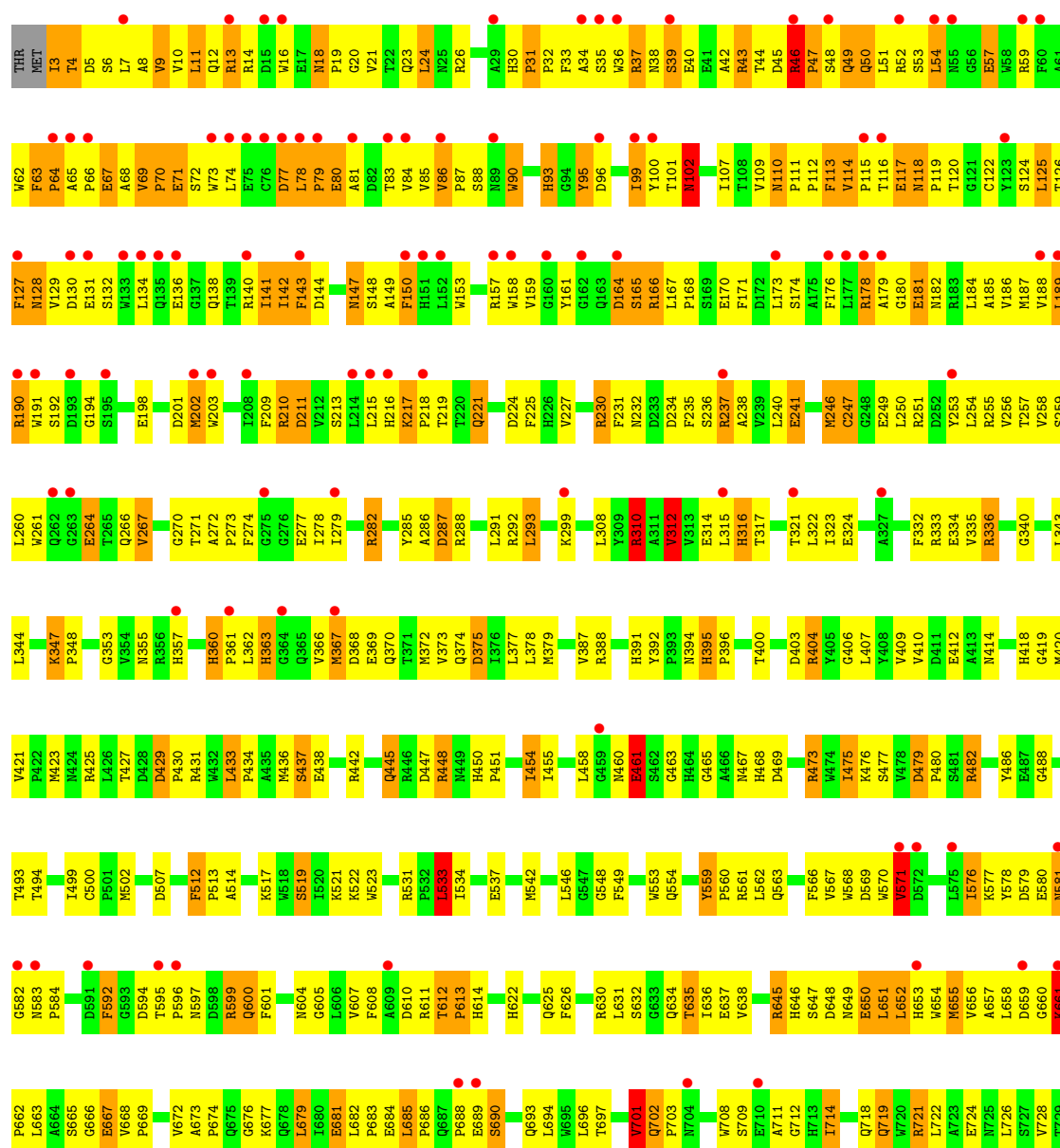
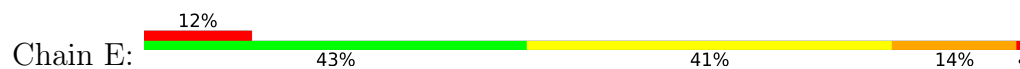
- Molecule 1: Beta-Galactosidase

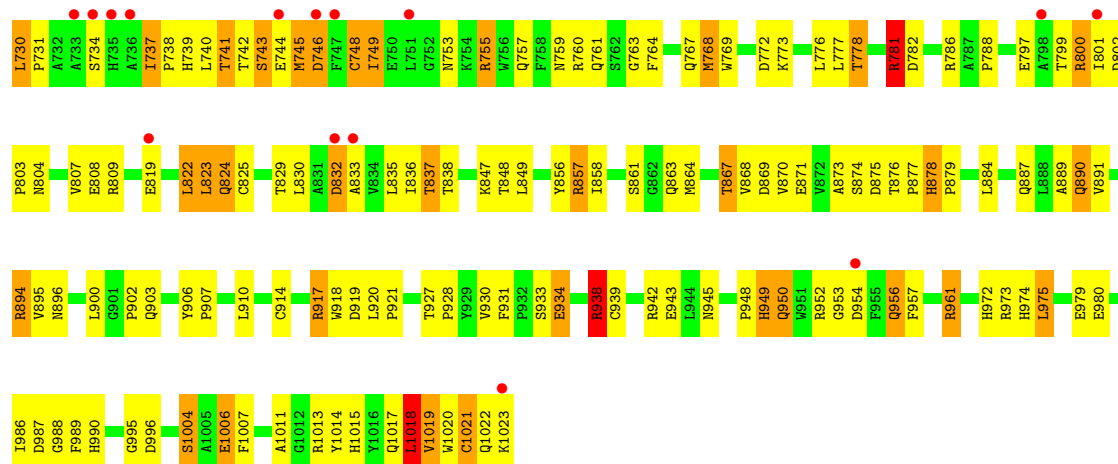




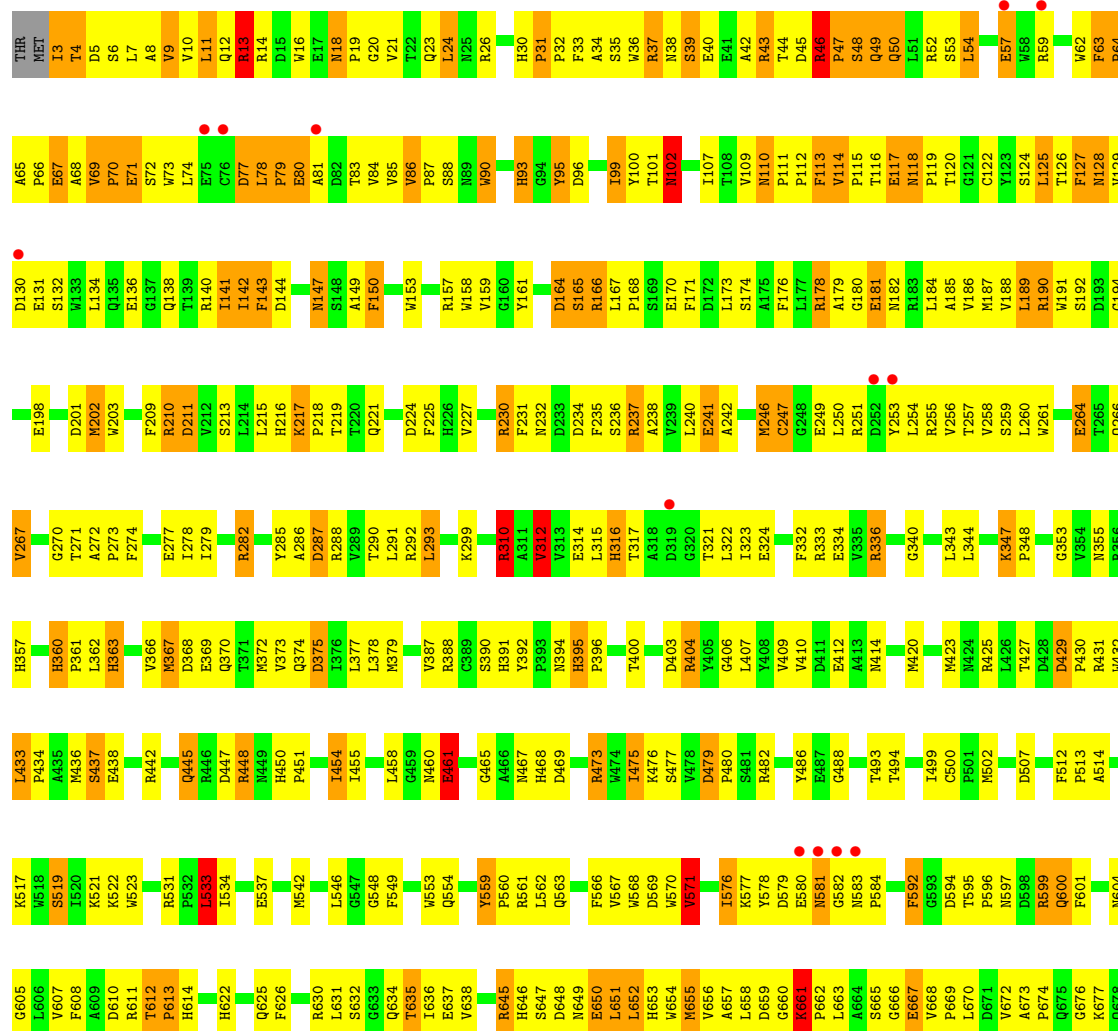
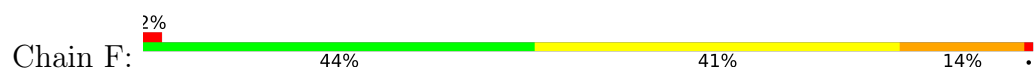
• Molecule 1: Beta-Galactosidase

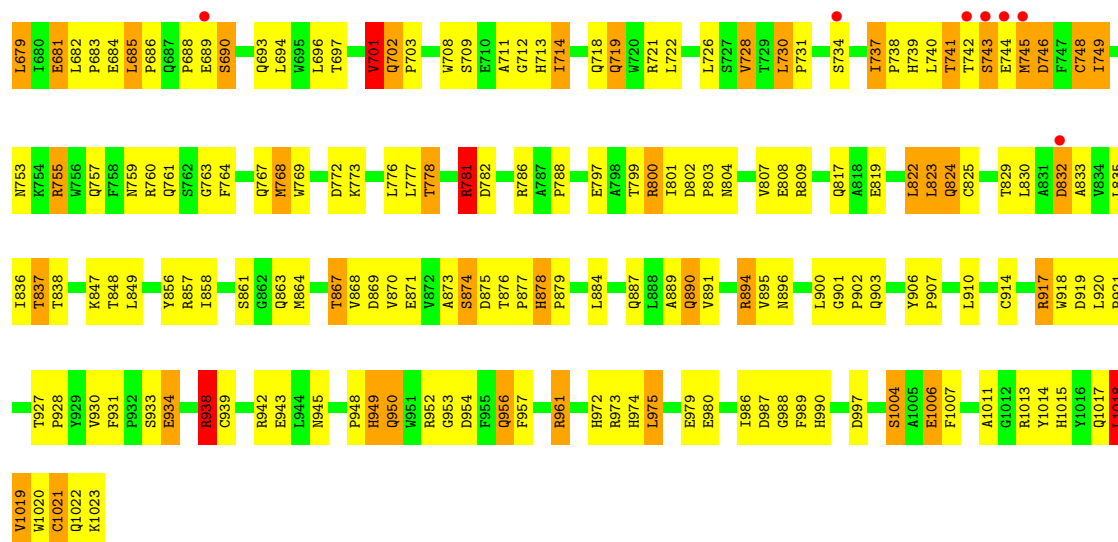




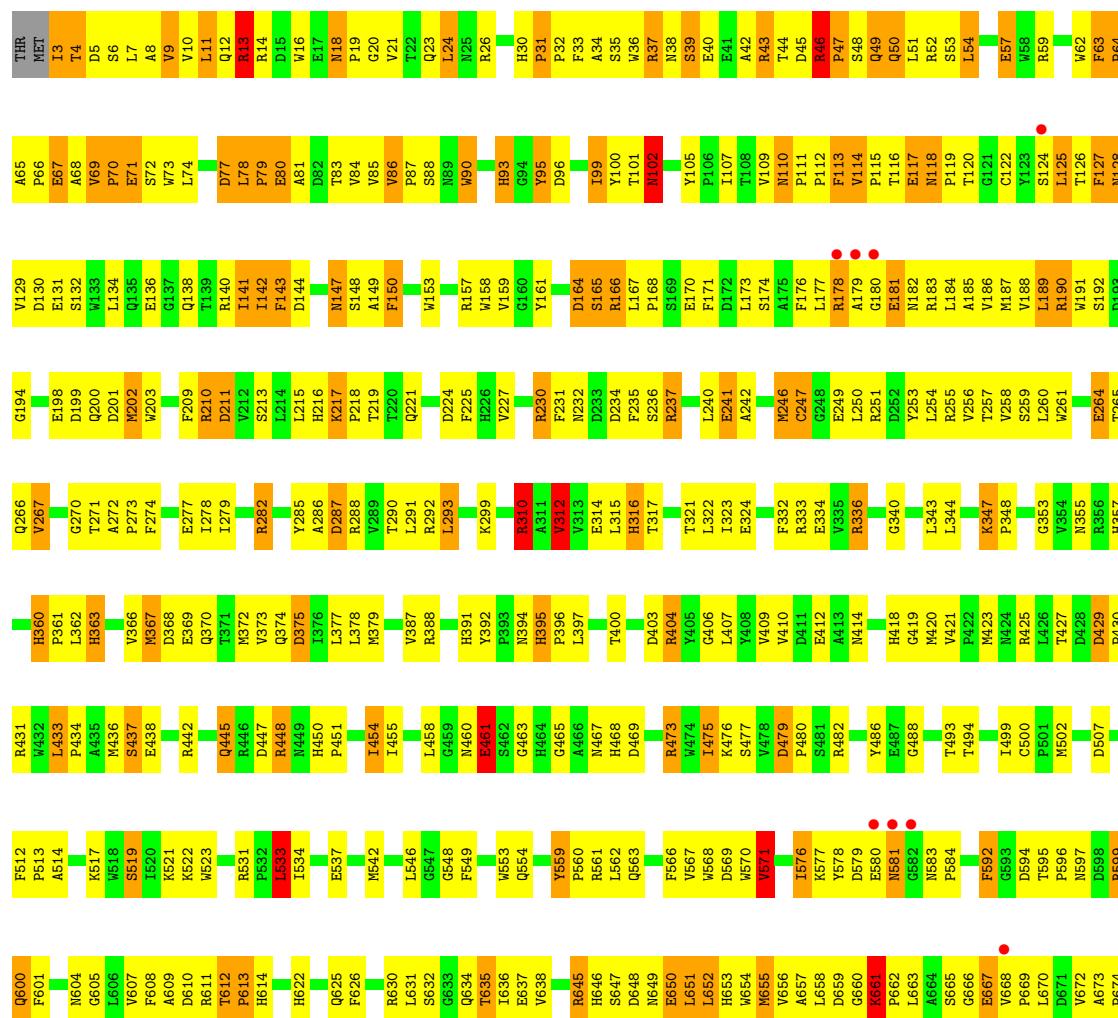
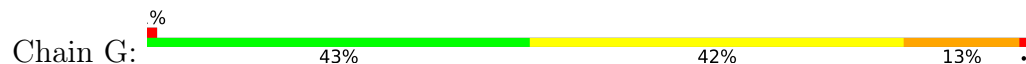


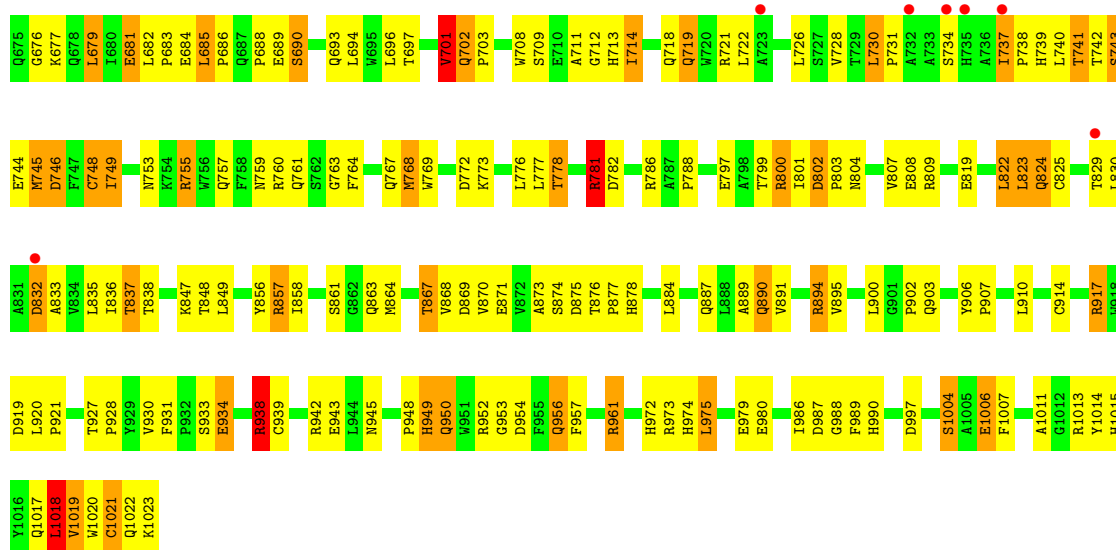
• Molecule 1: Beta-Galactosidase



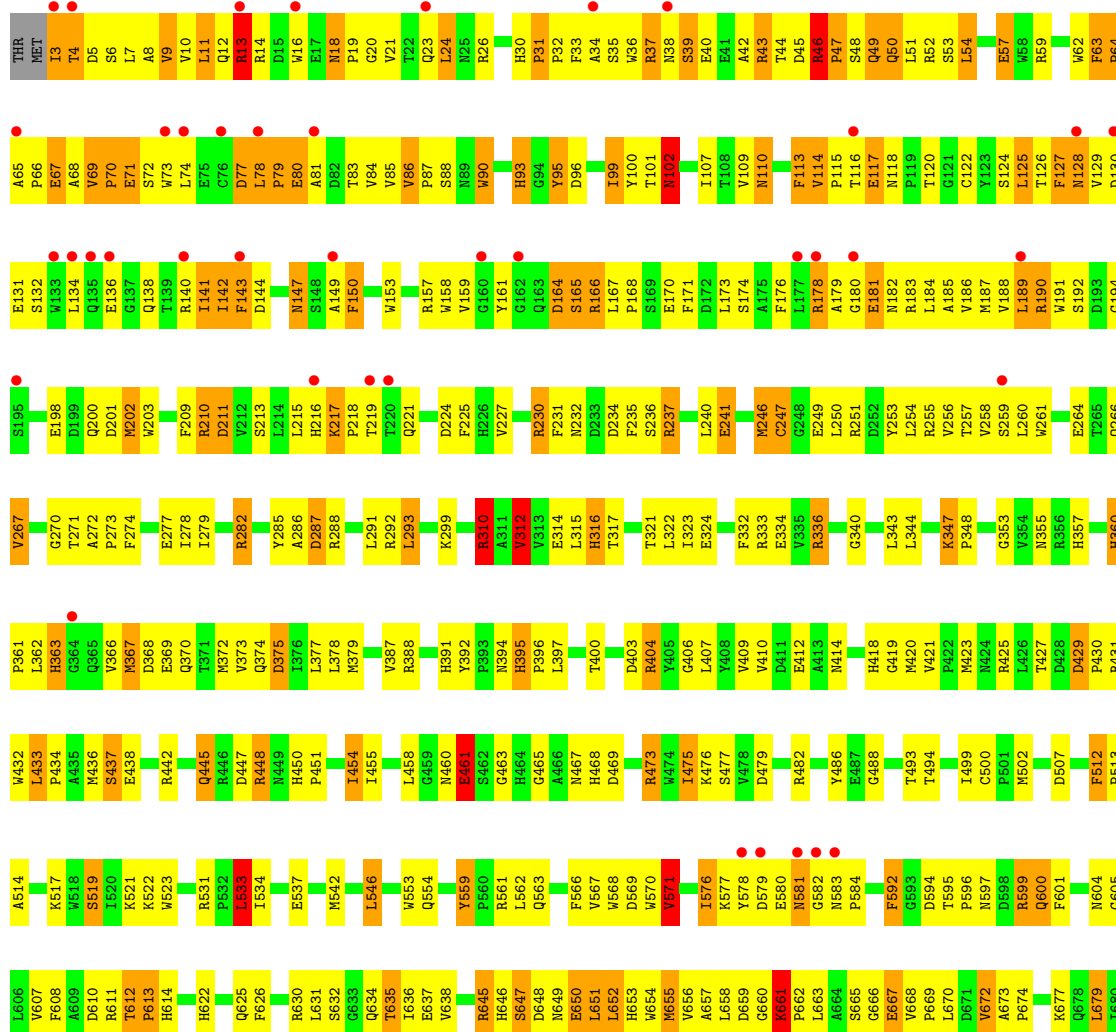


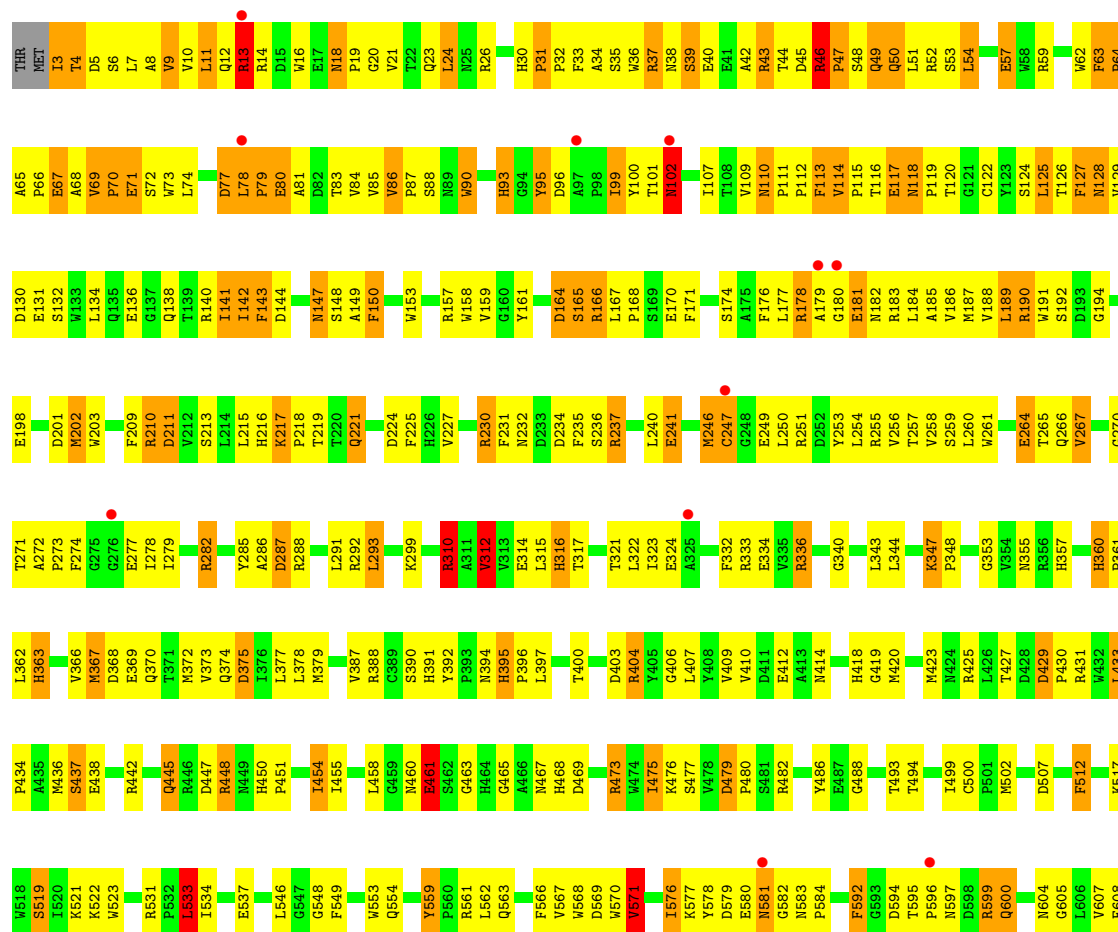
• Molecule 1: Beta-Galactosidase

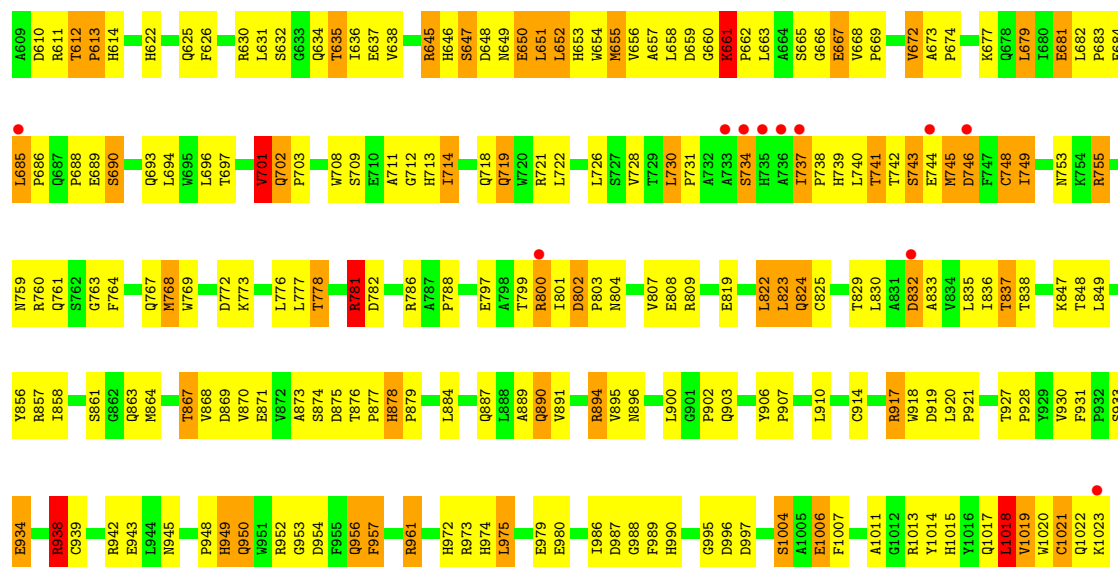




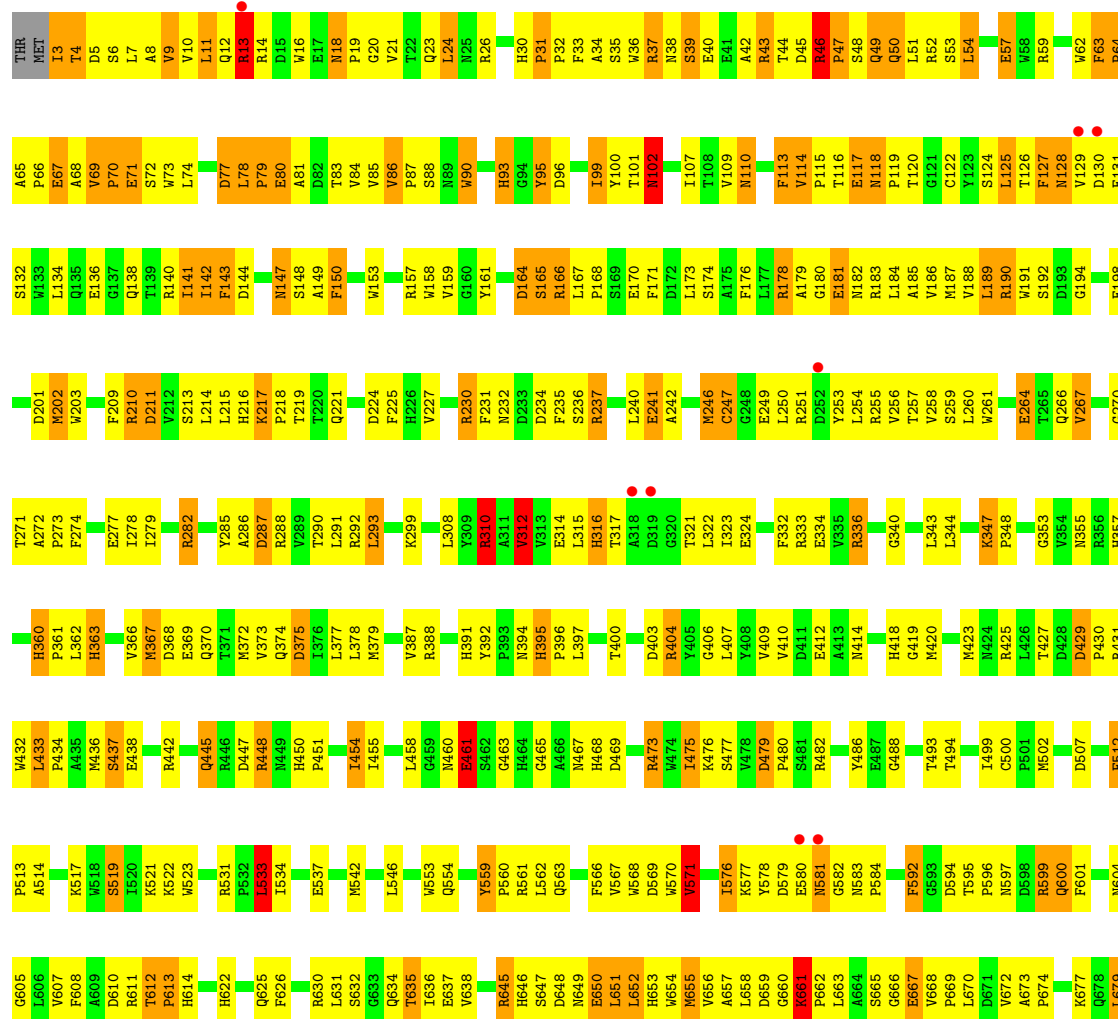
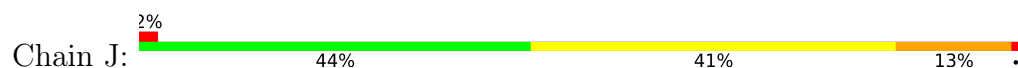
• Molecule 1: Beta-Galactosidase





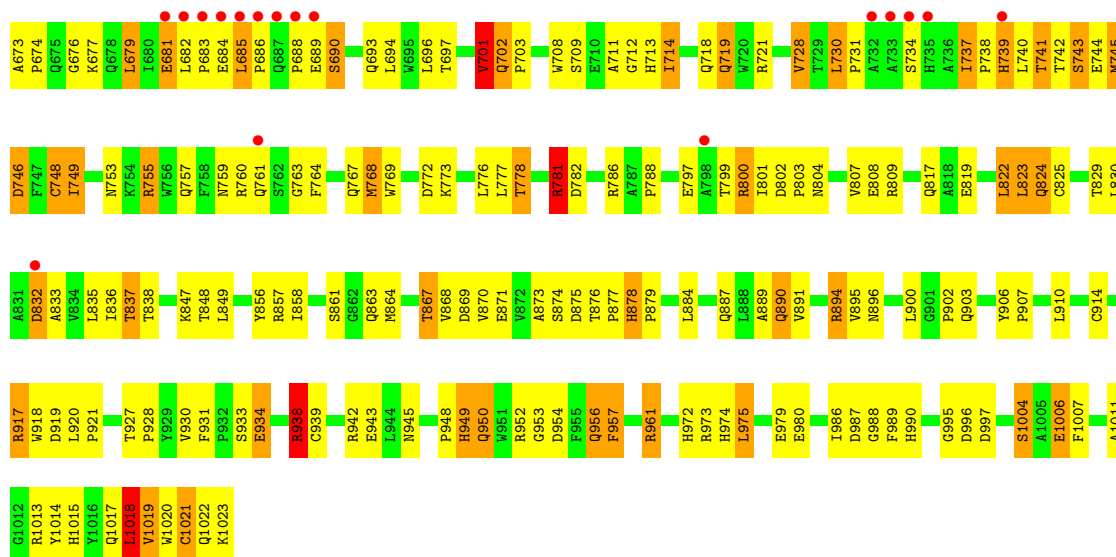


• Molecule 1: Beta-Galactosidase

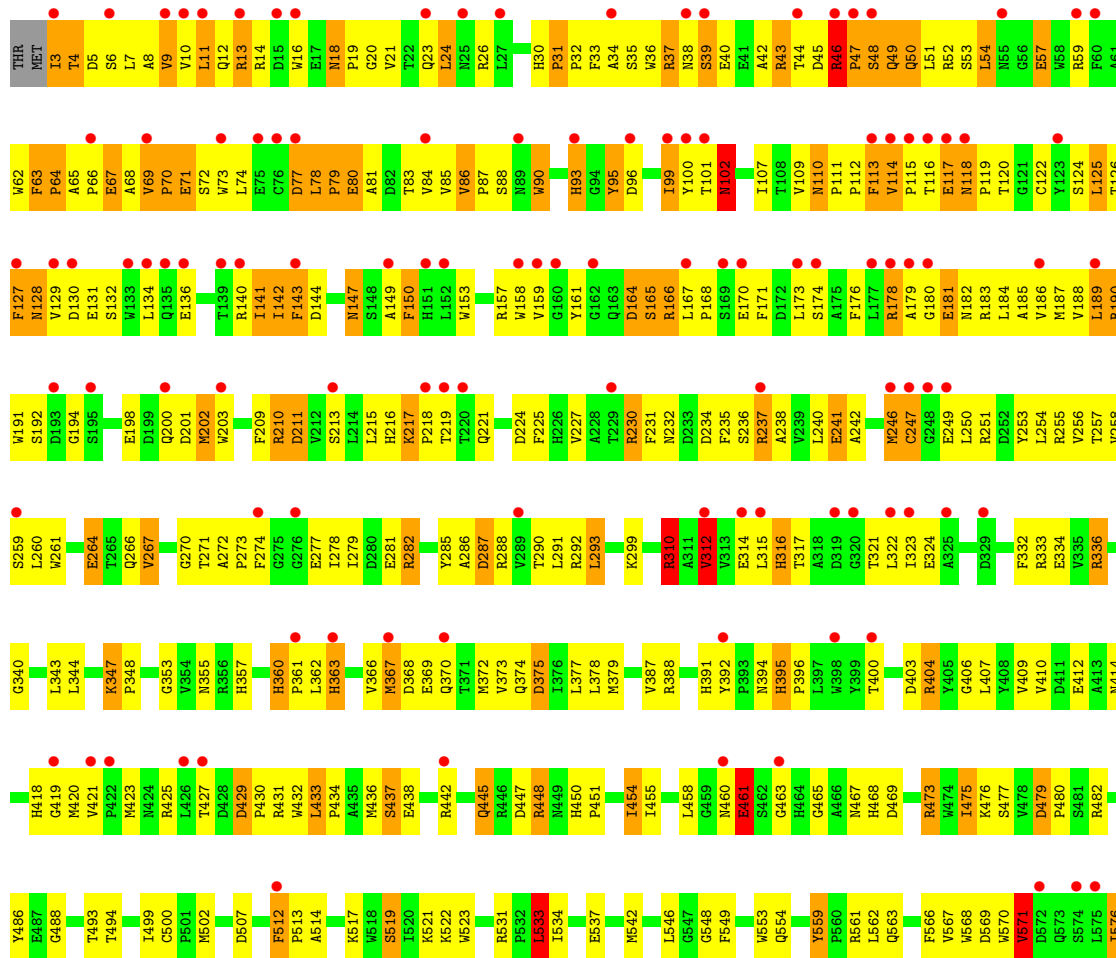
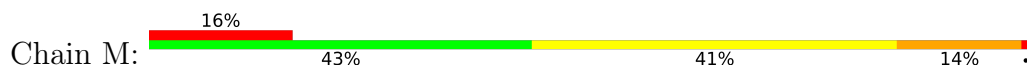






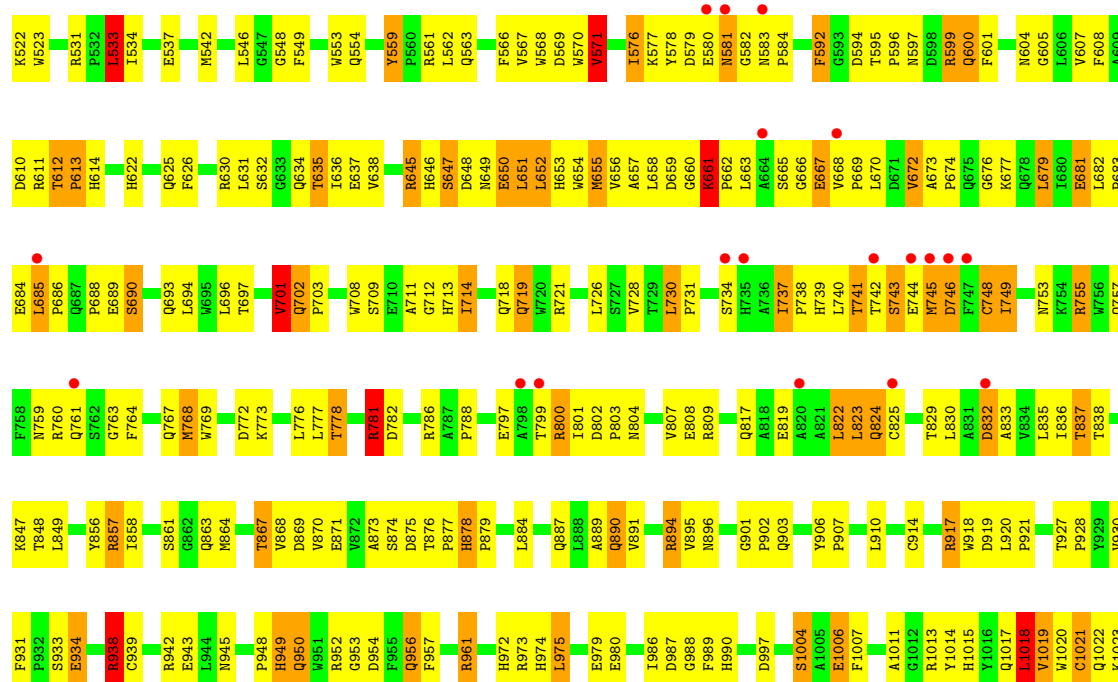


• Molecule 1: Beta-Galactosidase

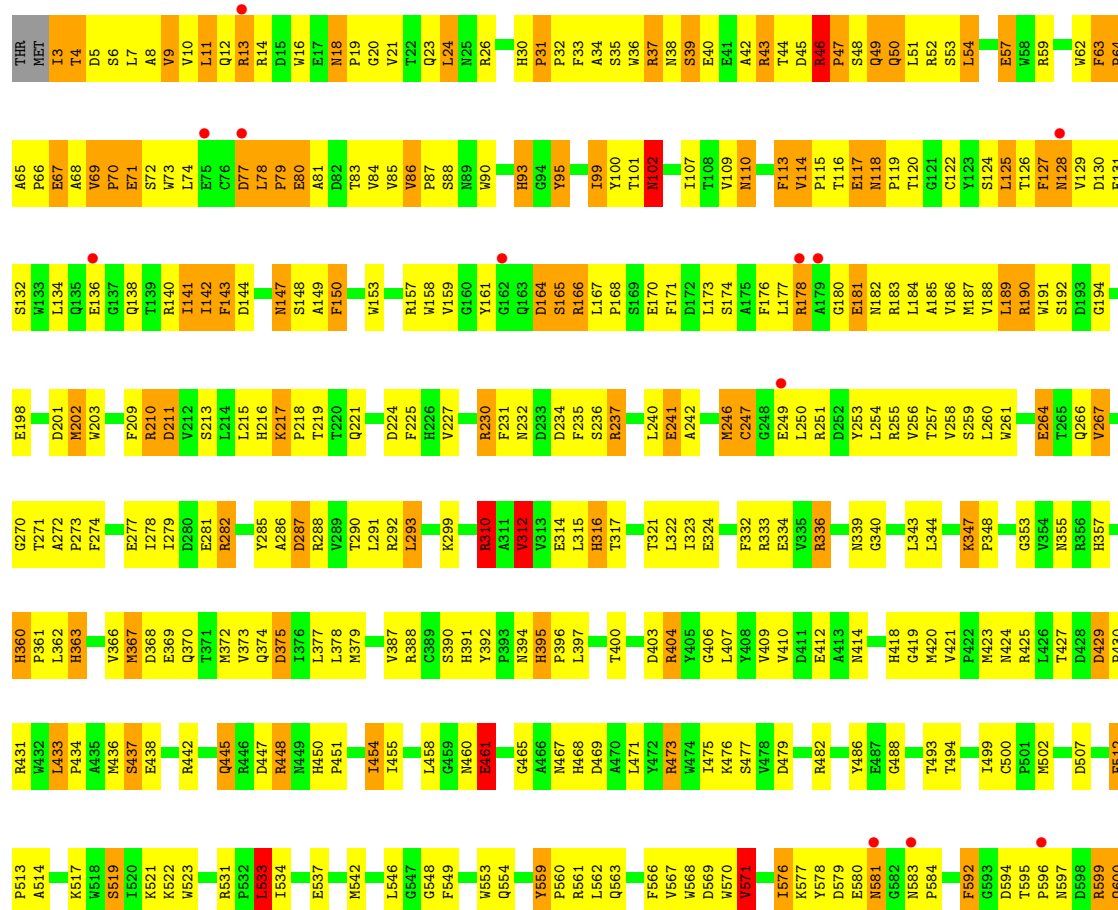


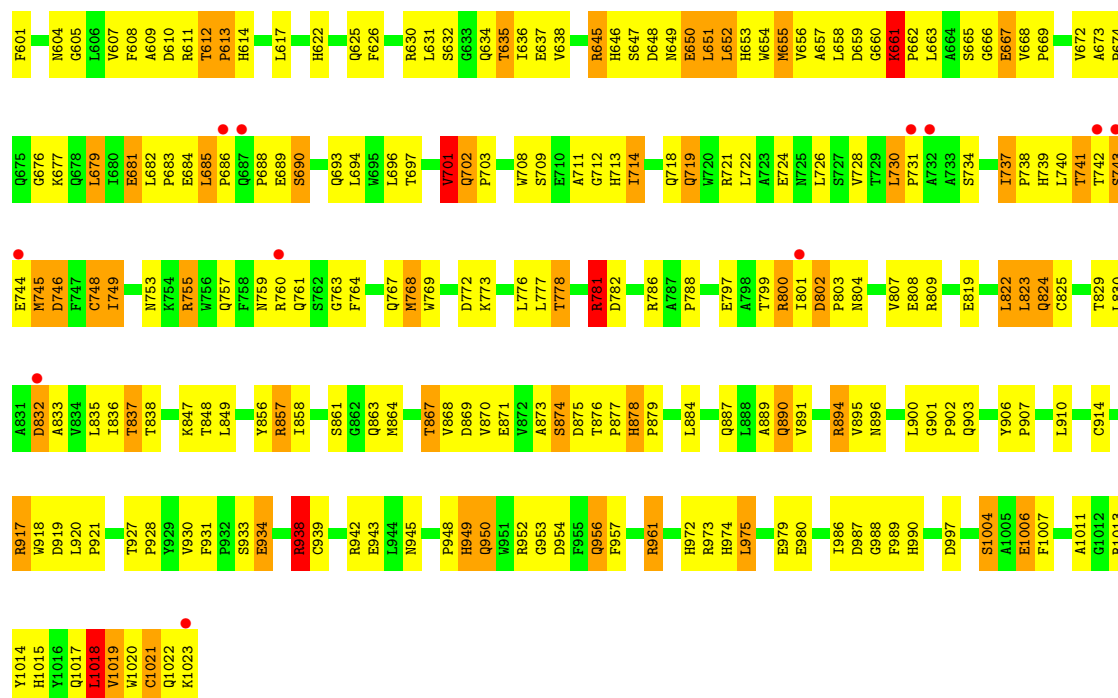


E438	H363	A272	D201	E131	A65
R442	V366	F274	W203	M132	P66
Q445	M367	E277	F209	L134	E67
R446	D368	I278	R210	Q135	A68
R448	E369	I279	D211	E136	V69
R449	Q370		V212	R140	P70
R450	M372	R282	G213	I141	E71
P451	V374		L214	F143	S72
	D375	A286	H216	D144	W73
I454	L376	R287	K217		V9
I455	L377	R288	F218	I142	W10
	L378		T219	F143	L11
L458	M379	L291	T220	D144	Q12
		R292	Q221		R13
		L293		M147	R14
M460	V387		D224	S148	D15
R461	R388	K299	F225	A149	W16
Q465	C389		H226	F150	E17
A466	S390	R310	W227		M18
M467	H391	A311		R157	P19
M468	V392	U312		W158	V21
	F393	V313	R230	G160	T22
	N394	E314	F231	Y161	S88
R473	H395	L315	N232		R89
W474	P396	H316	D234	D164	W90
K476	L397	T317	F235	S165	
		A318	S236	R166	H93
S477	T400	D319	R237	L167	G94
W478	D403	G320	A238	P168	Y95
P480	R404	R321	W239		P31
S481	Y405	L322	L240	I101	P32
R482	G406	I323	E241	F171	F33
	L407	E324		D172	A34
	Y408	F332	M246	L173	W36
E487	V409	R333	C247	S174	R37
Q488	V410	E334	G248	F176	S39
	D411	E249	L177	I108	E40
T493	E412	V335	L250	N110	E41
T494	A413	R336	R251	P111	A42
	M414		D252	R178	R43
		G340	V253	A179	T44
I499	M420	L343	R254	G180	D45
P501	V421	L344	L255	E181	R46
M502	M423		R256	N182	P47
		K347	V257	R183	S48
	T427	P348	T258	L184	Q49
	D428		V186	A185	Q50
F512	Q429	G353	M187	N118	L51
A514	P430	V354	L280	P119	R52
V515	R431	N355	S259	T120	S53
P516	W432	R356	L261	G121	L54
K517	L433	H357		C122	
W518	P434			Y123	
S519	A435	H360	E264	R189	E57
T520	M436	P361	T265	W191	W58
	R437	L362	Q266	S192	R59
			V267	D193	
				G194	W62
					F63
				E198	P64

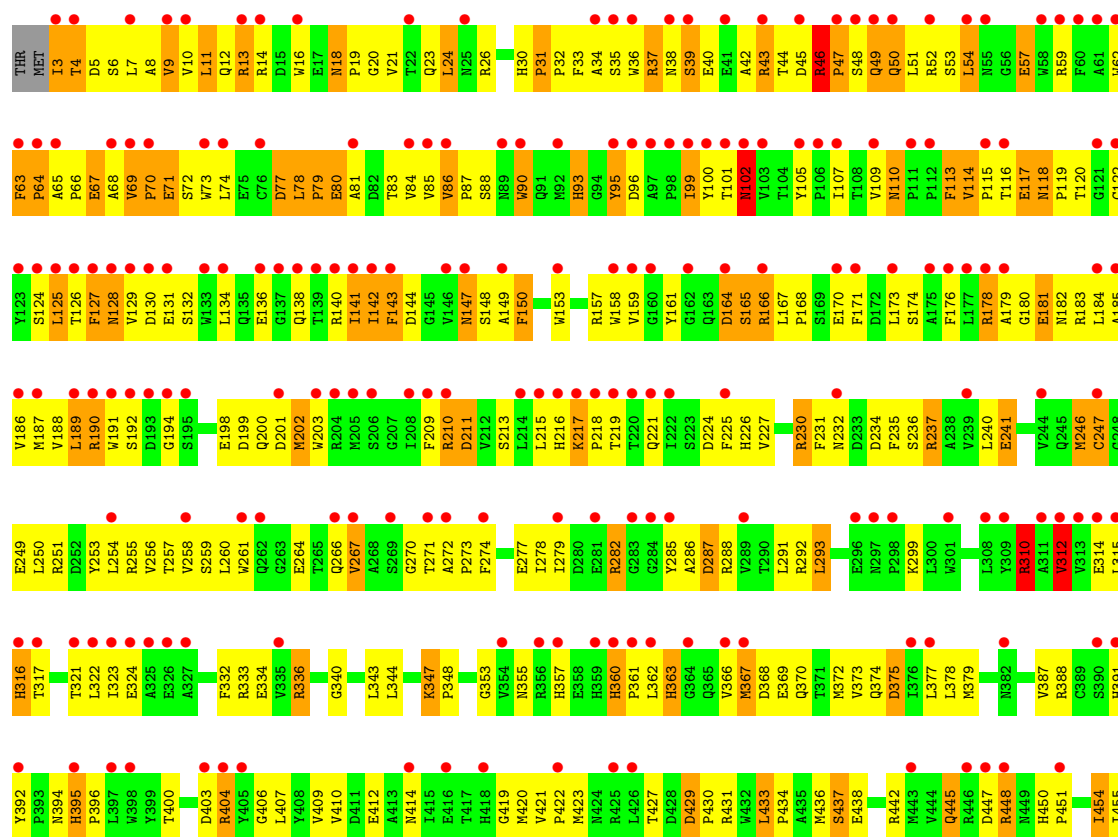


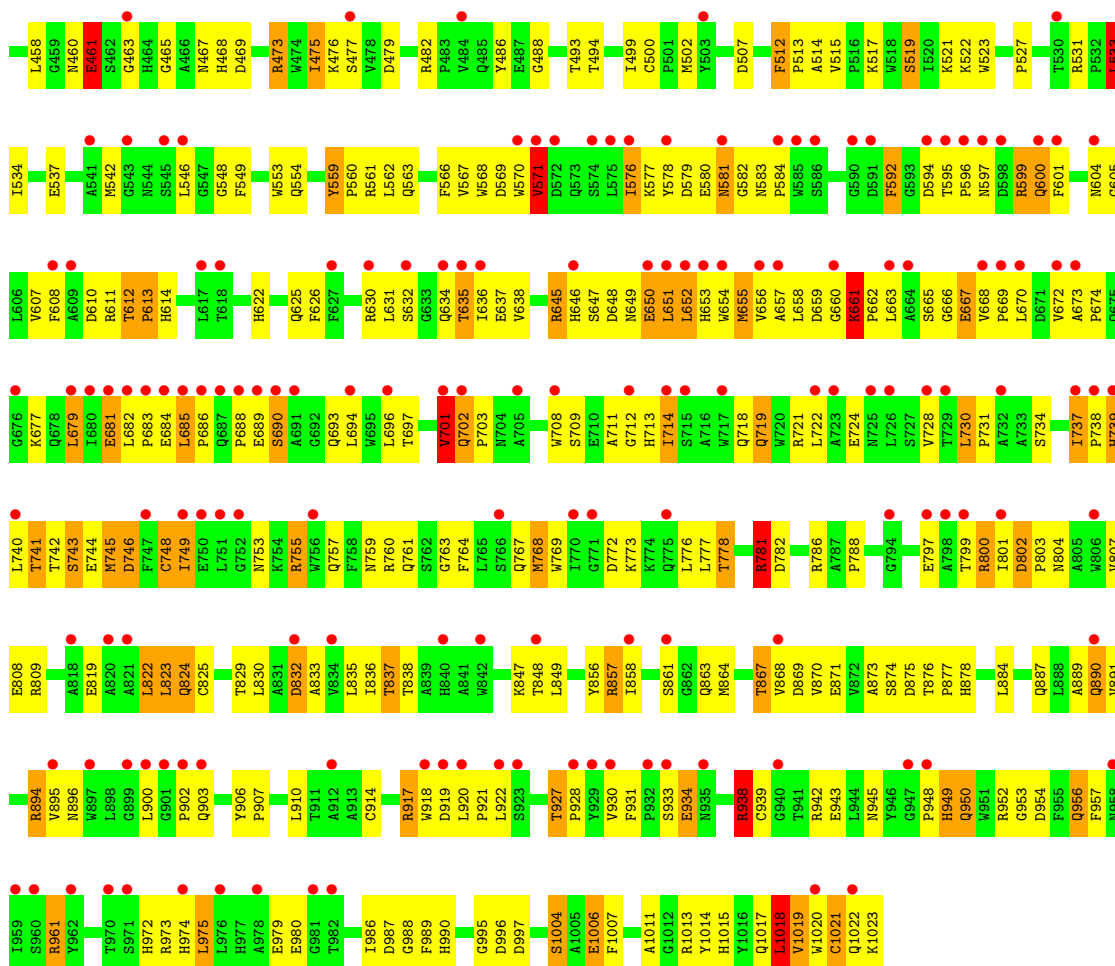
● Molecule 1: Beta-Galactosidase





• Molecule 1: Beta-Galactosidase





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

Chain Q: 50% 50%



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

Chain R: 50% 50%



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

Chain S: 50% 50%



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

Chain T:  50% 50%



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

Chain U:  50% 50%



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

Chain V:  50% 50%



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

Chain W:  50% 50%



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

Chain X:  50% 50%



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

Chain Y:  50% 50%



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

Chain Z:  50% 50%



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

Chain a:  50% 50%



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

Chain b:



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

Chain c:



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

Chain d:



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

Chain e:



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

Chain f:



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) 65.8 (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 , 0.212	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)	0.30 , 95.7	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: 2FG, MG, NA, BGC, 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	1.37	5/8439 (0.1%)	1.70	117/11510 (1.0%)
1	B	1.37	5/8439 (0.1%)	1.70	119/11510 (1.0%)
1	C	1.37	5/8439 (0.1%)	1.70	119/11510 (1.0%)
1	D	1.37	6/8439 (0.1%)	1.70	117/11510 (1.0%)
1	E	1.37	5/8439 (0.1%)	1.70	117/11510 (1.0%)
1	F	1.37	5/8439 (0.1%)	1.70	117/11510 (1.0%)
1	G	1.37	5/8439 (0.1%)	1.70	119/11510 (1.0%)
1	H	1.37	5/8439 (0.1%)	1.70	118/11510 (1.0%)
1	I	1.37	5/8439 (0.1%)	1.70	120/11510 (1.0%)
1	J	1.37	5/8439 (0.1%)	1.70	117/11510 (1.0%)
1	K	1.37	5/8439 (0.1%)	1.70	118/11510 (1.0%)
1	L	1.37	5/8439 (0.1%)	1.70	119/11510 (1.0%)
1	M	1.37	5/8439 (0.1%)	1.70	118/11510 (1.0%)
1	N	1.37	5/8439 (0.1%)	1.70	118/11510 (1.0%)
1	O	1.37	5/8439 (0.1%)	1.70	119/11510 (1.0%)
1	P	1.37	6/8439 (0.1%)	1.70	118/11510 (1.0%)
All	All	1.37	82/135024 (0.1%)	1.70	1890/184160 (1.0%)

The worst 5 of 82 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	479	ASP	C-N	-6.90	1.27	1.33
1	P	479	ASP	C-N	-6.85	1.27	1.33
1	C	479	ASP	C-N	-6.83	1.27	1.33
1	E	479	ASP	C-N	-6.83	1.27	1.33
1	M	479	ASP	C-N	-6.83	1.27	1.33

The worst 5 of 1890 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	363	HIS	CA-CB-CG	-10.47	103.33	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	363	HIS	CA-CB-CG	-10.46	103.34	113.80
1	J	363	HIS	CA-CB-CG	-10.45	103.35	113.80
1	O	363	HIS	CA-CB-CG	-10.45	103.35	113.80
1	E	363	HIS	CA-CB-CG	-10.43	103.37	113.80

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	614	3
1	B	8219	0	7811	596	5
1	C	8219	0	7811	578	1
1	D	8219	0	7811	610	0
1	E	8219	0	7811	600	0
1	F	8219	0	7811	591	1
1	G	8219	0	7811	600	1
1	H	8219	0	7811	591	0
1	I	8219	0	7811	600	1
1	J	8219	0	7811	598	0
1	K	8219	0	7811	593	0
1	L	8219	0	7811	606	1
1	M	8219	0	7811	610	0
1	N	8219	0	7811	602	0
1	O	8219	0	7811	606	0
1	P	8219	0	7811	610	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	9467	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 37.

The worst 5 of 9467 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:I:427:THR:HA	1:I:436:MET:HE1	1.17	1.16
1:J:427:THR:HA	1:J:436:MET:HE1	1.17	1.16
1:N:427:THR:HA	1:N:436:MET:HE1	1.17	1.16
1:F:427:THR:HA	1:F:436:MET:HE1	1.17	1.16
1:C:427:THR:HA	1:C:436:MET:HE1	1.17	1.15

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%)	14	35
1	B	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	C	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	D	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	E	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	F	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	G	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	H	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	I	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	J	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	K	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	L	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	M	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	N	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	O	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	P	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
All	All	16288/16368 (100%)	15296 (94%)	848 (5%)	144 (1%)	14	35

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%)	734 (84%)	138 (16%)	2	7
1	B	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	C	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	D	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	E	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	F	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	G	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	H	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	I	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	J	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	K	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	L	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	M	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	N	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	O	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	P	872/872 (100%)	734 (84%)	138 (16%)	2	7
All	All	13952/13952 (100%)	11744 (84%)	2208 (16%)	2	7

5 of 2208 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	310	ARG
1	N	799	THR
1	N	293	LEU
1	P	49	GLN
1	F	635	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 379 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	977	HIS
1	M	128	ASN
1	K	226	HIS
1	L	102	ASN
1	M	761	GLN

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	748	1	8,9,10	0.92	0	6,9,11	1.62	2 (33%)
1	CME	M	1021	1	8,9,10	0.67	0	6,9,11	1.51	1 (16%)
1	CME	B	748	1	8,9,10	0.92	0	6,9,11	1.62	2 (33%)
1	CME	I	1021	1	8,9,10	0.66	0	6,9,11	1.52	1 (16%)
1	CME	P	914	1	8,9,10	0.93	0	6,9,11	1.58	1 (16%)
1	CME	I	748	1	8,9,10	0.93	0	6,9,11	1.62	2 (33%)
1	CME	N	748	1	8,9,10	0.93	0	6,9,11	1.62	2 (33%)
1	CME	P	748	1	8,9,10	0.93	0	6,9,11	1.62	2 (33%)
1	CME	N	914	1	8,9,10	0.93	0	6,9,11	1.57	1 (16%)
1	CME	E	1021	1	8,9,10	0.66	0	6,9,11	1.52	1 (16%)
1	CME	C	748	1	8,9,10	0.92	0	6,9,11	1.62	2 (33%)
1	CME	K	914	1	8,9,10	0.93	0	6,9,11	1.58	1 (16%)
1	CME	C	914	1	8,9,10	0.93	0	6,9,11	1.57	1 (16%)
1	CME	K	1021	1	8,9,10	0.66	0	6,9,11	1.52	1 (16%)
1	CME	C	1021	1	8,9,10	0.66	0	6,9,11	1.52	1 (16%)
1	CME	J	914	1	8,9,10	0.93	0	6,9,11	1.57	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CME	D	914	1	8,9,10	0.93	0	6,9,11	1.57	1 (16%)
1	CME	L	748	1	8,9,10	0.92	0	6,9,11	1.61	2 (33%)
1	CME	G	914	1	8,9,10	0.93	0	6,9,11	1.58	1 (16%)
1	CME	I	914	1	8,9,10	0.92	0	6,9,11	1.58	1 (16%)
1	CME	E	914	1	8,9,10	0.93	0	6,9,11	1.58	1 (16%)
1	CME	O	914	1	8,9,10	0.93	0	6,9,11	1.57	1 (16%)
1	CME	O	1021	1	8,9,10	0.66	0	6,9,11	1.52	1 (16%)
1	CME	G	1021	1	8,9,10	0.66	0	6,9,11	1.52	1 (16%)
1	CME	H	914	1	8,9,10	0.93	0	6,9,11	1.57	1 (16%)
1	CME	J	748	1	8,9,10	0.93	0	6,9,11	1.62	2 (33%)
1	CME	L	1021	1	8,9,10	0.66	0	6,9,11	1.52	1 (16%)
1	CME	A	914	1	8,9,10	0.93	0	6,9,11	1.57	1 (16%)
1	CME	D	1021	1	8,9,10	0.67	0	6,9,11	1.52	1 (16%)
1	CME	J	1021	1	8,9,10	0.67	0	6,9,11	1.52	1 (16%)
1	CME	K	748	1	8,9,10	0.93	0	6,9,11	1.61	2 (33%)
1	CME	H	1021	1	8,9,10	0.67	0	6,9,11	1.52	1 (16%)
1	CME	B	914	1	8,9,10	0.93	0	6,9,11	1.58	1 (16%)
1	CME	F	748	1	8,9,10	0.93	0	6,9,11	1.62	2 (33%)
1	CME	M	914	1	8,9,10	0.93	0	6,9,11	1.57	1 (16%)
1	CME	D	748	1	8,9,10	0.93	0	6,9,11	1.62	2 (33%)
1	CME	F	914	1	8,9,10	0.92	0	6,9,11	1.58	1 (16%)
1	CME	L	914	1	8,9,10	0.93	0	6,9,11	1.57	1 (16%)
1	CME	B	1021	1	8,9,10	0.66	0	6,9,11	1.52	1 (16%)
1	CME	G	748	1	8,9,10	0.92	0	6,9,11	1.62	2 (33%)
1	CME	N	1021	1	8,9,10	0.67	0	6,9,11	1.52	1 (16%)
1	CME	P	1021	1	8,9,10	0.66	0	6,9,11	1.52	1 (16%)
1	CME	A	748	1	8,9,10	0.92	0	6,9,11	1.62	2 (33%)
1	CME	O	748	1	8,9,10	0.93	0	6,9,11	1.62	2 (33%)
1	CME	M	748	1	8,9,10	0.92	0	6,9,11	1.62	2 (33%)
1	CME	A	1021	1	8,9,10	0.66	0	6,9,11	1.52	1 (16%)
1	CME	F	1021	1	8,9,10	0.67	0	6,9,11	1.51	1 (16%)
1	CME	E	748	1	8,9,10	0.92	0	6,9,11	1.62	2 (33%)

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	748	1	-	4/5/8/10	-
1	CME	M	1021	1	-	5/5/8/10	-
1	CME	B	748	1	-	4/5/8/10	-
1	CME	I	1021	1	-	5/5/8/10	-
1	CME	P	914	1	-	3/5/8/10	-
1	CME	I	748	1	-	4/5/8/10	-
1	CME	N	748	1	-	4/5/8/10	-
1	CME	P	748	1	-	4/5/8/10	-
1	CME	N	914	1	-	3/5/8/10	-
1	CME	E	1021	1	-	5/5/8/10	-
1	CME	C	748	1	-	4/5/8/10	-
1	CME	K	914	1	-	3/5/8/10	-
1	CME	C	914	1	-	3/5/8/10	-
1	CME	K	1021	1	-	5/5/8/10	-
1	CME	C	1021	1	-	5/5/8/10	-
1	CME	J	914	1	-	3/5/8/10	-
1	CME	D	914	1	-	3/5/8/10	-
1	CME	L	748	1	-	4/5/8/10	-
1	CME	G	914	1	-	3/5/8/10	-
1	CME	I	914	1	-	3/5/8/10	-
1	CME	E	914	1	-	2/5/8/10	-
1	CME	O	914	1	-	3/5/8/10	-
1	CME	O	1021	1	-	5/5/8/10	-
1	CME	G	1021	1	-	5/5/8/10	-
1	CME	H	914	1	-	3/5/8/10	-
1	CME	J	748	1	-	4/5/8/10	-
1	CME	L	1021	1	-	5/5/8/10	-
1	CME	A	914	1	-	3/5/8/10	-
1	CME	D	1021	1	-	5/5/8/10	-
1	CME	J	1021	1	-	5/5/8/10	-
1	CME	K	748	1	-	4/5/8/10	-
1	CME	H	1021	1	-	5/5/8/10	-
1	CME	B	914	1	-	3/5/8/10	-

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

There are no bond length outliers.

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	914	CME	CB-SG-SD	-3.45	94.94	103.86
1	I	914	CME	CB-SG-SD	-3.44	94.95	103.86
1	E	914	CME	CB-SG-SD	-3.44	94.95	103.86
1	K	914	CME	CB-SG-SD	-3.44	94.95	103.86
1	F	914	CME	CB-SG-SD	-3.44	94.95	103.86

There are no chirality outliers.

5 of 189 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	748	CME	SD-CE-CZ-OH
1	A	1021	CME	N-CA-CB-SG
1	A	1021	CME	SD-CE-CZ-OH
1	B	748	CME	SD-CE-CZ-OH
1	B	1021	CME	N-CA-CB-SG

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	M	1021	CME	6	0
1	B	748	CME	2	0
1	I	1021	CME	7	0
1	I	748	CME	2	0
1	N	748	CME	2	0
1	P	748	CME	2	0
1	E	1021	CME	7	0
1	C	748	CME	2	0
1	K	1021	CME	6	0
1	C	1021	CME	6	0
1	L	748	CME	2	0
1	O	1021	CME	7	0
1	G	1021	CME	7	0
1	J	748	CME	2	0
1	L	1021	CME	6	0
1	D	1021	CME	6	0
1	J	1021	CME	7	0
1	K	748	CME	2	0
1	H	1021	CME	6	0
1	F	748	CME	2	0
1	D	748	CME	2	0
1	B	1021	CME	7	0
1	G	748	CME	2	0
1	N	1021	CME	7	0
1	P	1021	CME	6	0
1	A	748	CME	2	0
1	O	748	CME	2	0
1	M	748	CME	2	0
1	A	1021	CME	7	0
1	F	1021	CME	6	0
1	E	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	0.65	0	17,17,17	0.72	0
2	2FG	Q	2	2,4	11,11,12	0.88	0	12,15,17	1.35	2 (16%)
2	BGC	R	1	2	12,12,12	0.65	0	17,17,17	0.71	0
2	2FG	R	2	2,4	11,11,12	0.88	0	12,15,17	1.36	2 (16%)
2	BGC	S	1	2	12,12,12	0.66	0	17,17,17	0.72	0
2	2FG	S	2	2,4	11,11,12	0.88	0	12,15,17	1.37	2 (16%)
2	BGC	T	1	2	12,12,12	0.65	0	17,17,17	0.72	0
2	2FG	T	2	2,4	11,11,12	0.87	0	12,15,17	1.36	2 (16%)
2	BGC	U	1	2	12,12,12	0.66	0	17,17,17	0.72	0
2	2FG	U	2	2,4	11,11,12	0.88	0	12,15,17	1.36	2 (16%)
2	BGC	V	1	2	12,12,12	0.66	0	17,17,17	0.72	0
2	2FG	V	2	2,4	11,11,12	0.89	0	12,15,17	1.35	2 (16%)
2	BGC	W	1	2	12,12,12	0.66	0	17,17,17	0.72	0
2	2FG	W	2	2,4	11,11,12	0.90	0	12,15,17	1.35	2 (16%)
2	BGC	X	1	2	12,12,12	0.66	0	17,17,17	0.72	0
2	2FG	X	2	2,4	11,11,12	0.88	0	12,15,17	1.35	2 (16%)
2	BGC	Y	1	2	12,12,12	0.66	0	17,17,17	0.72	0
2	2FG	Y	2	2,4	11,11,12	0.87	0	12,15,17	1.37	2 (16%)
2	BGC	Z	1	2	12,12,12	0.66	0	17,17,17	0.72	0
2	2FG	Z	2	2,4	11,11,12	0.89	0	12,15,17	1.35	2 (16%)
2	BGC	a	1	2	12,12,12	0.65	0	17,17,17	0.72	0
2	2FG	a	2	2,4	11,11,12	0.87	0	12,15,17	1.36	2 (16%)
2	BGC	b	1	2	12,12,12	0.66	0	17,17,17	0.73	0
2	2FG	b	2	2,4	11,11,12	0.87	0	12,15,17	1.36	2 (16%)
2	BGC	c	1	2	12,12,12	0.65	0	17,17,17	0.72	0
2	2FG	c	2	2,4	11,11,12	0.88	0	12,15,17	1.37	2 (16%)
2	BGC	d	1	2	12,12,12	0.65	0	17,17,17	0.72	0
2	2FG	d	2	2,4	11,11,12	0.88	0	12,15,17	1.35	2 (16%)
2	BGC	e	1	2	12,12,12	0.65	0	17,17,17	0.72	0
2	2FG	e	2	2,4	11,11,12	0.87	0	12,15,17	1.37	2 (16%)
2	BGC	f	1	2	12,12,12	0.66	0	17,17,17	0.72	0
2	2FG	f	2	2,4	11,11,12	0.88	0	12,15,17	1.36	2 (16%)

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
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.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	2	2FG	C2-C3-C4	-3.48	105.39	109.59
2	e	2	2FG	C2-C3-C4	-3.47	105.40	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	2	2FG	C2-C3-C4	-3.47	105.40	109.59
2	S	2	2FG	C2-C3-C4	-3.46	105.42	109.59
2	T	2	2FG	C2-C3-C4	-3.46	105.42	109.59

There are no chirality outliers.

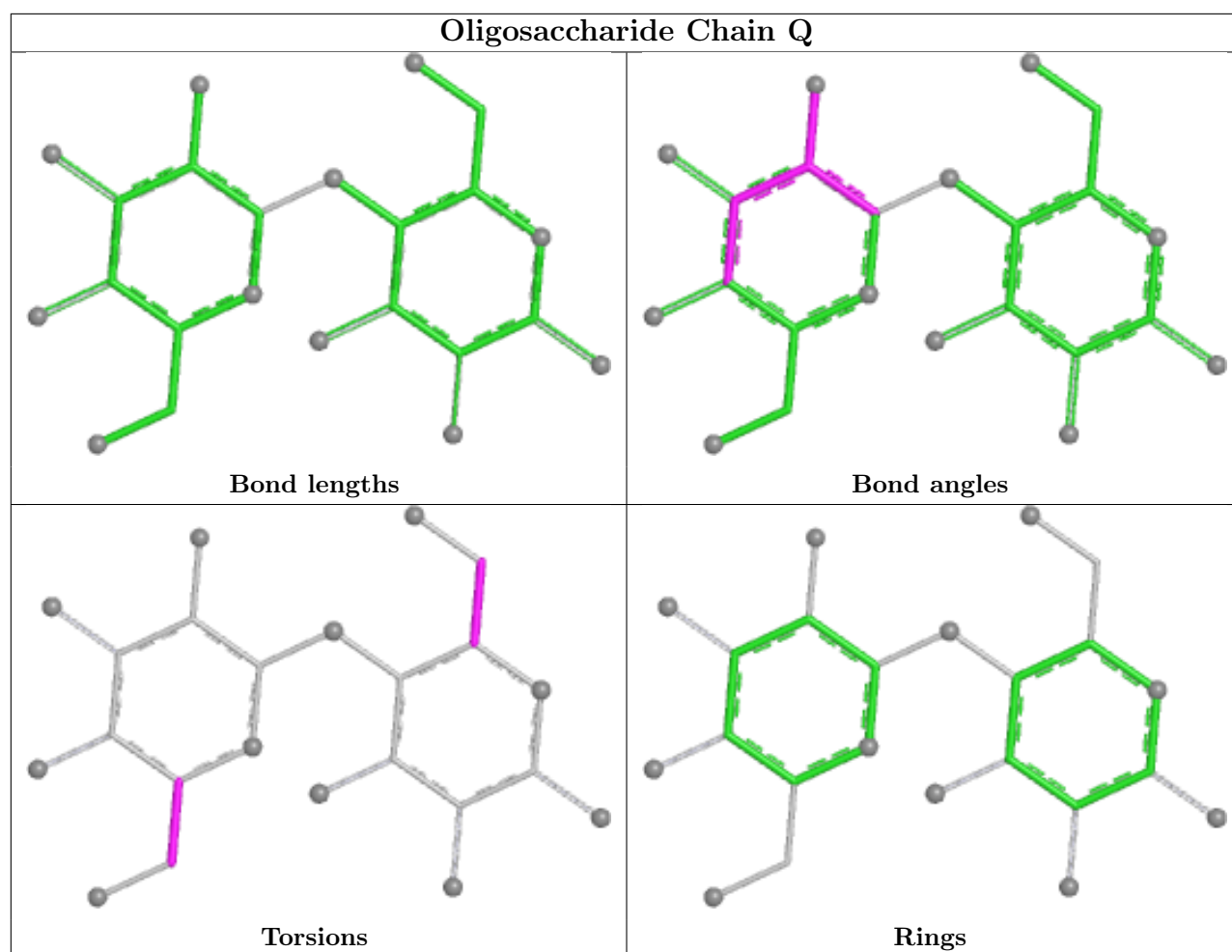
5 of 48 torsion outliers are listed below:

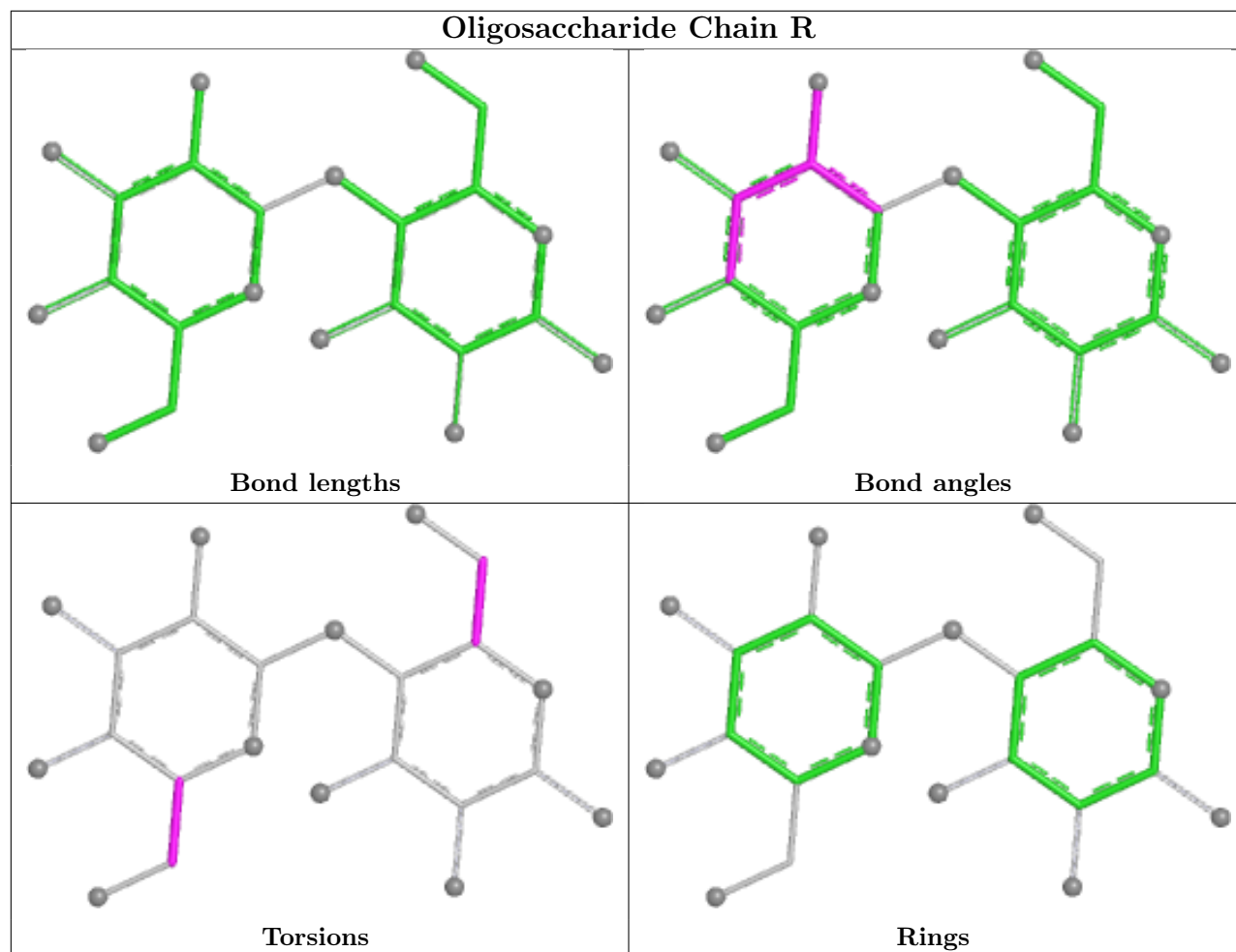
Mol	Chain	Res	Type	Atoms
2	Q	1	BGC	O5-C5-C6-O6
2	R	1	BGC	O5-C5-C6-O6
2	T	1	BGC	O5-C5-C6-O6
2	b	1	BGC	O5-C5-C6-O6
2	c	1	BGC	O5-C5-C6-O6

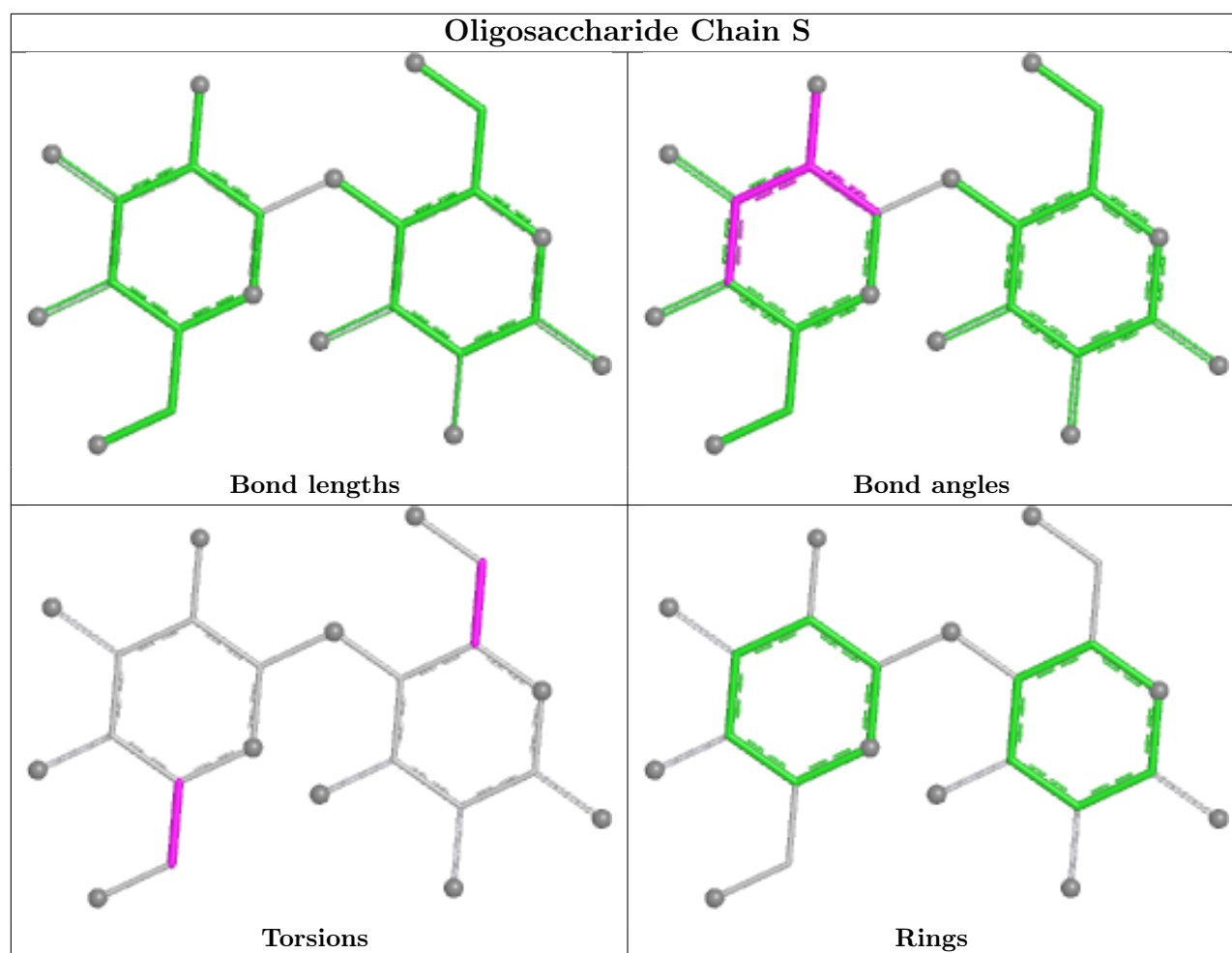
There are no ring outliers.

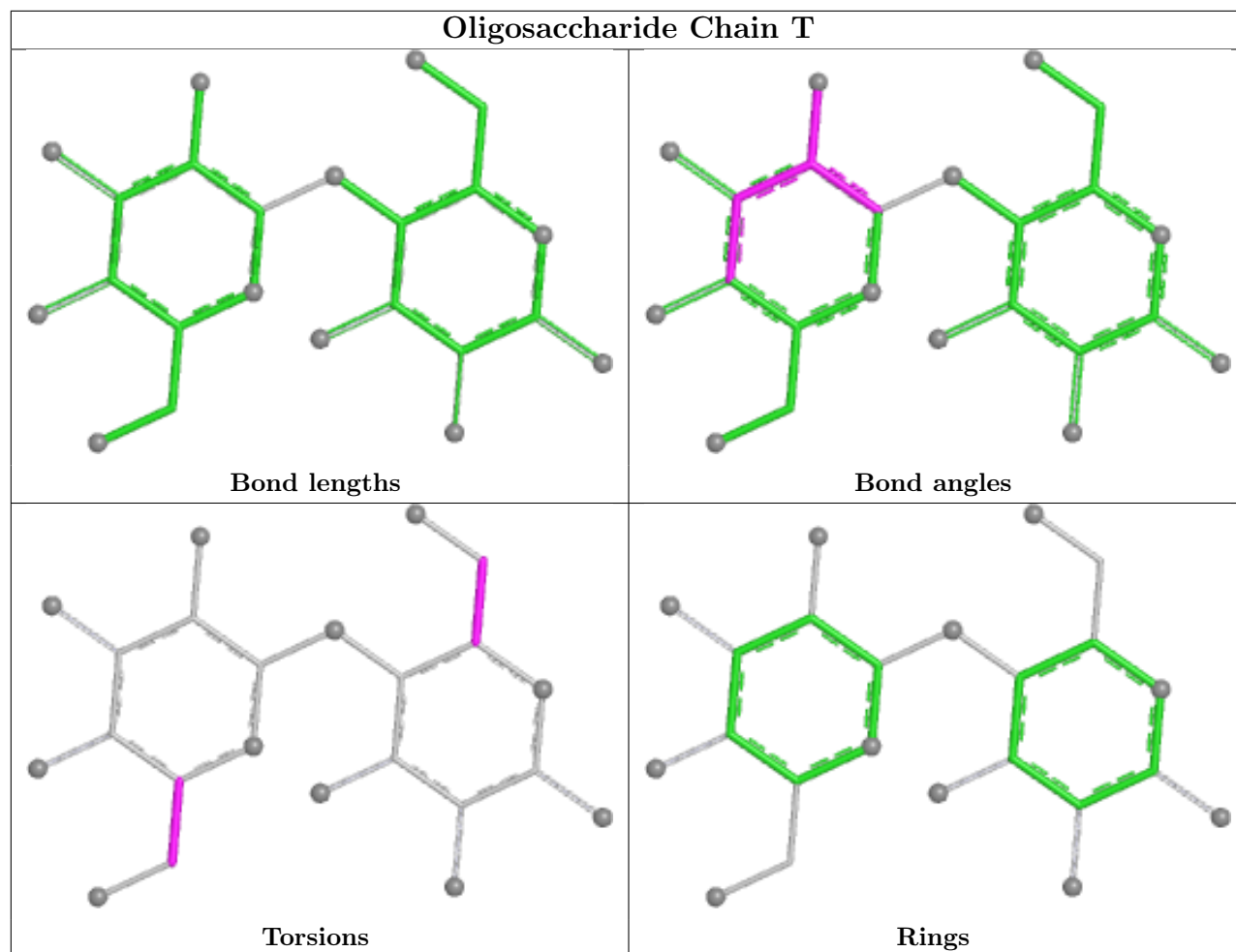
No monomer is involved in short contacts.

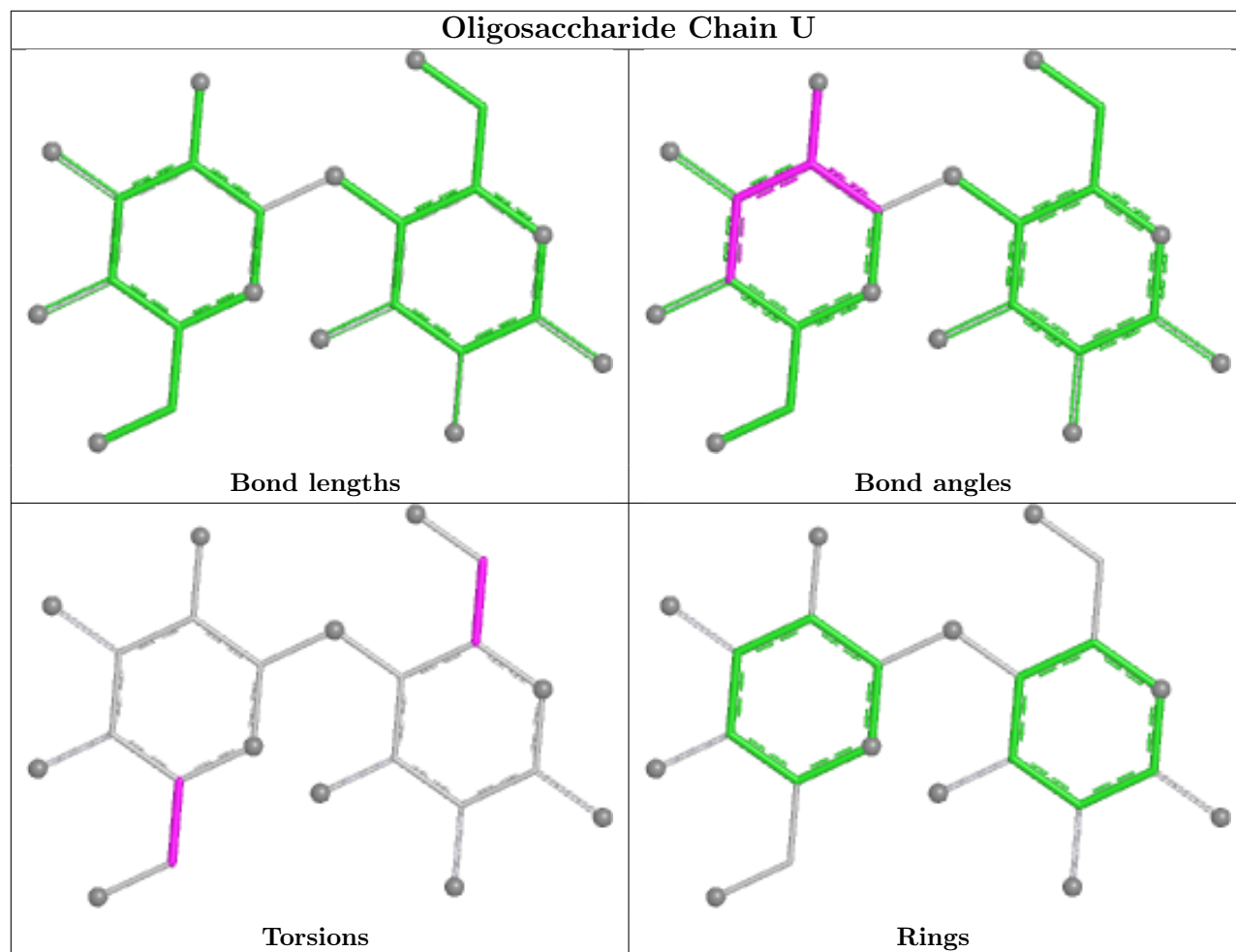
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

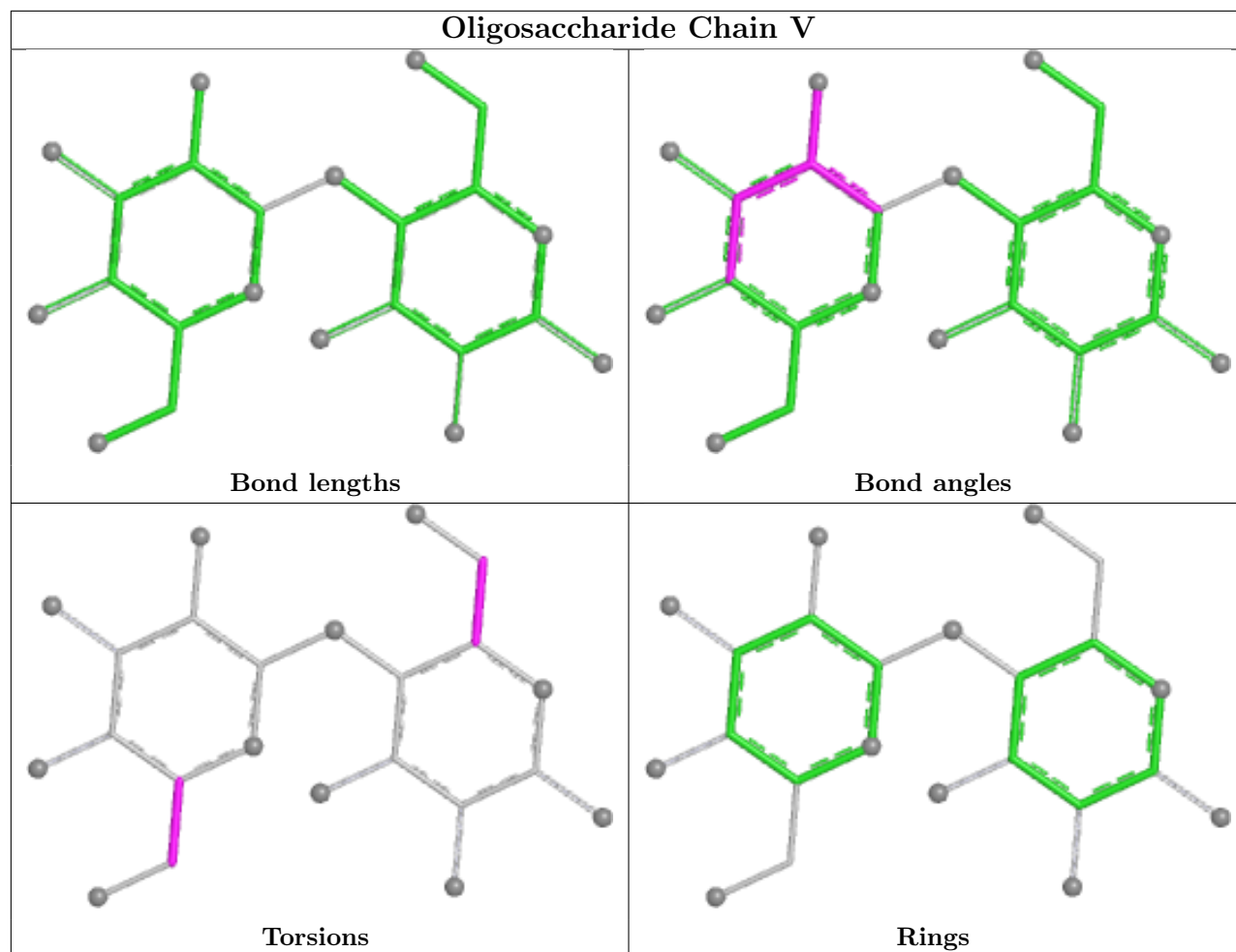


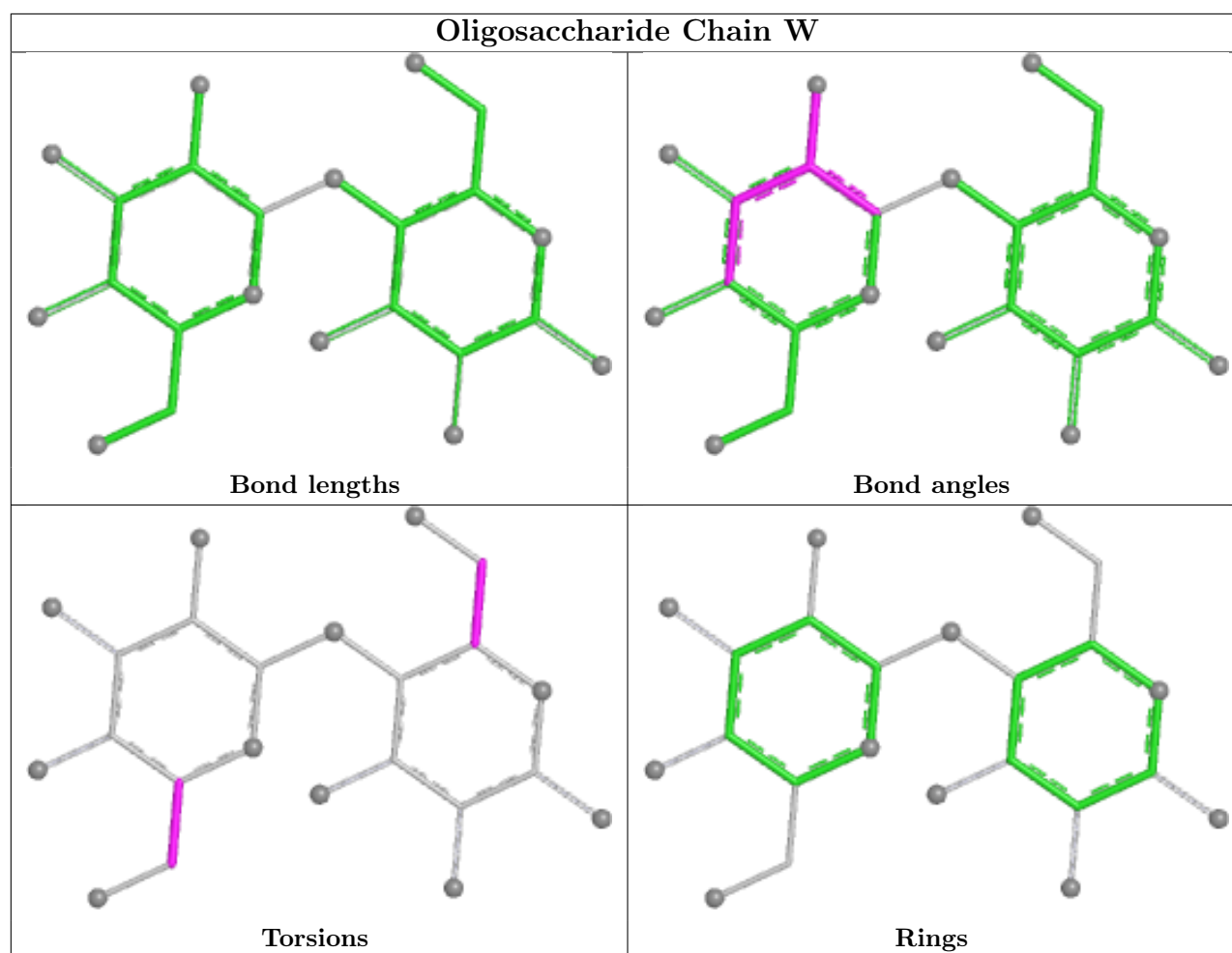


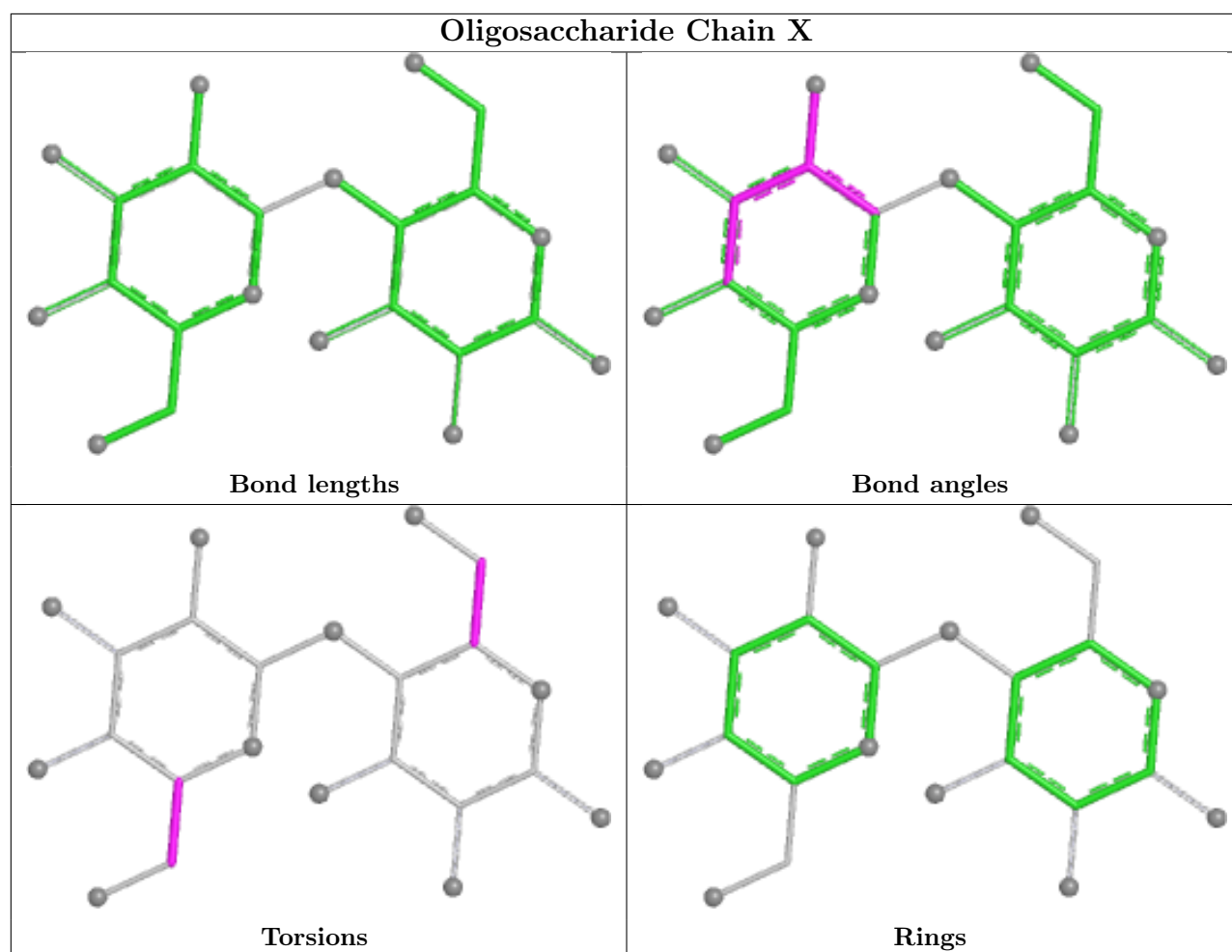


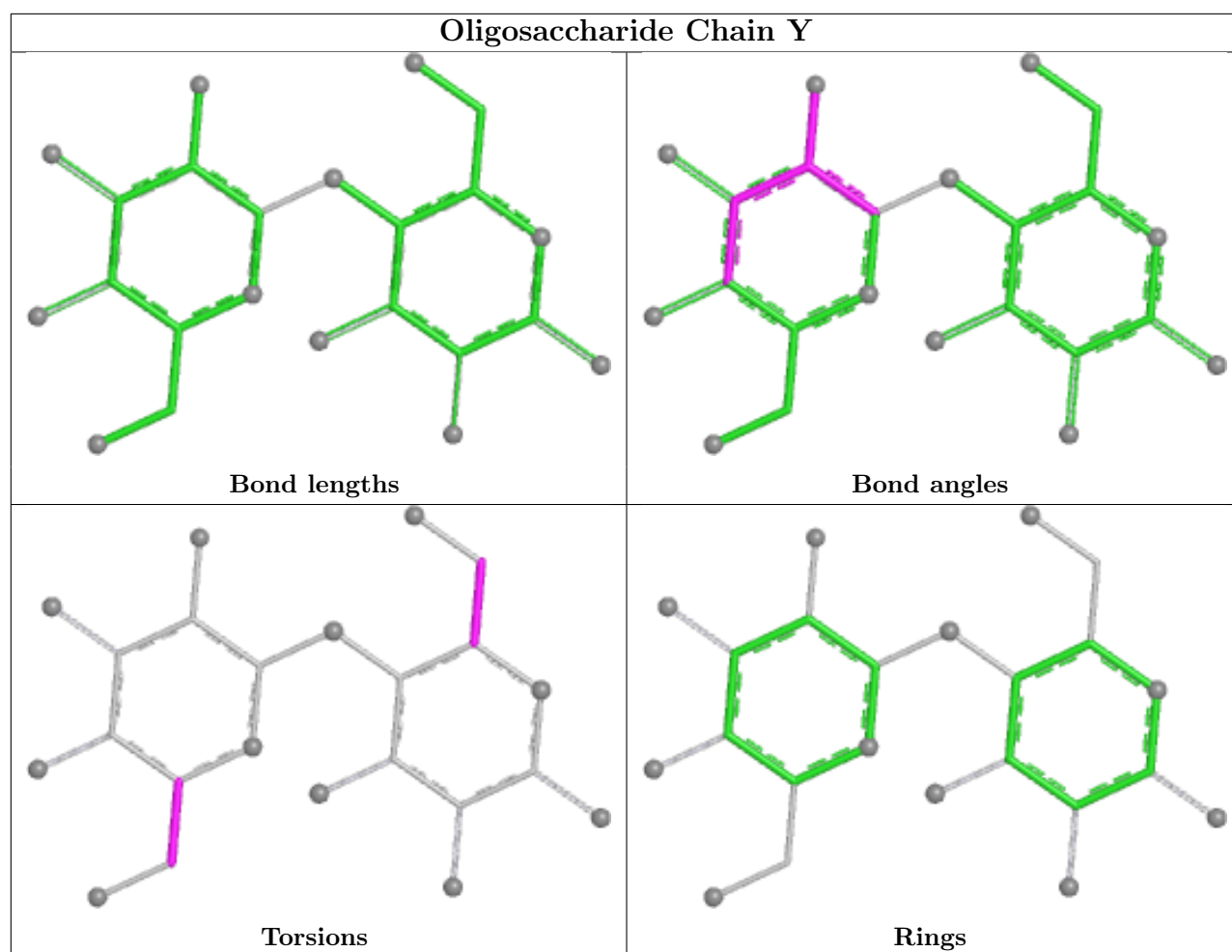


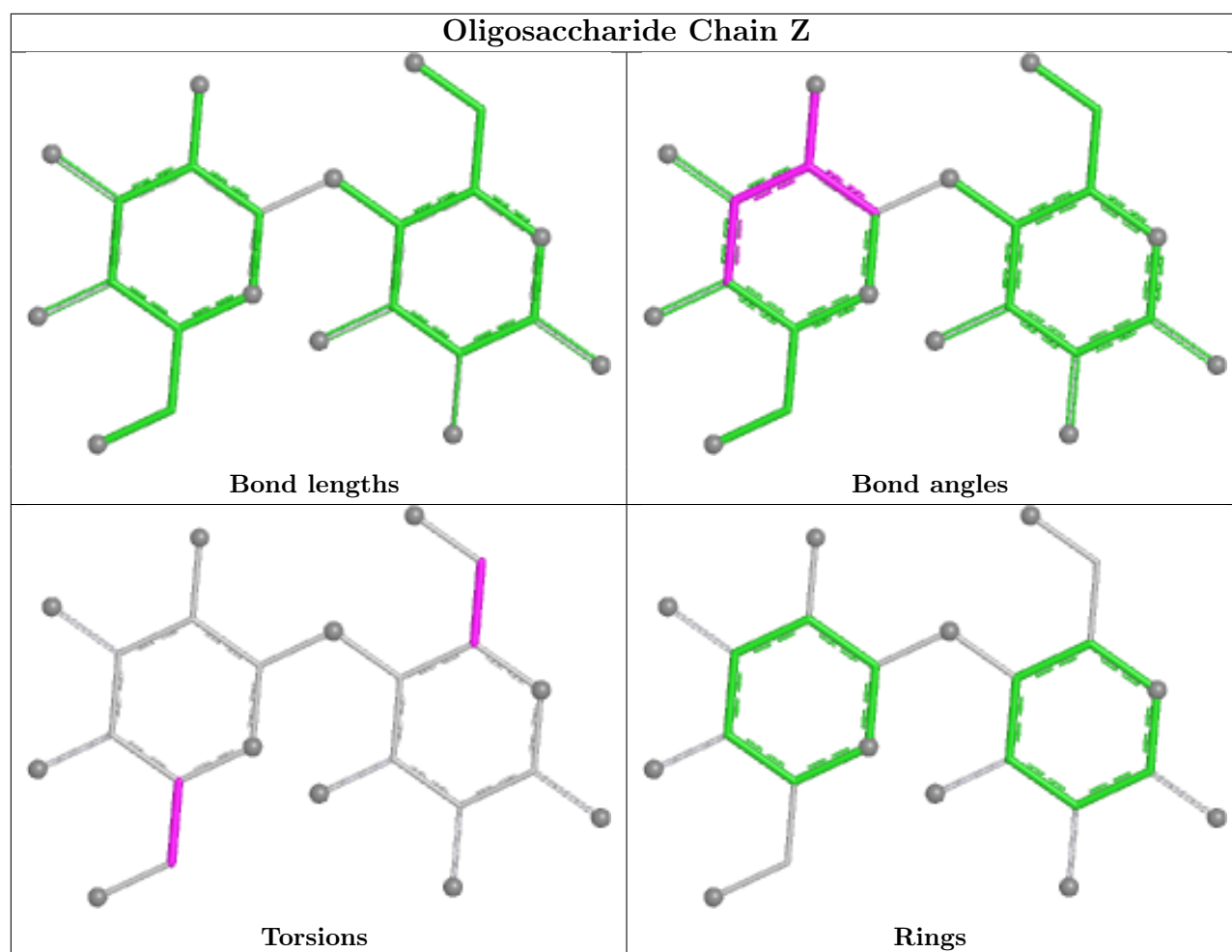


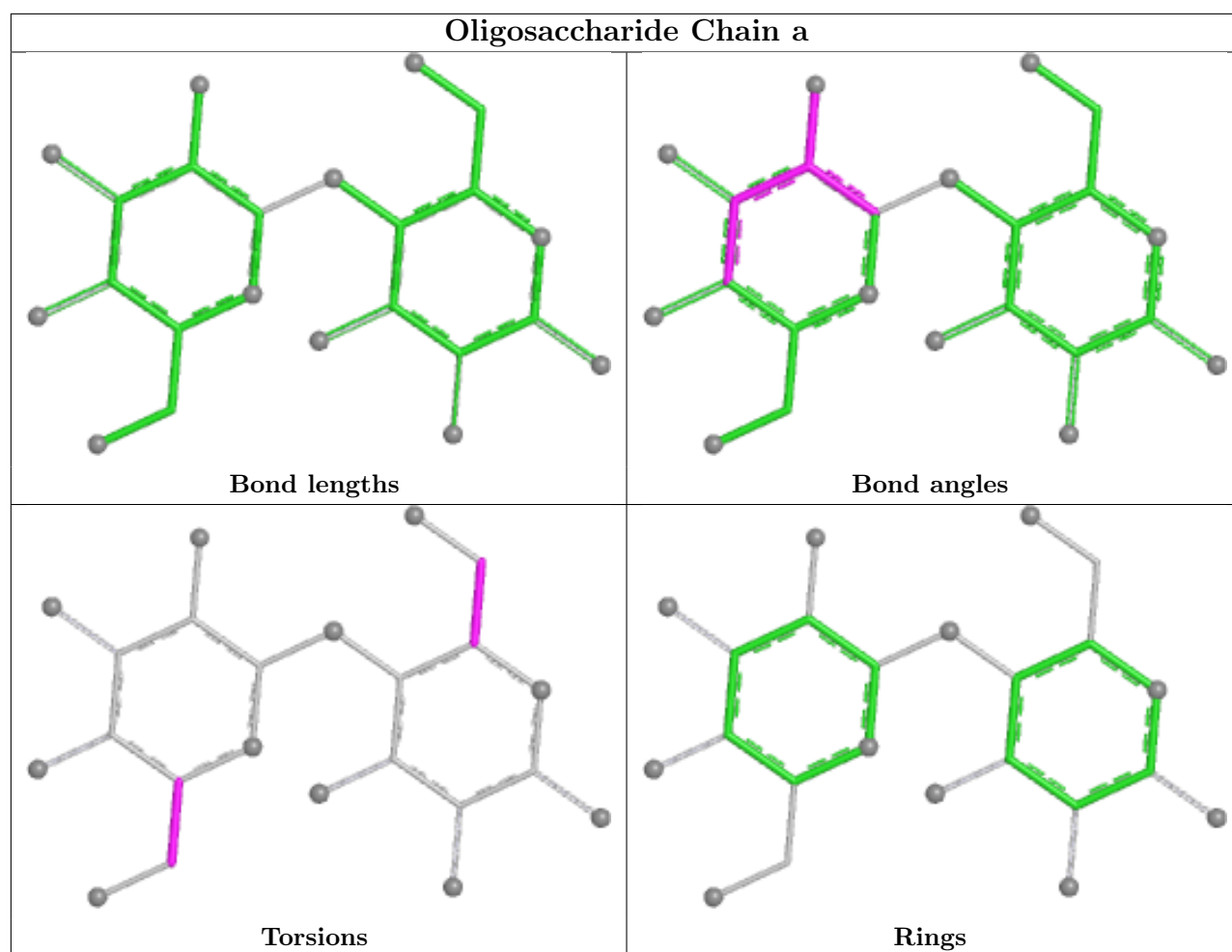


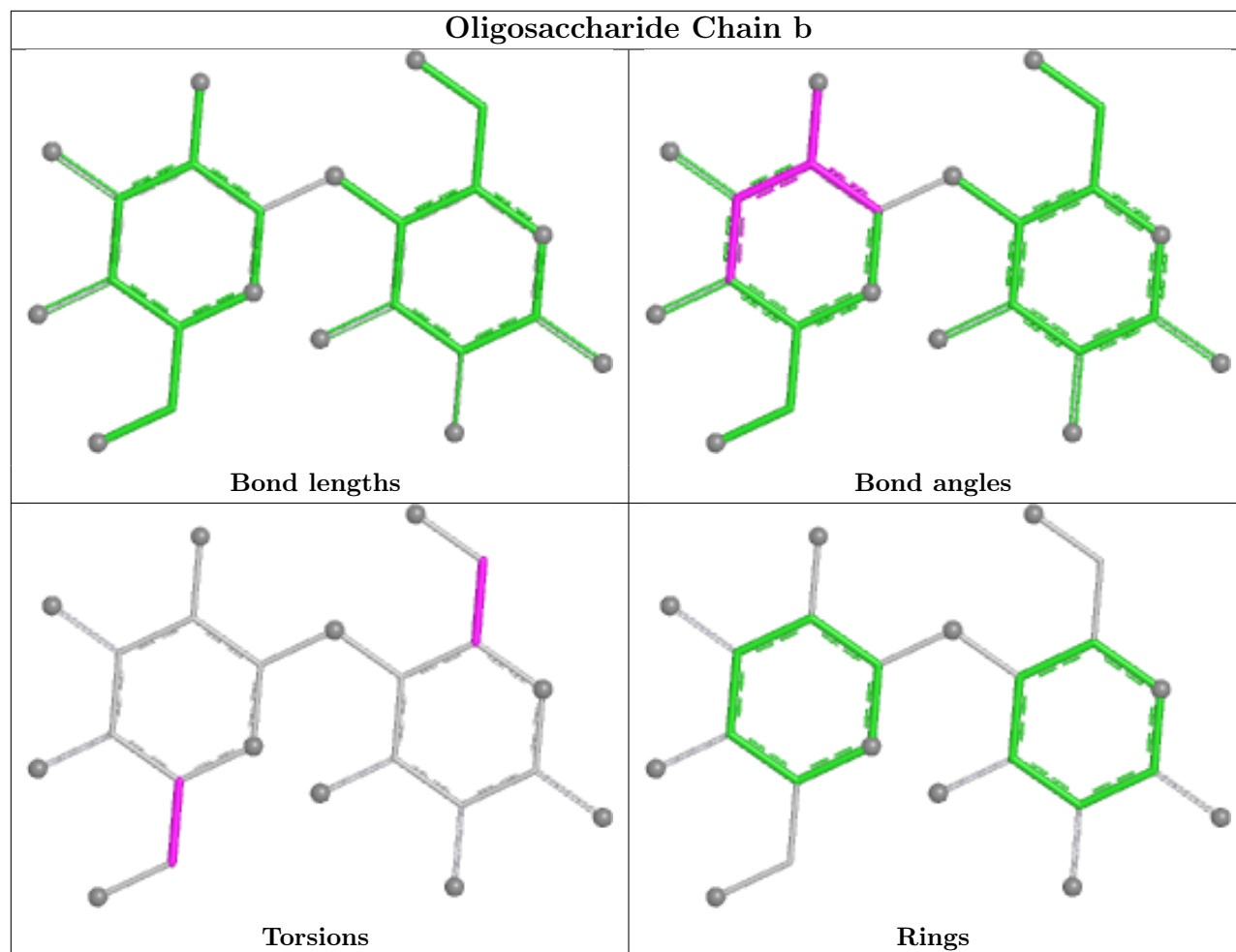


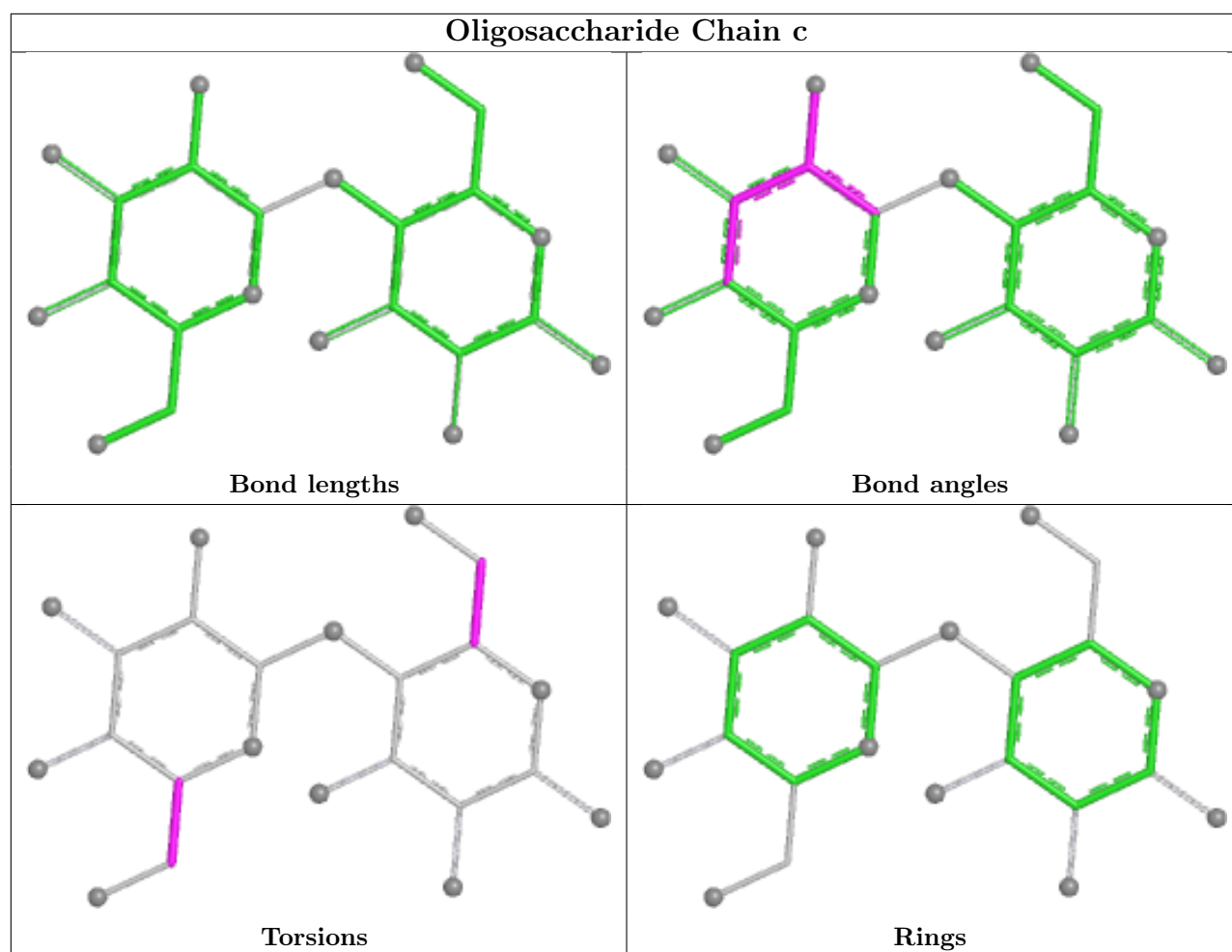


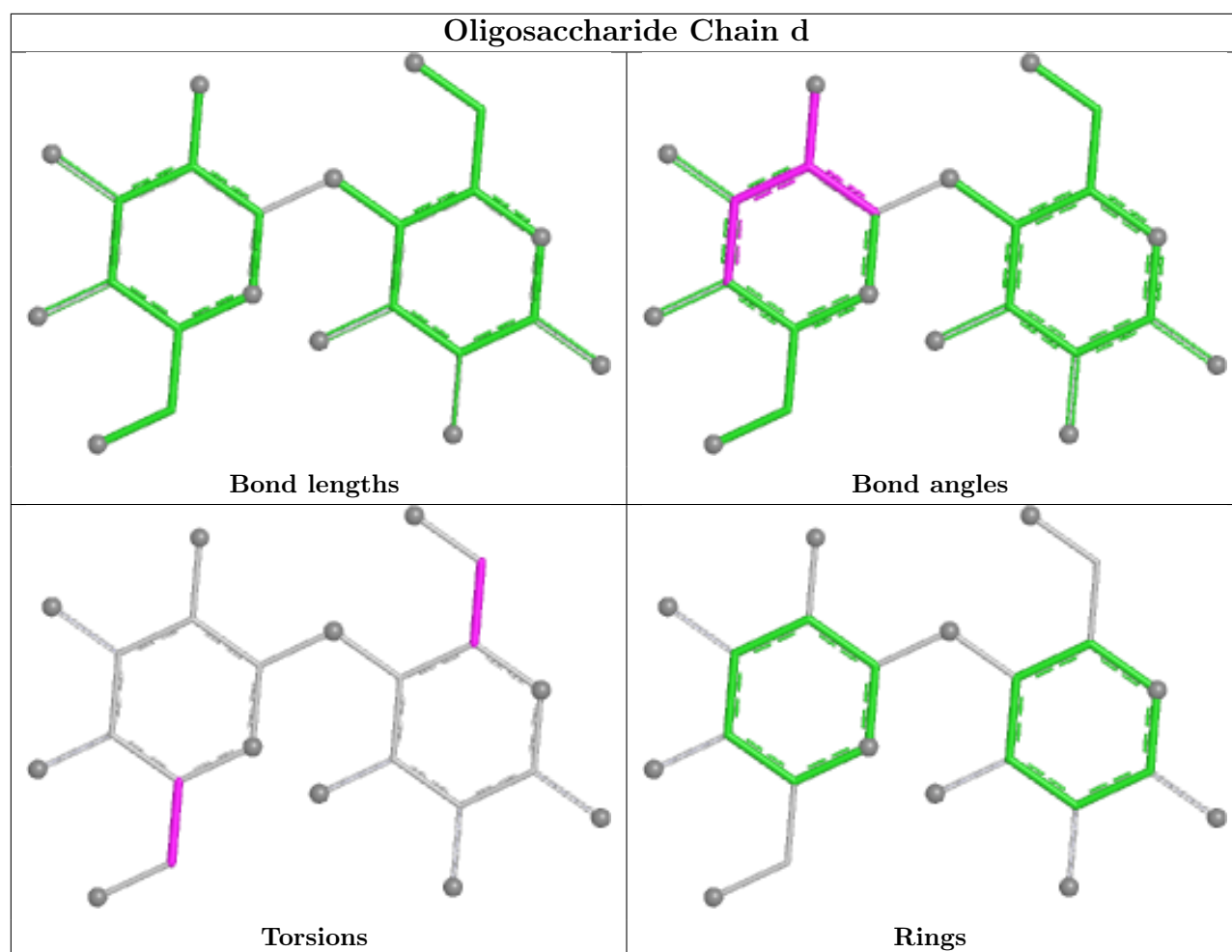


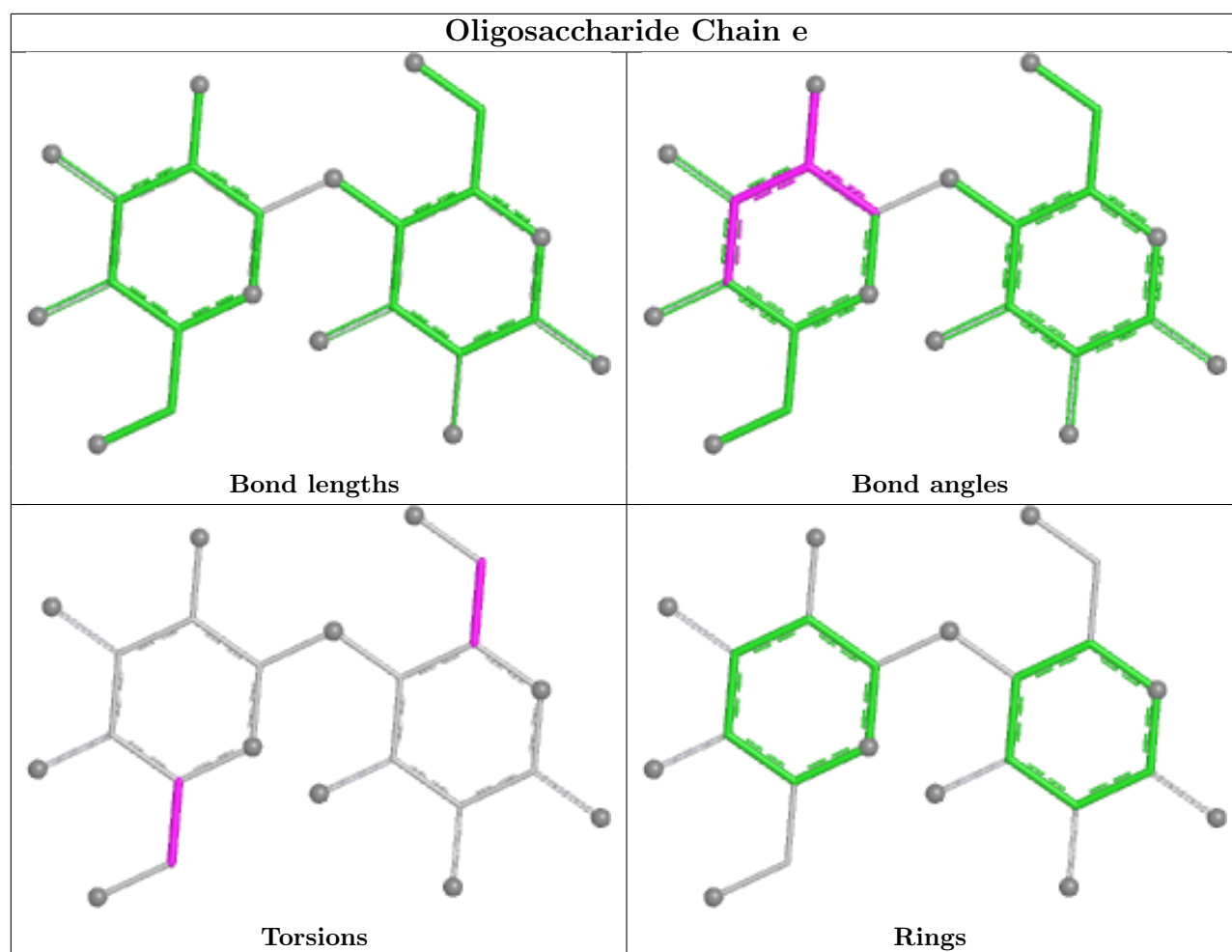


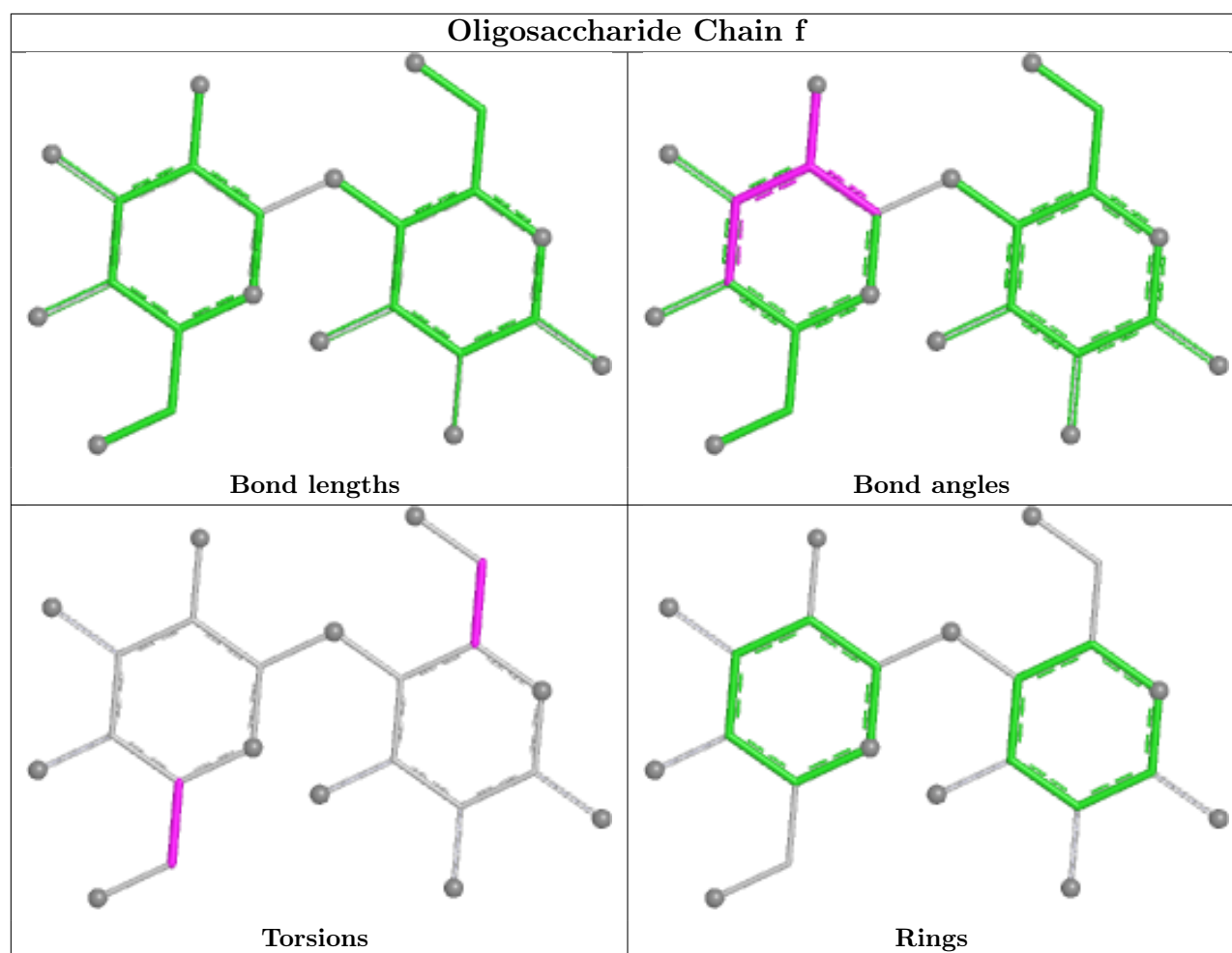












5.6 Ligand geometry [i](#)

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%)	-0.08	24 (2%)	59	56	2, 23, 63, 99	2 (0%)
1	B	1018/1023 (99%)	-0.13	14 (1%)	73	72	1, 21, 61, 98	2 (0%)
1	C	1018/1023 (99%)	-0.11	22 (2%)	62	59	1, 21, 61, 98	2 (0%)
1	D	1018/1023 (99%)	0.22	39 (3%)	44	40	10, 31, 69, 100	2 (0%)
1	E	1018/1023 (99%)	0.93	119 (11%)	9	7	27, 48, 83, 100	2 (0%)
1	F	1018/1023 (99%)	-0.03	20 (1%)	65	62	8, 28, 67, 100	2 (0%)
1	G	1018/1023 (99%)	-0.00	15 (1%)	72	70	8, 28, 68, 100	2 (0%)
1	H	1018/1023 (99%)	0.48	48 (4%)	36	33	18, 38, 75, 100	2 (0%)
1	I	1018/1023 (99%)	0.14	22 (2%)	62	59	11, 32, 70, 100	2 (0%)
1	J	1018/1023 (99%)	-0.05	16 (1%)	70	68	10, 30, 69, 100	2 (0%)
1	K	1018/1023 (99%)	0.32	17 (1%)	69	67	24, 45, 81, 100	2 (0%)
1	L	1018/1023 (99%)	0.50	42 (4%)	41	37	25, 45, 81, 100	2 (0%)
1	M	1018/1023 (99%)	1.16	166 (16%)	4	4	27, 48, 83, 100	2 (0%)
1	N	1018/1023 (99%)	0.19	31 (3%)	52	49	16, 36, 74, 100	2 (0%)
1	O	1018/1023 (99%)	0.31	23 (2%)	61	58	21, 42, 78, 100	2 (0%)
1	P	1018/1023 (99%)	1.72	359 (35%)	1	1	37, 60, 91, 100	2 (0%)
All	All	16288/16368 (99%)	0.35	977 (5%)	27	24	1, 37, 76, 100	32 (0%)

The worst 5 of 977 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	582	GLY	8.7
1	P	739	HIS	6.4
1	P	364	GLY	5.8
1	I	735	HIS	5.7
1	A	580	GLU	5.6

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CME	P	914	10/11	0.72	0.22	54,62,98,100	0
1	CME	P	1021	10/11	0.77	0.19	72,87,100,100	0
1	CME	P	748	10/11	0.81	0.17	68,80,100,100	0
1	CME	M	748	10/11	0.83	0.18	56,68,100,100	0
1	CME	O	748	10/11	0.84	0.24	50,62,95,100	0
1	CME	L	748	10/11	0.85	0.16	53,65,99,100	0
1	CME	B	1021	10/11	0.85	0.17	33,49,84,97	0
1	CME	K	1021	10/11	0.85	0.13	57,73,100,100	0
1	CME	L	1021	10/11	0.86	0.12	57,73,100,100	0
1	CME	J	1021	10/11	0.86	0.16	42,58,93,100	0
1	CME	M	914	10/11	0.87	0.14	42,50,86,92	0
1	CME	N	1021	10/11	0.87	0.14	48,64,99,100	0
1	CME	E	748	10/11	0.87	0.20	56,68,100,100	0
1	CME	G	1021	10/11	0.87	0.14	41,56,91,100	0
1	CME	I	748	10/11	0.87	0.16	40,52,85,97	0
1	CME	B	748	10/11	0.87	0.14	29,41,75,86	0
1	CME	N	748	10/11	0.88	0.18	44,56,90,100	0
1	CME	H	1021	10/11	0.88	0.13	50,66,100,100	0
1	CME	C	1021	10/11	0.88	0.14	33,49,84,97	0
1	CME	J	748	10/11	0.88	0.14	38,50,84,95	0
1	CME	D	748	10/11	0.88	0.17	39,51,84,95	0
1	CME	K	748	10/11	0.88	0.14	53,65,98,100	0
1	CME	E	1021	10/11	0.89	0.16	60,76,100,100	0
1	CME	F	748	10/11	0.89	0.14	36,48,81,93	0
1	CME	F	1021	10/11	0.89	0.12	40,56,91,100	0
1	CME	D	1021	10/11	0.89	0.16	43,58,93,100	0
1	CME	C	748	10/11	0.90	0.15	29,41,74,86	0
1	CME	H	748	10/11	0.90	0.14	46,58,92,100	0
1	CME	O	1021	10/11	0.90	0.13	54,69,100,100	0
1	CME	A	1021	10/11	0.90	0.12	35,50,85,99	0
1	CME	M	1021	10/11	0.90	0.16	60,75,100,100	0
1	CME	L	914	10/11	0.90	0.13	40,47,84,89	0
1	CME	I	1021	10/11	0.91	0.12	44,60,94,100	0
1	CME	A	748	10/11	0.91	0.14	31,43,76,87	0
1	CME	A	914	10/11	0.92	0.11	17,25,61,67	0
1	CME	K	914	10/11	0.92	0.11	40,47,84,89	0
1	CME	G	748	10/11	0.92	0.13	37,48,82,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CME	E	914	10/11	0.92	0.14	42,50,87,92	0
1	CME	J	914	10/11	0.93	0.11	25,32,69,75	0
1	CME	I	914	10/11	0.93	0.11	26,34,70,76	0
1	CME	N	914	10/11	0.94	0.10	31,38,75,81	0
1	CME	O	914	10/11	0.94	0.10	36,44,80,86	0
1	CME	H	914	10/11	0.94	0.10	33,40,77,82	0
1	CME	F	914	10/11	0.95	0.10	23,30,67,72	0
1	CME	D	914	10/11	0.95	0.11	25,33,69,75	0
1	CME	B	914	10/11	0.95	0.09	16,23,60,66	0
1	CME	G	914	10/11	0.95	0.09	23,31,67,73	0
1	CME	C	914	10/11	0.96	0.09	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.

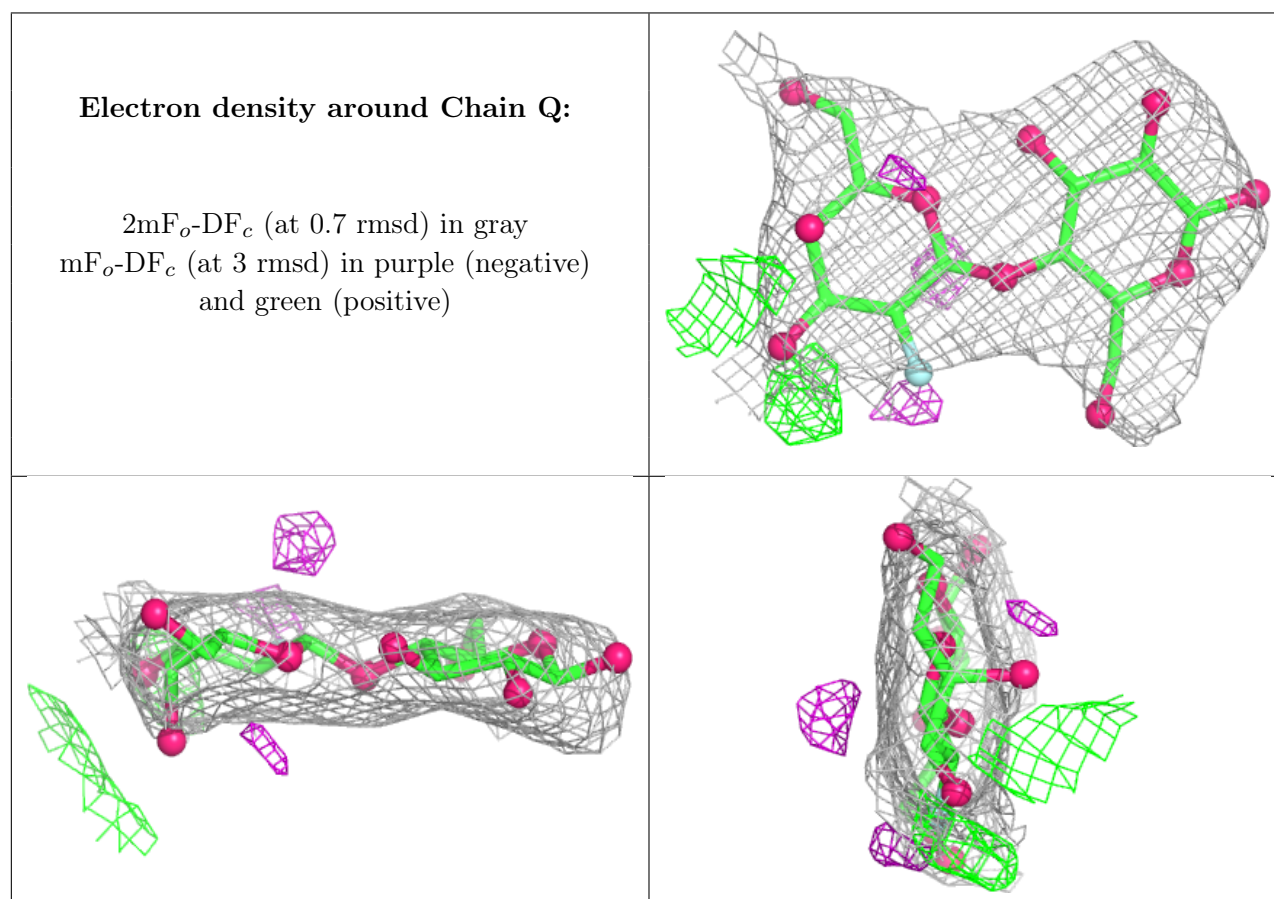
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	2FG	X	2	11/12	0.67	0.22	56,61,72,78	0
2	2FG	U	2	11/12	0.85	0.21	66,71,82,88	0
2	BGC	Z	1	12/12	0.85	0.14	50,65,82,99	0
2	BGC	R	1	12/12	0.86	0.15	41,56,73,90	0
2	2FG	Q	2	11/12	0.86	0.16	40,46,57,63	0
2	BGC	W	1	12/12	0.87	0.18	48,63,80,97	0
2	BGC	T	1	12/12	0.87	0.14	50,65,82,99	0
2	BGC	Y	1	12/12	0.87	0.14	51,67,84,100	0
2	BGC	S	1	12/12	0.87	0.13	41,56,73,89	0
2	2FG	R	2	11/12	0.88	0.13	39,44,55,61	0
2	2FG	S	2	11/12	0.89	0.14	39,44,55,61	0
2	BGC	V	1	12/12	0.89	0.13	48,63,80,96	0
2	BGC	X	1	12/12	0.90	0.13	58,73,90,100	0
2	2FG	Y	2	11/12	0.90	0.13	49,55,66,72	0
2	2FG	V	2	11/12	0.90	0.14	46,51,62,68	0
2	2FG	Z	2	11/12	0.90	0.13	48,53,64,70	0
2	BGC	U	1	12/12	0.91	0.15	67,83,100,100	0
2	2FG	W	2	11/12	0.91	0.12	46,51,63,68	0
2	BGC	Q	1	12/12	0.92	0.11	42,57,74,91	0
2	2FG	T	2	11/12	0.95	0.10	48,54,65,71	0
2	BGC	a	1	12/12	-	-	65,80,97,100	0
2	2FG	a	2	11/12	-	-	63,68,79,85	0

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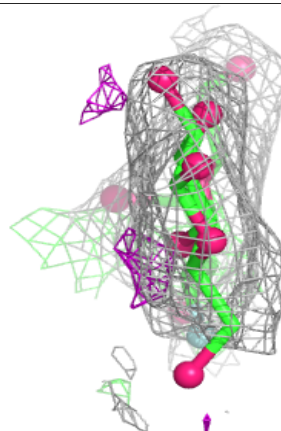
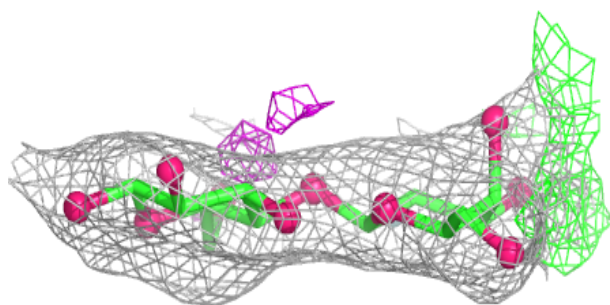
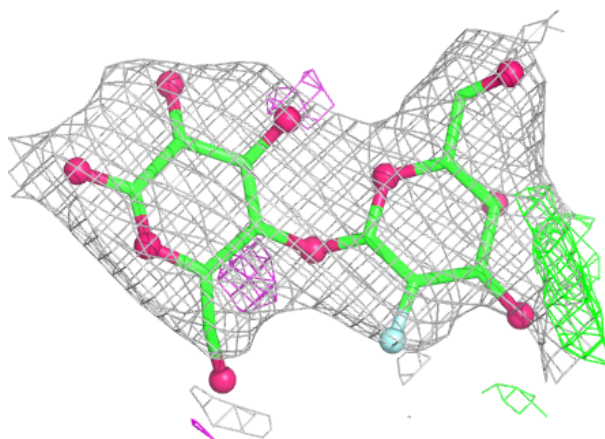
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	b	1	12/12	-	-	65,80,97,100	0
2	2FG	b	2	11/12	-	-	63,68,79,85	0
2	BGC	c	1	12/12	-	-	67,82,99,100	0
2	2FG	c	2	11/12	-	-	65,71,82,88	0
2	BGC	d	1	12/12	-	-	56,71,88,100	0
2	2FG	d	2	11/12	-	-	54,59,70,76	0
2	BGC	e	1	12/12	-	-	61,76,93,100	0
2	2FG	e	2	11/12	-	-	59,65,76,82	0
2	BGC	f	1	12/12	-	-	79,94,100,100	0
2	2FG	f	2	11/12	-	-	77,83,94,100	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.



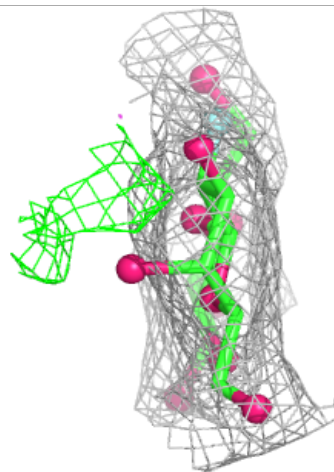
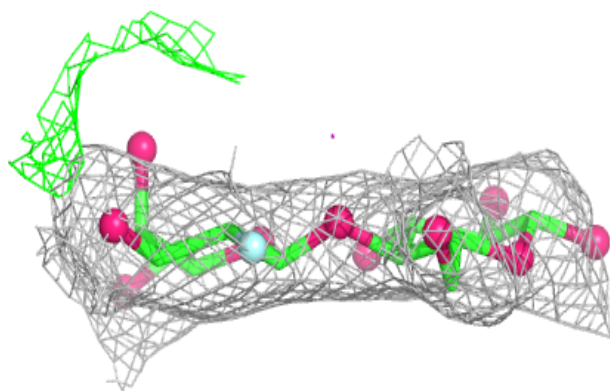
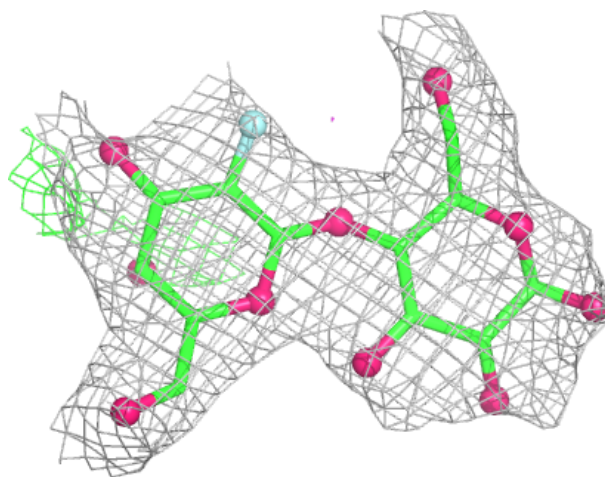
Electron density around Chain R:

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



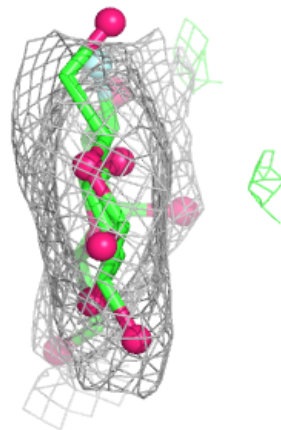
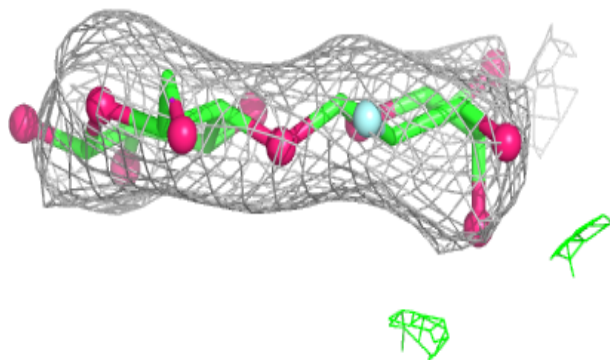
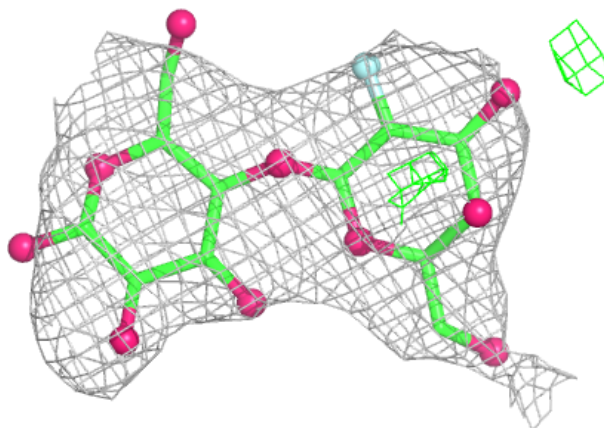
Electron density around Chain S:

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



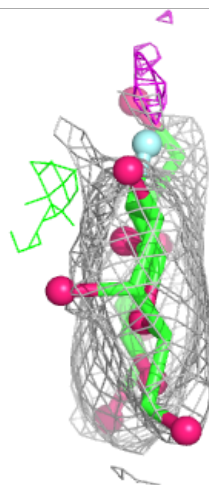
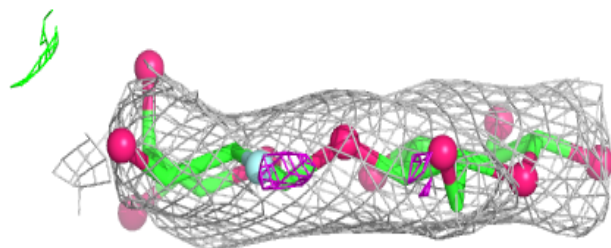
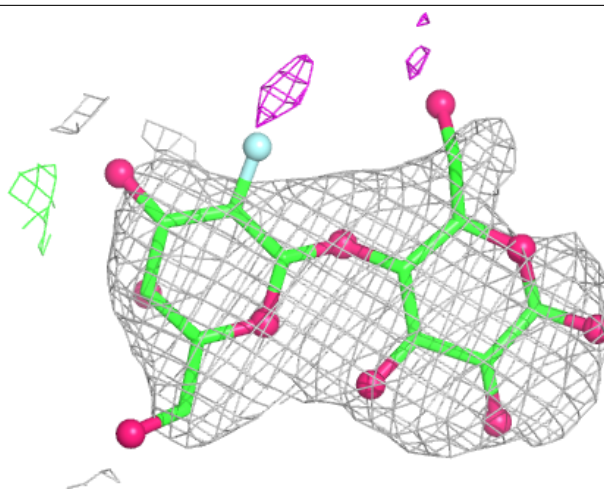
Electron density around Chain T:

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



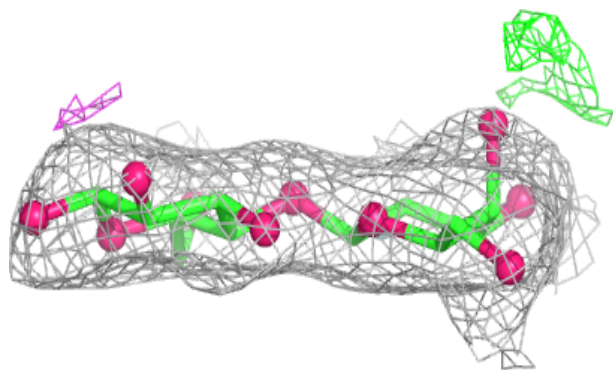
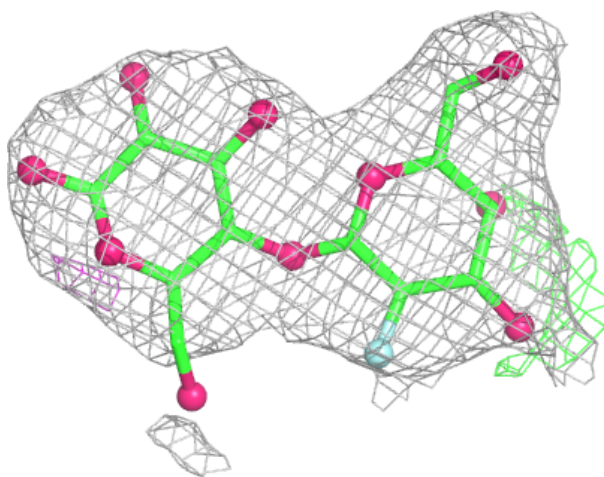
Electron density around Chain U:

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



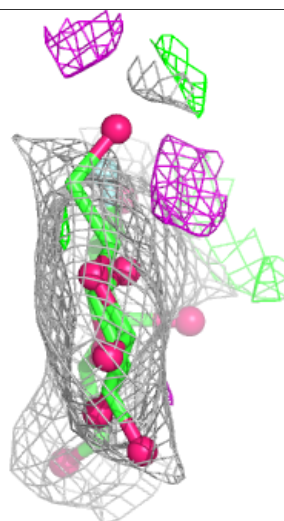
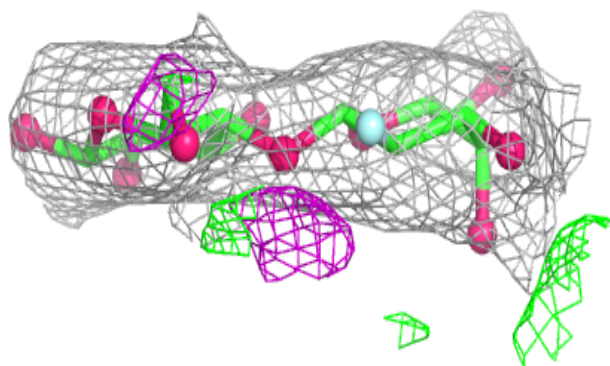
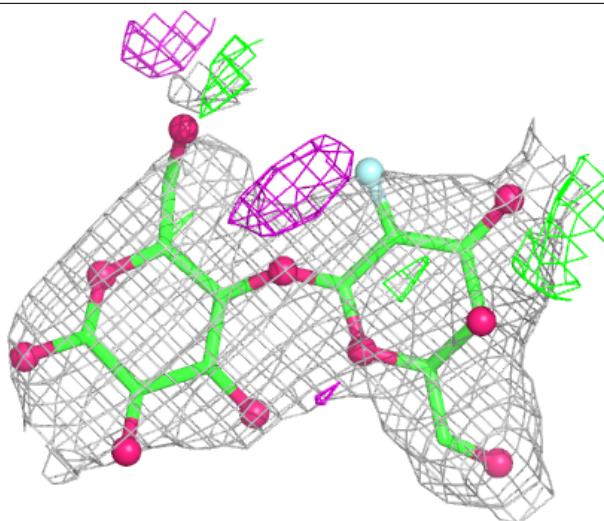
Electron density around Chain V:

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



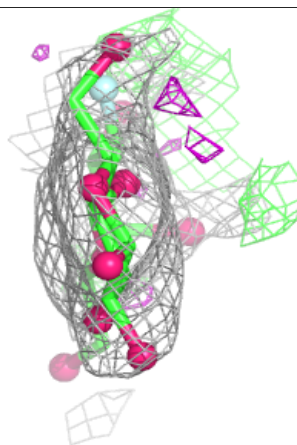
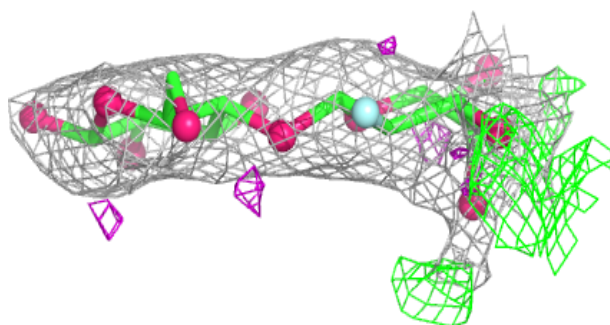
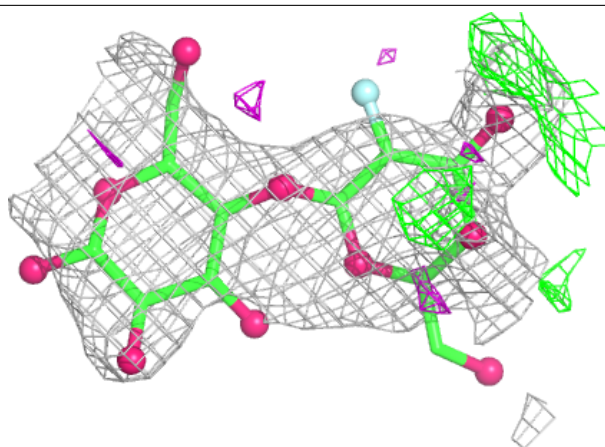
Electron density around Chain W:

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



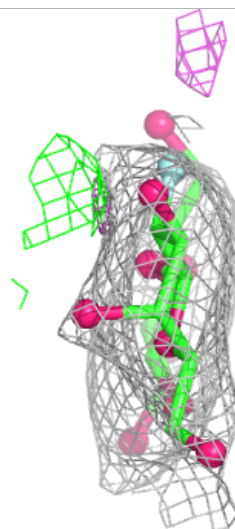
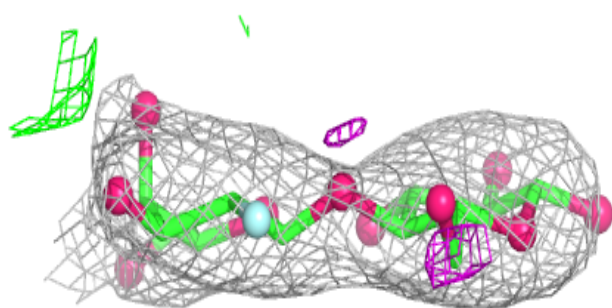
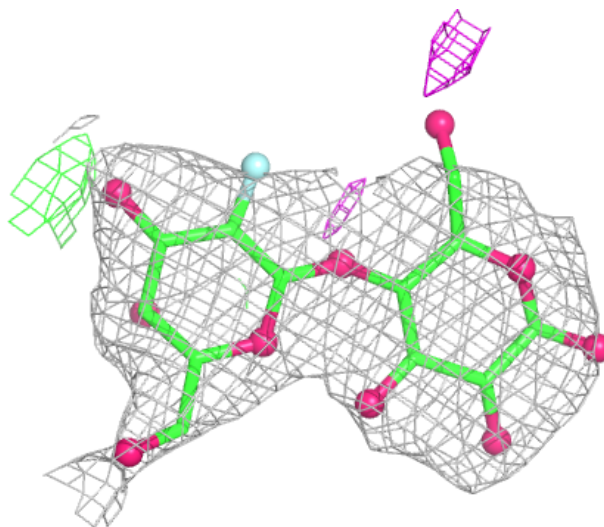
Electron density around Chain X:

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



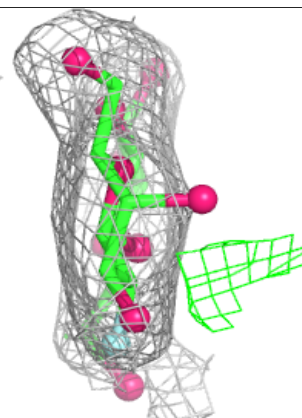
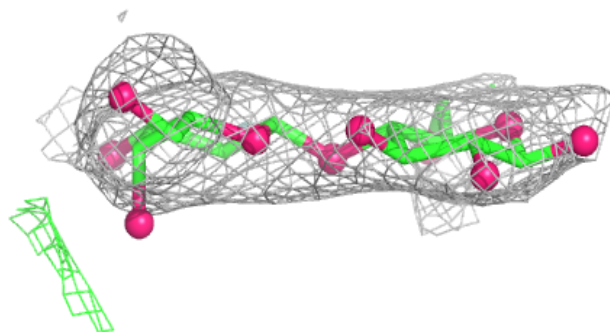
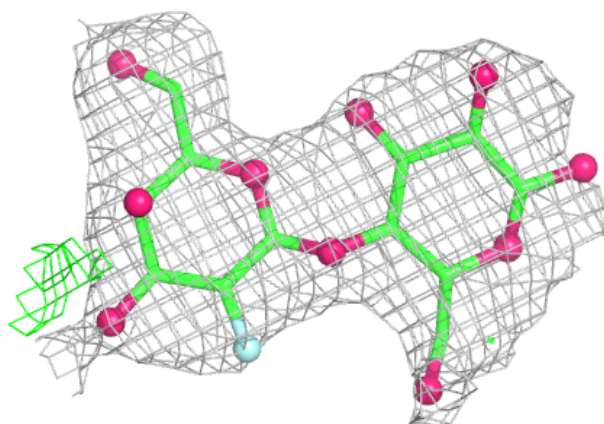
Electron density around Chain Y:

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



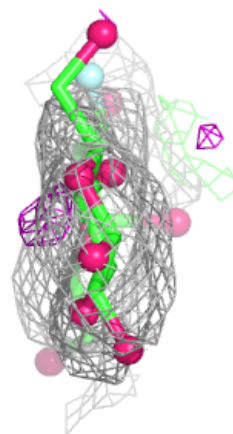
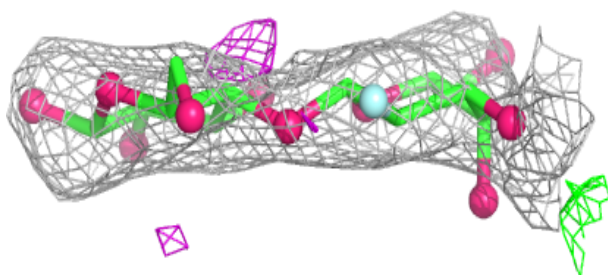
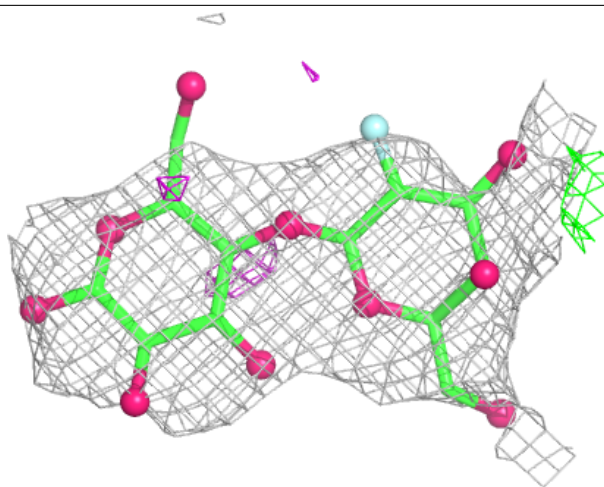
Electron density around Chain Z:

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



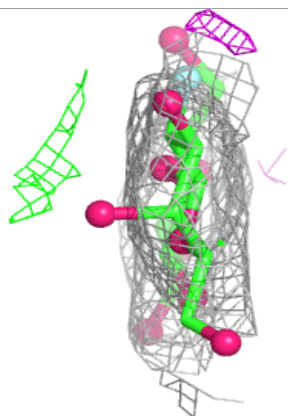
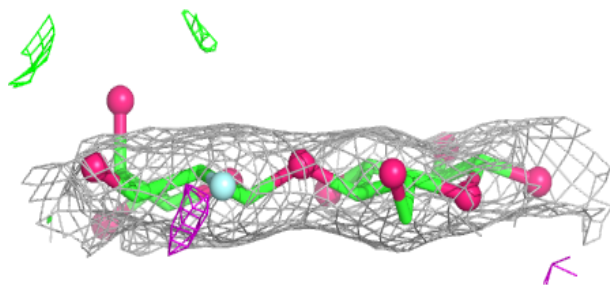
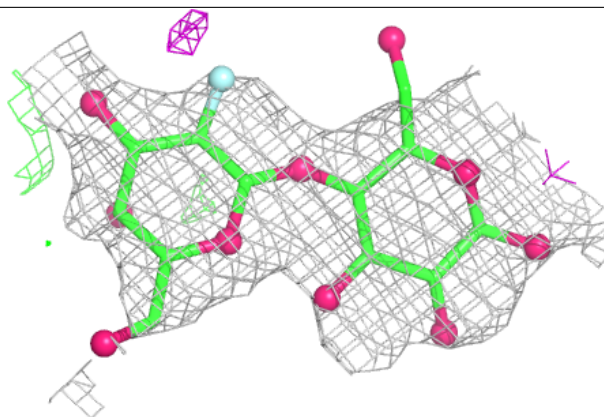
Electron density around Chain a:

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

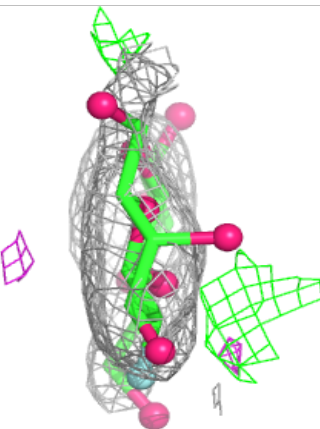
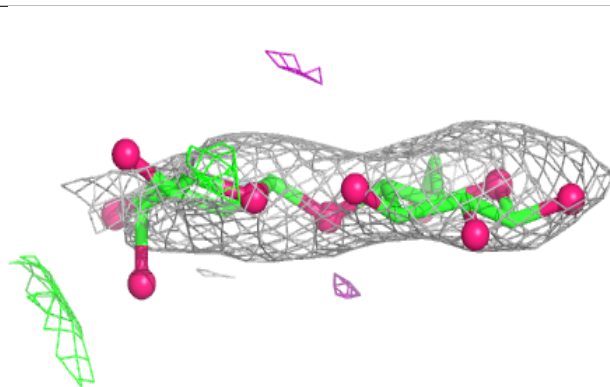
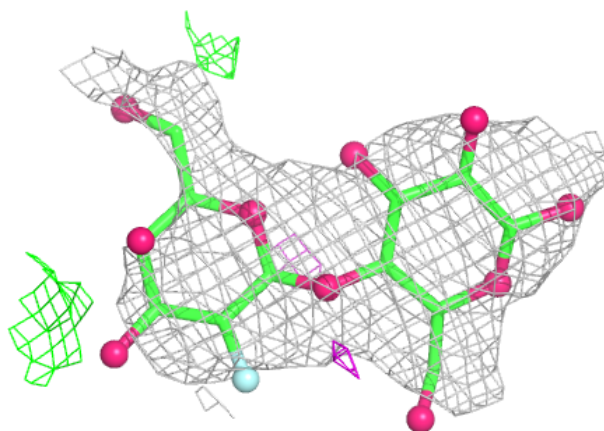


Electron density around Chain b:

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

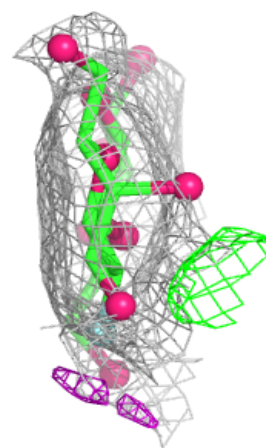
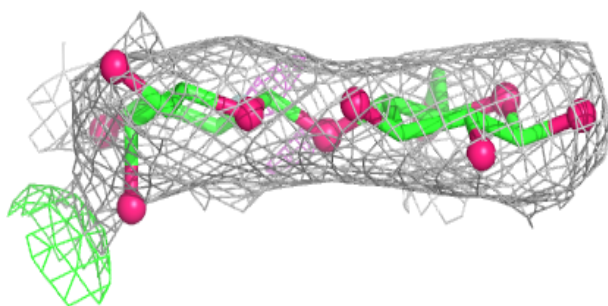
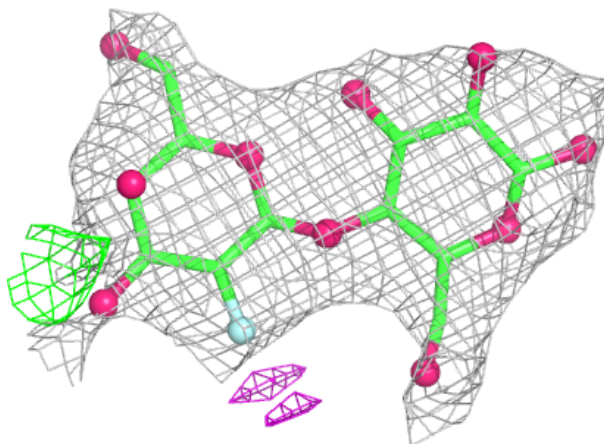
**Electron density around Chain c:**

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



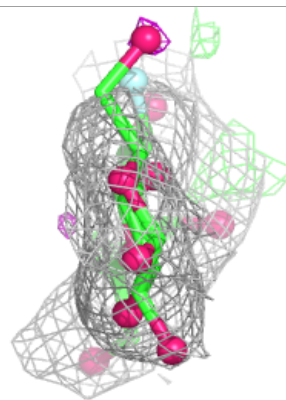
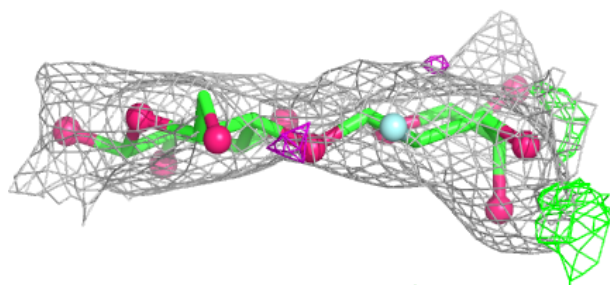
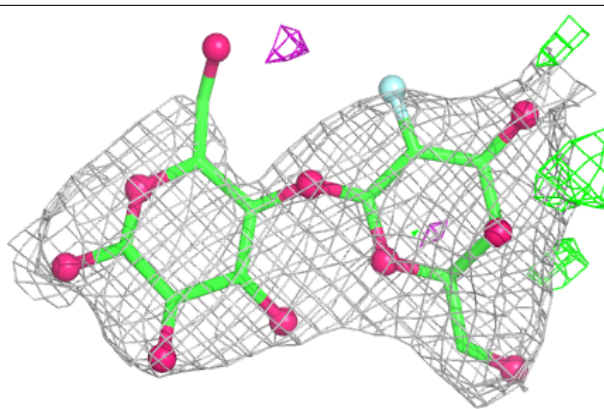
Electron density around Chain d:

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

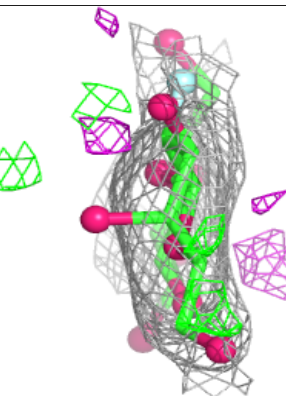
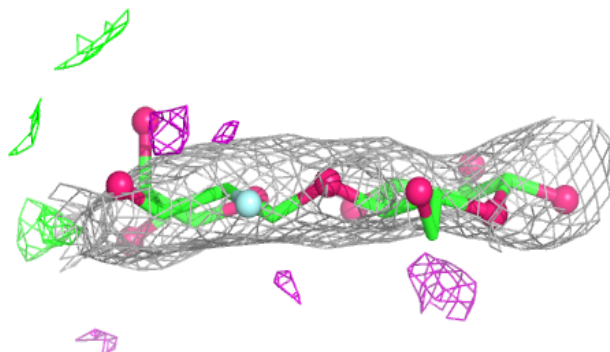
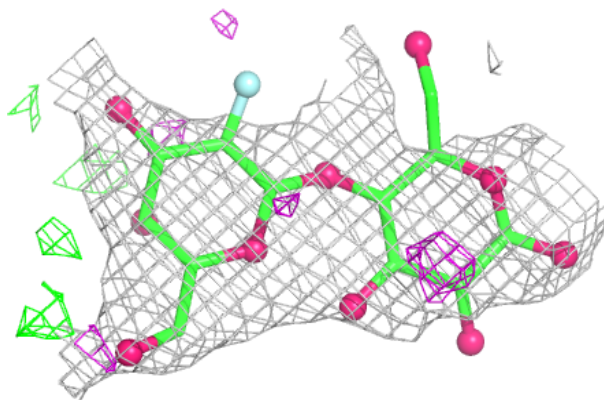


Electron density around Chain e:

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

**Electron density around Chain f:**

$2mF_o-DF_c$ (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	L	2004	1/1	0.71	0.18	53,53,53,53	0
4	NA	M	2004	1/1	0.78	0.20	55,55,55,55	0
4	NA	O	2005	1/1	0.80	0.10	37,37,37,37	0
4	NA	P	2004	1/1	0.80	0.16	67,67,67,67	0
4	NA	D	2004	1/1	0.83	0.09	38,38,38,38	0
4	NA	K	2004	1/1	0.83	0.12	53,53,53,53	0
4	NA	D	2005	1/1	0.85	0.08	26,26,26,26	0
4	NA	J	2004	1/1	0.86	0.13	38,38,38,38	0
4	NA	J	2005	1/1	0.87	0.06	25,25,25,25	0
3	MG	P	2002	1/1	0.87	0.18	60,60,60,60	0
3	MG	E	2003	1/1	0.88	0.10	42,42,42,42	0
3	MG	L	2003	1/1	0.88	0.11	39,39,39,39	0
3	MG	C	2003	1/1	0.89	0.12	15,15,15,15	0
4	NA	O	2004	1/1	0.89	0.10	49,49,49,49	0
3	MG	M	2002	1/1	0.89	0.14	48,48,48,48	0
3	MG	H	2003	1/1	0.89	0.06	32,32,32,32	0
4	NA	I	2005	1/1	0.90	0.09	27,27,27,27	0
3	MG	I	2003	1/1	0.90	0.09	26,26,26,26	0
4	NA	E	2004	1/1	0.90	0.20	55,55,55,55	0
4	NA	N	2004	1/1	0.91	0.10	44,44,44,44	0
3	MG	G	2002	1/1	0.91	0.20	29,29,29,29	0
3	MG	H	2002	1/1	0.91	0.24	39,39,39,39	0
3	MG	L	2002	1/1	0.91	0.17	46,46,46,46	0
3	MG	F	2003	1/1	0.92	0.11	22,22,22,22	0
4	NA	A	2004	1/1	0.92	0.07	30,30,30,30	0
4	NA	C	2005	1/1	0.92	0.06	16,16,16,16	0
3	MG	A	2002	1/1	0.92	0.08	23,23,23,23	0
3	MG	J	2002	1/1	0.93	0.08	31,31,31,31	0
3	MG	G	2003	1/1	0.93	0.08	22,22,22,22	0
4	NA	G	2004	1/1	0.93	0.07	36,36,36,36	0
4	NA	M	2005	1/1	0.93	0.10	43,43,43,43	0
4	NA	K	2005	1/1	0.94	0.04	40,40,40,40	0
4	NA	F	2004	1/1	0.94	0.14	36,36,36,36	0
3	MG	F	2002	1/1	0.94	0.17	29,29,29,29	0
4	NA	H	2004	1/1	0.94	0.12	46,46,46,46	0
3	MG	E	2002	1/1	0.94	0.15	48,48,48,48	0
4	NA	N	2005	1/1	0.94	0.10	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	N	2003	1/1	0.94	0.06	30,30,30,30	0
3	MG	C	2002	1/1	0.94	0.15	22,22,22,22	0
3	MG	P	2003	1/1	0.94	0.07	53,53,53,53	0
3	MG	O	2003	1/1	0.95	0.08	35,35,35,35	0
3	MG	D	2003	1/1	0.95	0.07	24,24,24,24	0
4	NA	E	2005	1/1	0.95	0.09	43,43,43,43	0
3	MG	O	2002	1/1	0.95	0.18	42,42,42,42	0
4	NA	F	2005	1/1	0.95	0.05	23,23,23,23	0
4	NA	P	2005	1/1	0.95	0.12	55,55,55,55	0
4	NA	G	2005	1/1	0.96	0.04	24,24,24,24	0
3	MG	N	2002	1/1	0.96	0.12	37,37,37,37	0
3	MG	I	2002	1/1	0.96	0.15	32,32,32,32	0
3	MG	D	2002	1/1	0.96	0.11	31,31,31,31	0
4	NA	A	2005	1/1	0.96	0.05	18,18,18,18	0
4	NA	B	2005	1/1	0.96	0.10	16,16,16,16	0
4	NA	C	2004	1/1	0.96	0.08	29,29,29,29	0
3	MG	B	2003	1/1	0.96	0.08	15,15,15,15	0
3	MG	B	2002	1/1	0.97	0.17	22,22,22,22	0
3	MG	J	2003	1/1	0.97	0.11	24,24,24,24	0
3	MG	M	2003	1/1	0.97	0.15	41,41,41,41	0
3	MG	K	2002	1/1	0.97	0.16	45,45,45,45	0
3	MG	K	2003	1/1	0.97	0.05	39,39,39,39	0
4	NA	L	2005	1/1	0.97	0.08	40,40,40,40	0
3	MG	A	2003	1/1	0.97	0.09	16,16,16,16	0
4	NA	H	2005	1/1	0.98	0.06	33,33,33,33	0
4	NA	B	2004	1/1	0.98	0.06	29,29,29,29	0
4	NA	I	2004	1/1	0.99	0.06	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.