



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 28, 2026 – 09:36 PM UTC

PDB ID : 4V41 / pdb_00004v41
Title : E. COLI (LAC Z) BETA-GALACTOSIDASE (NCS CONSTRAINED MONOMER-MONOCLINIC)
Authors : Juers, D.H.; Jacobson, R.H.; Wigley, D.; Zhang, X.J.; Huber, R.E.; Tronrud, D.E.; Matthews, B.W.
Deposited on : 2000-06-07
Resolution : 2.50 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

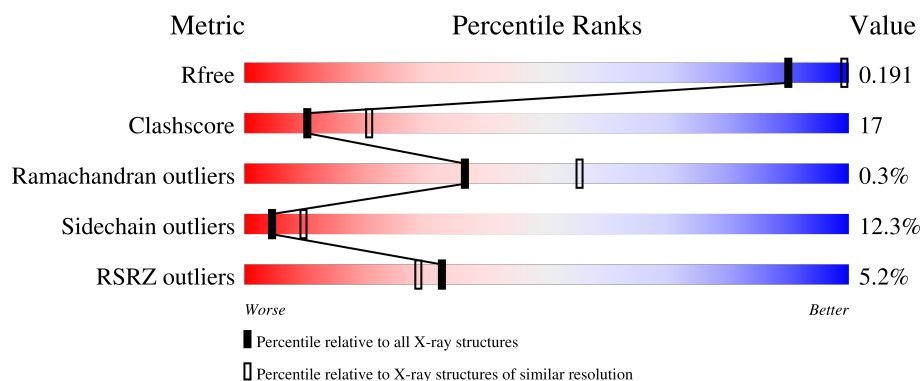
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	4% 60% 28% 10% .
1	B	1023	4% 60% 29% 10% .
1	C	1023	3% 58% 30% 10% .
1	D	1023	4% 60% 28% 10% .
1	E	1023	5% 59% 29% 9% .

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Mol	Chain	Length	Quality of chain				
1	F	1023	3%	59%	29%	10%	•
1	G	1023	2%	60%	28%	10%	•
1	H	1023	4%	59%	29%	10%	•
1	I	1023	2%	59%	29%	10%	•
1	J	1023	3%	59%	29%	10%	•
1	K	1023	•	59%	29%	10%	•
1	L	1023	3%	59%	29%	10%	•
1	M	1023	15%	60%	28%	10%	•
1	N	1023	3%	59%	29%	10%	•
1	O	1023	2%	59%	29%	10%	•
1	P	1023	26%	59%	29%	10%	•

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 138704 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	5	0
			8232	5201	1462	1528	41			
1	B	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	C	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	D	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	E	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	F	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	G	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	H	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	I	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	J	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	K	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	L	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	M	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	N	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	O	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	P	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

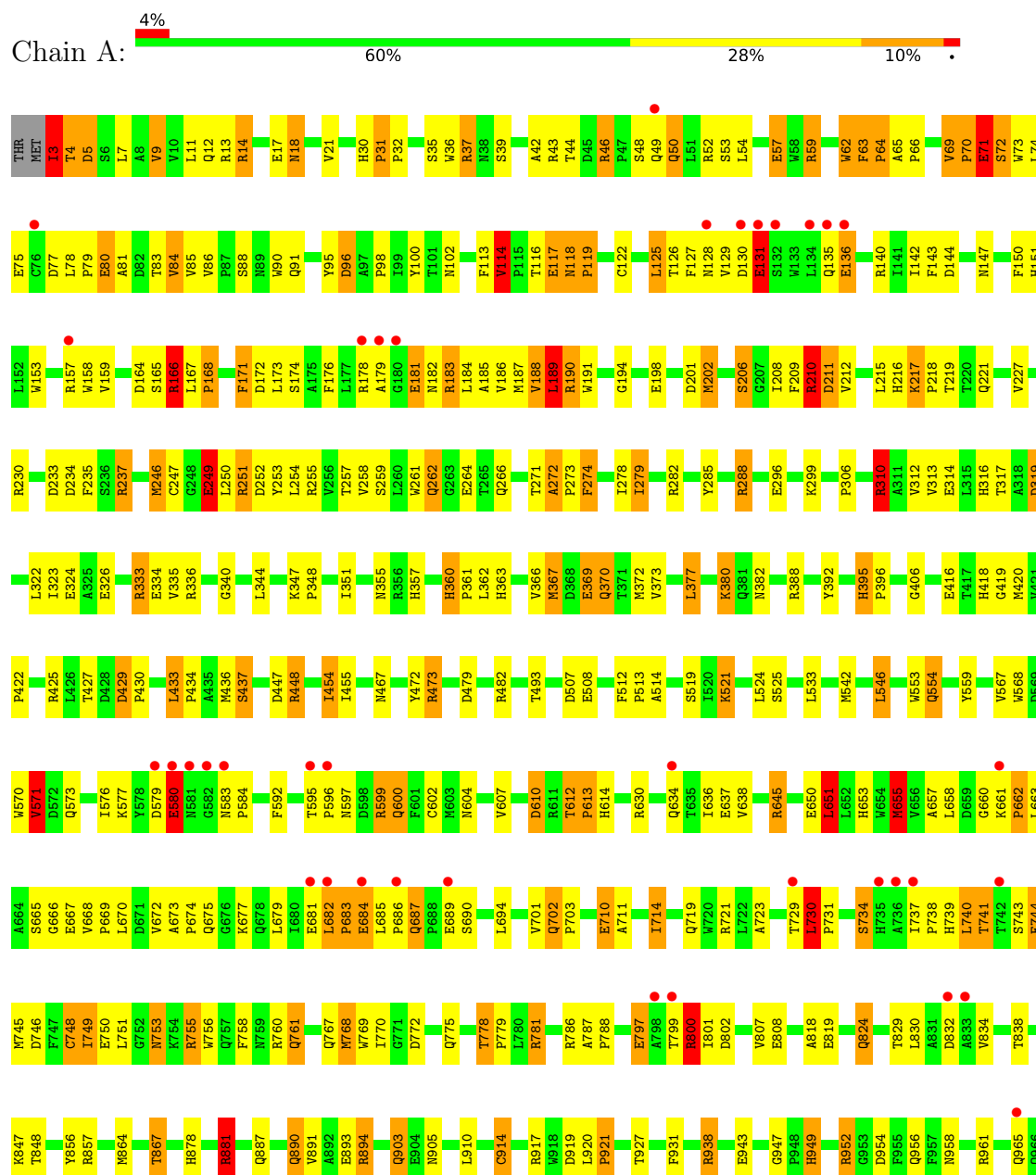
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	434	Total O 434 434	0	0
3	B	436	Total O 436 436	0	0
3	C	433	Total O 433 433	0	0
3	D	437	Total O 437 437	0	0
3	E	435	Total O 435 435	0	0
3	F	436	Total O 436 436	0	0
3	G	434	Total O 434 434	0	0
3	H	435	Total O 435 435	0	0
3	I	434	Total O 434 434	0	0
3	J	436	Total O 436 436	0	0
3	K	435	Total O 435 435	0	0
3	L	435	Total O 435 435	0	0
3	M	434	Total O 434 434	0	0
3	N	436	Total O 436 436	0	0
3	O	433	Total O 433 433	0	0
3	P	437	Total O 437 437	0	0

3 Residue-property plots [i](#)

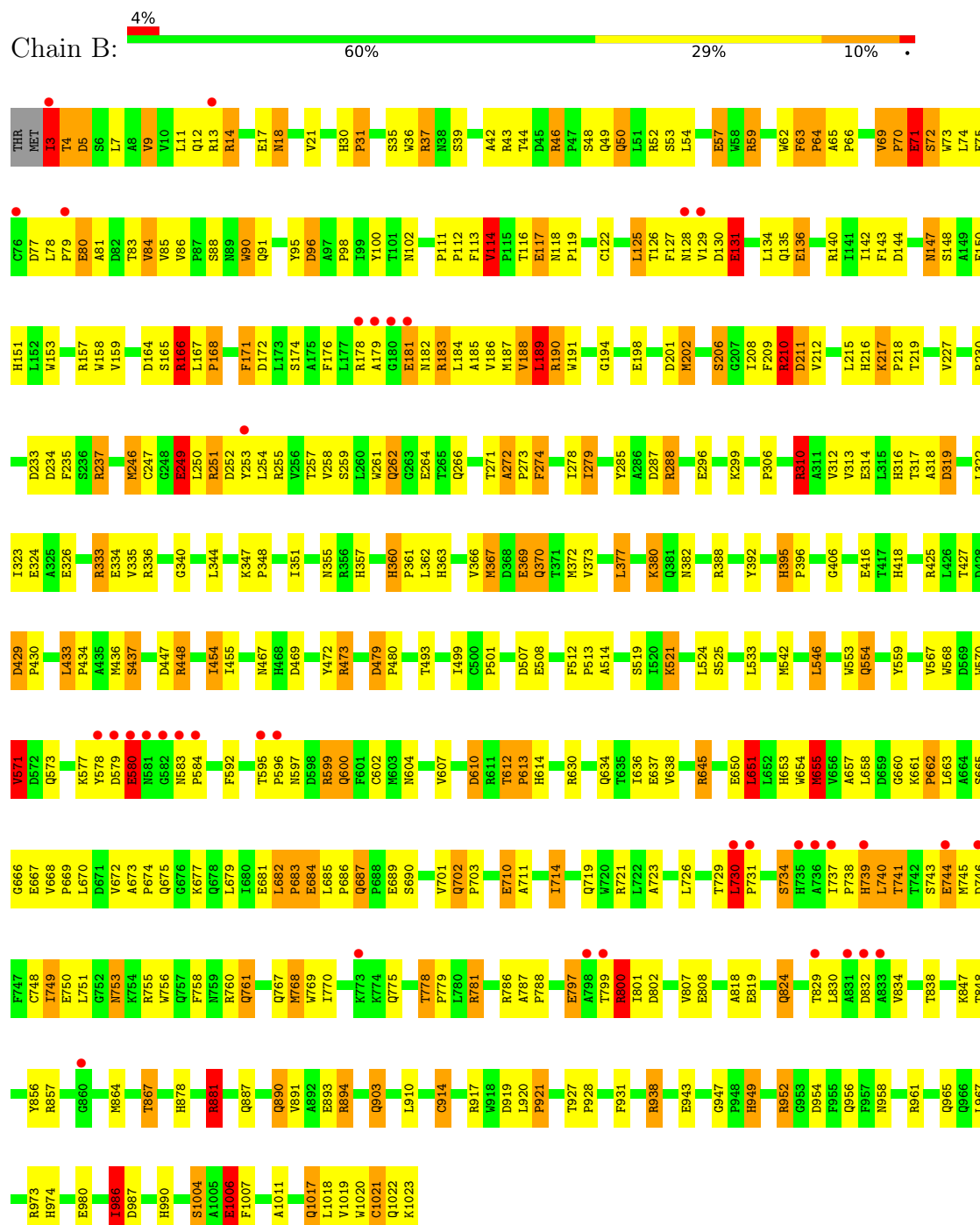
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: BETA-GALACTOSIDASE



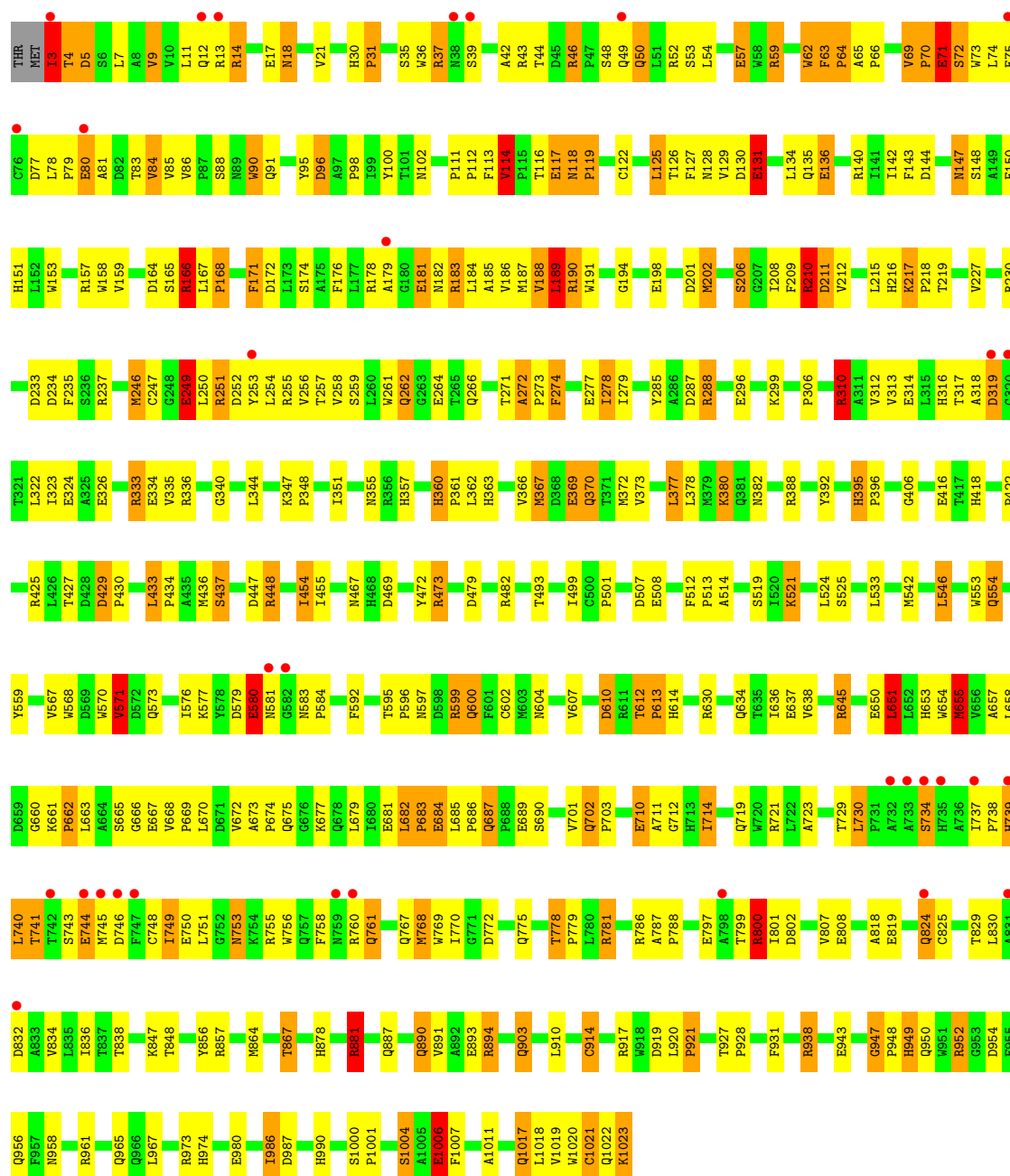


● Molecule 1: BETA-GALACTOSIDASE

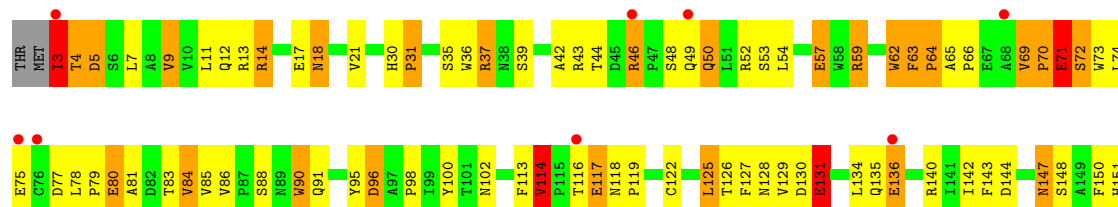


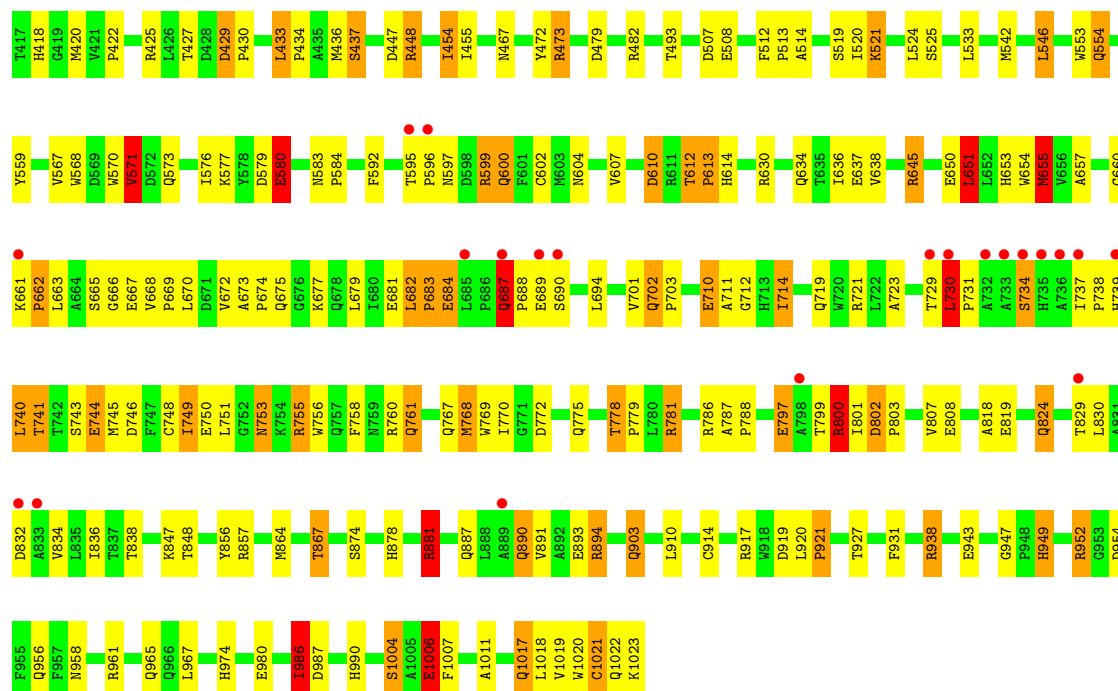
● Molecule 1: BETA-GALACTOSIDASE



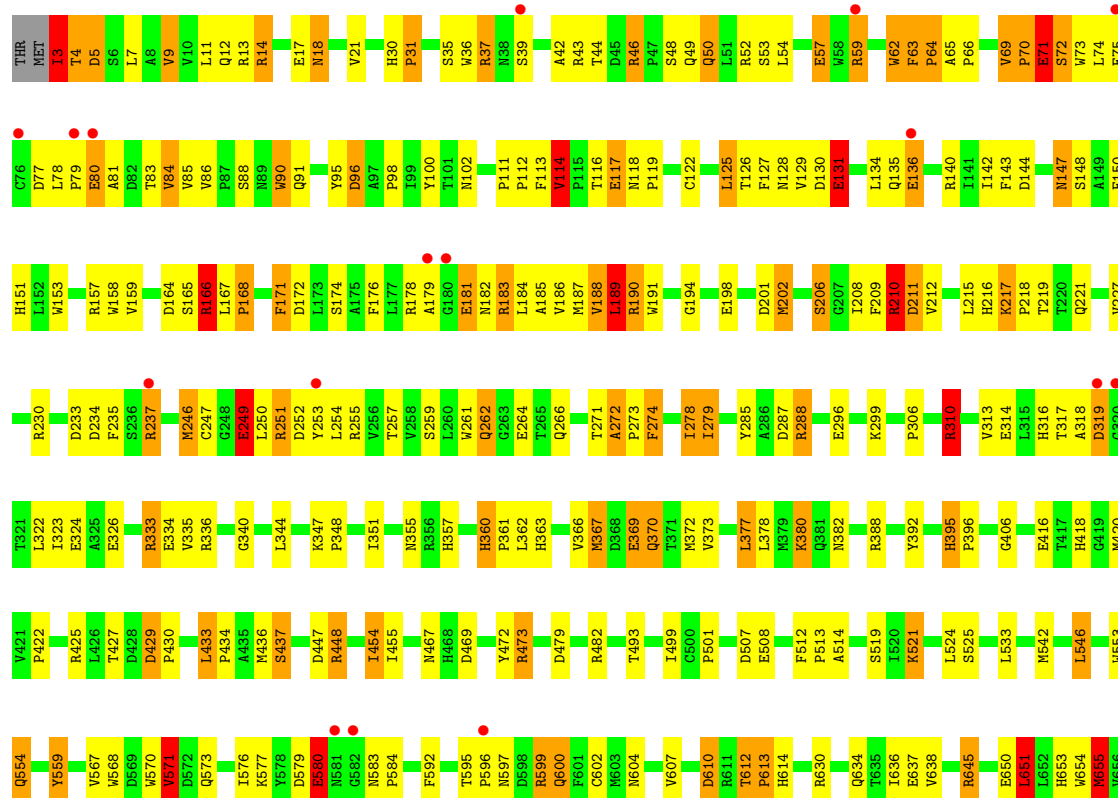


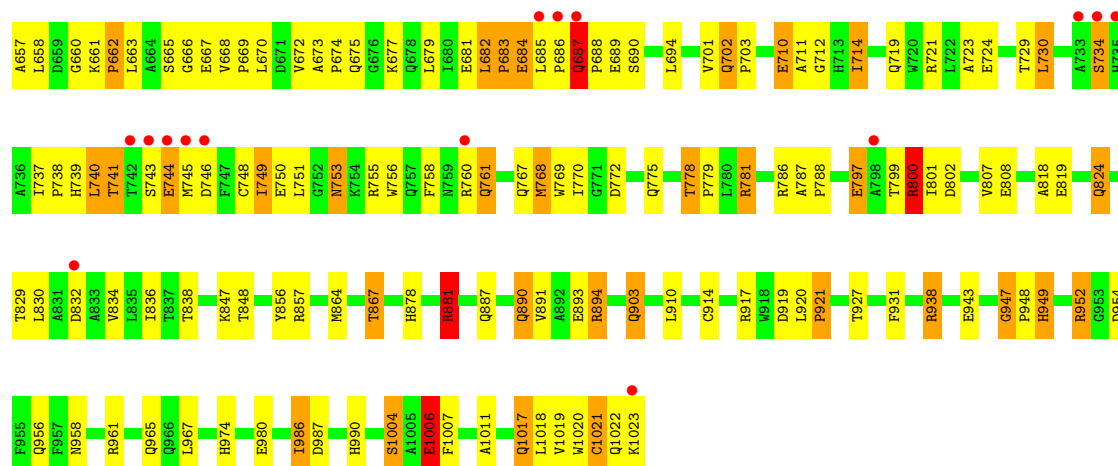
● Molecule 1: BETA-GALACTOSIDASE



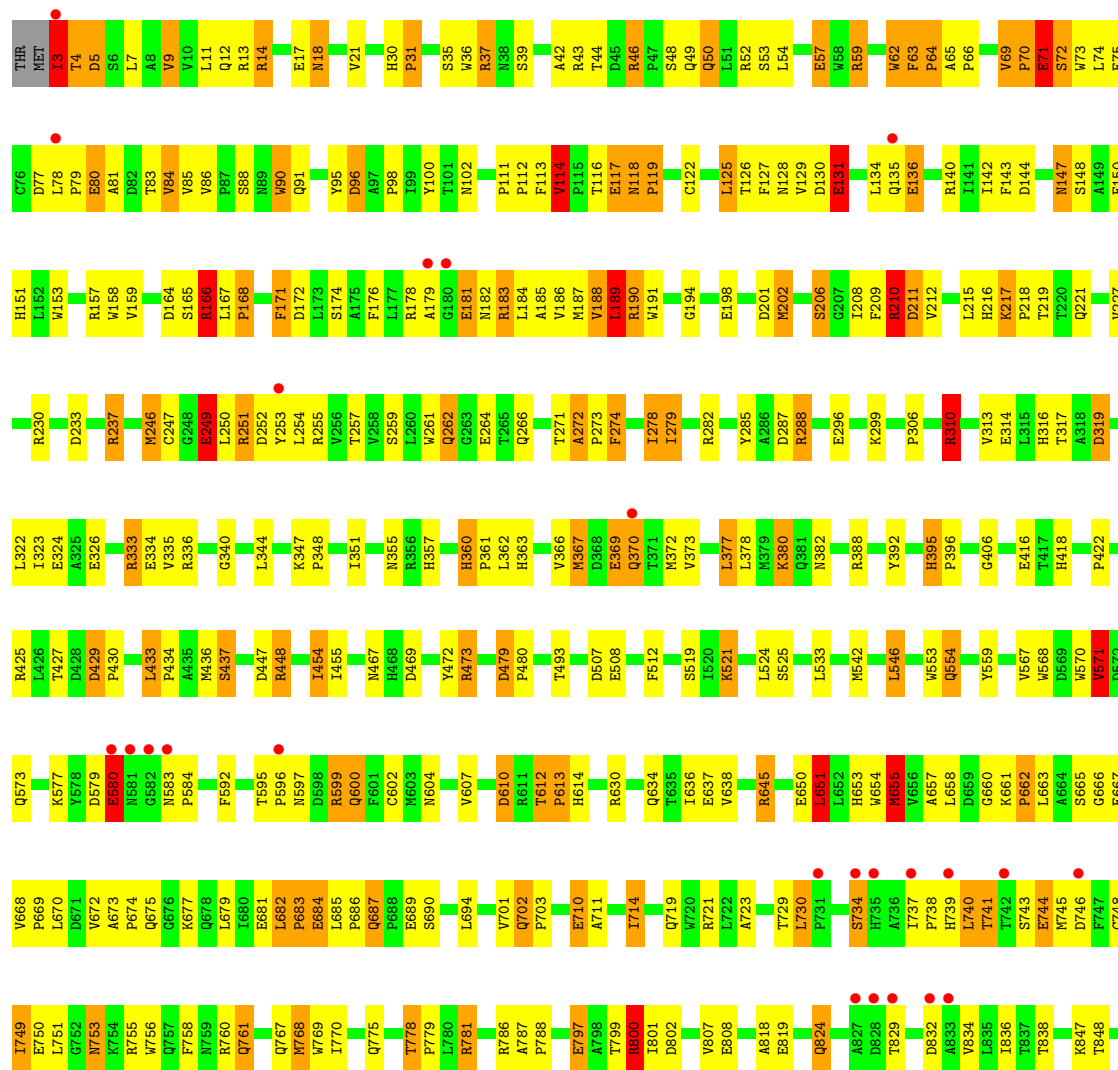


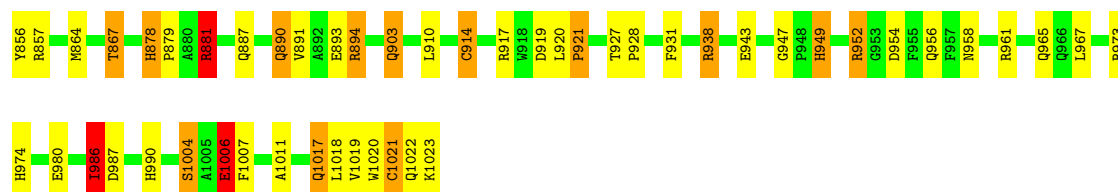
• Molecule 1: BETA-GALACTOSIDASE



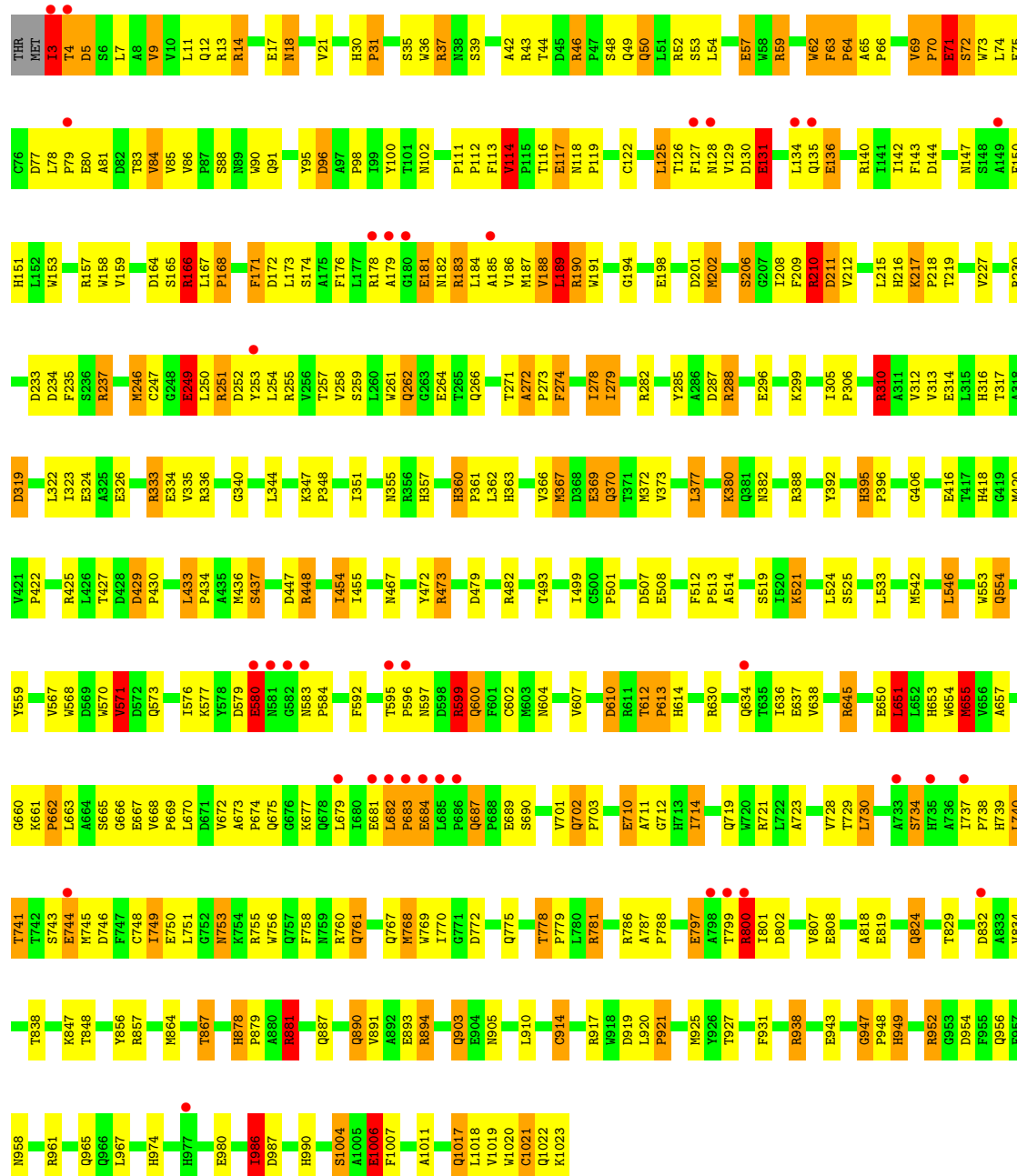


• Molecule 1: BETA-GALACTOSIDASE

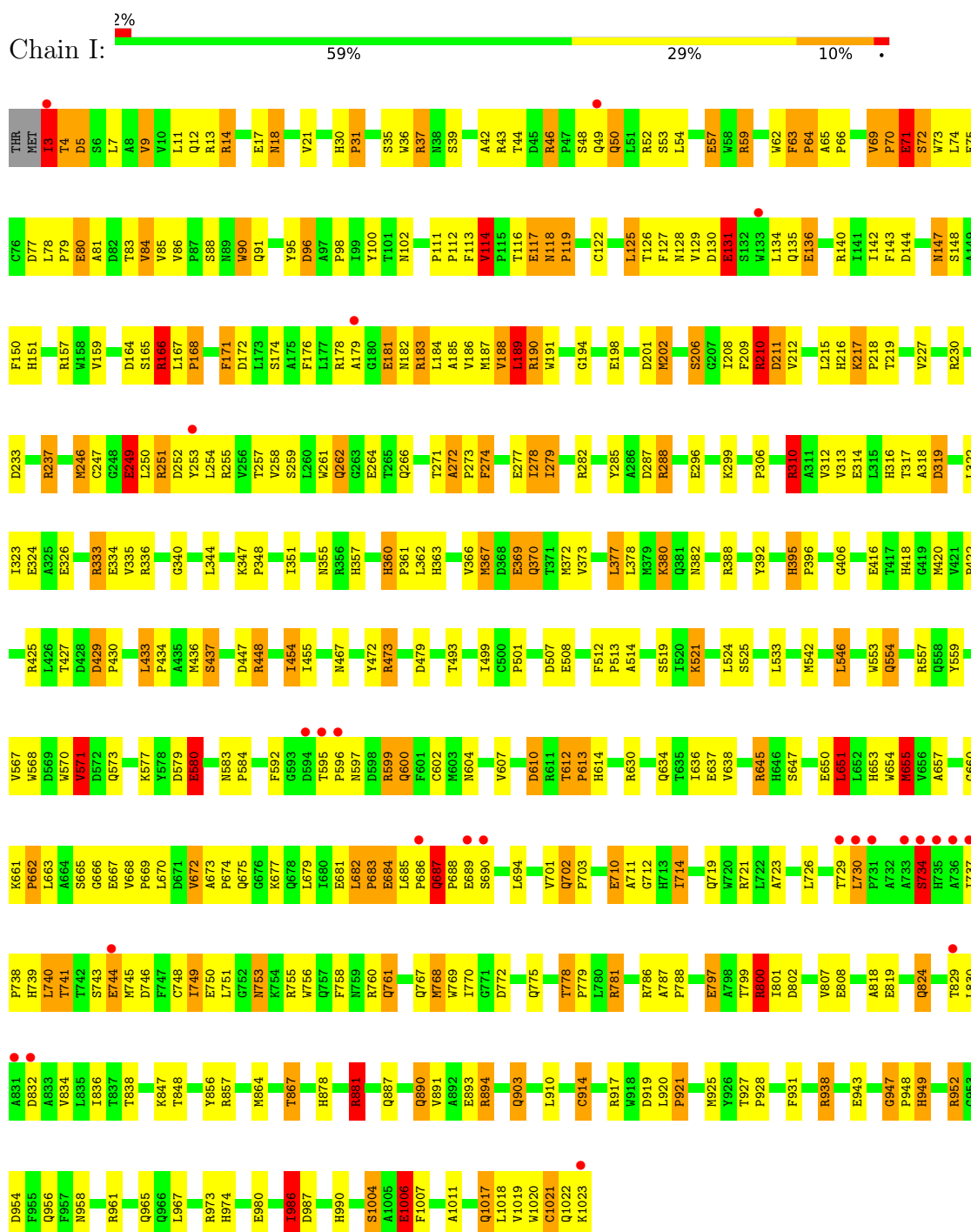




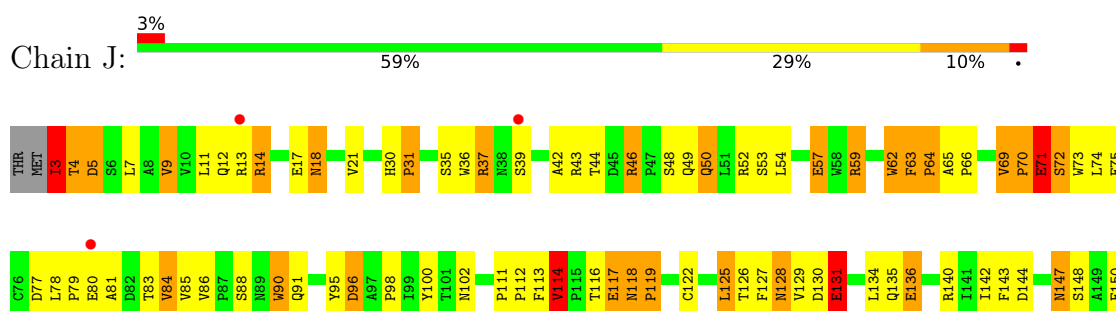
• Molecule 1: BETA-GALACTOSIDASE

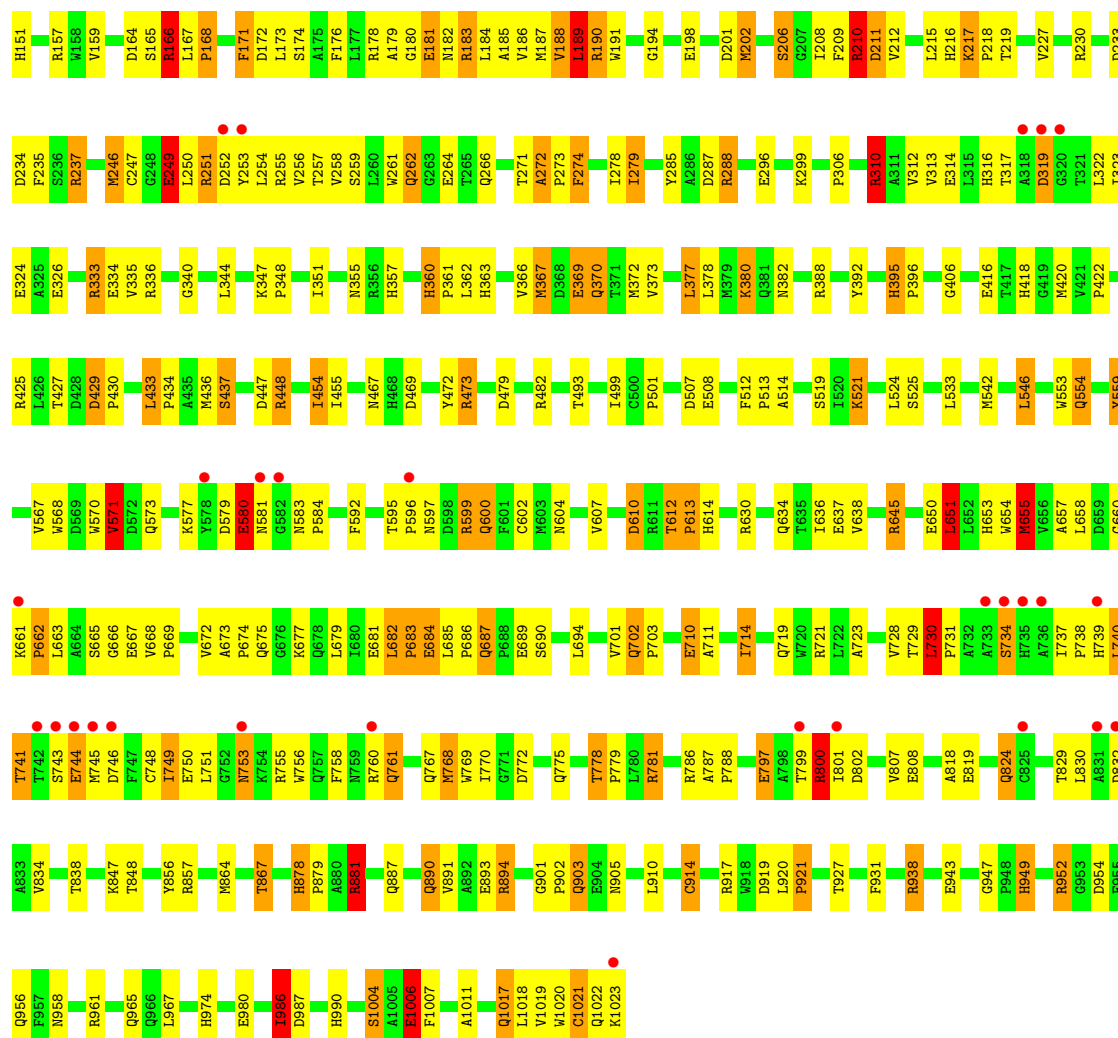


• Molecule 1: BETA-GALACTOSIDASE

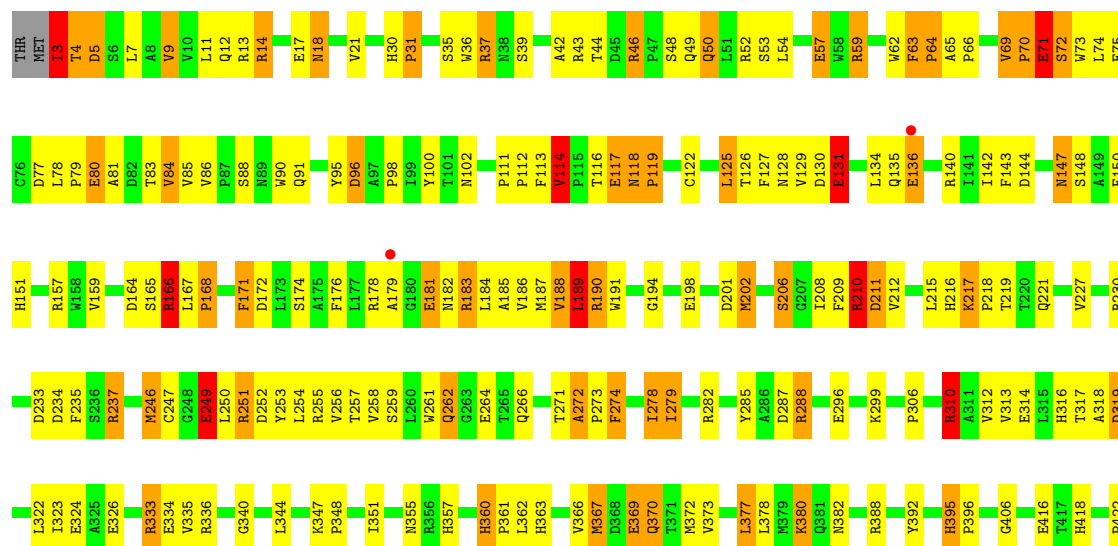


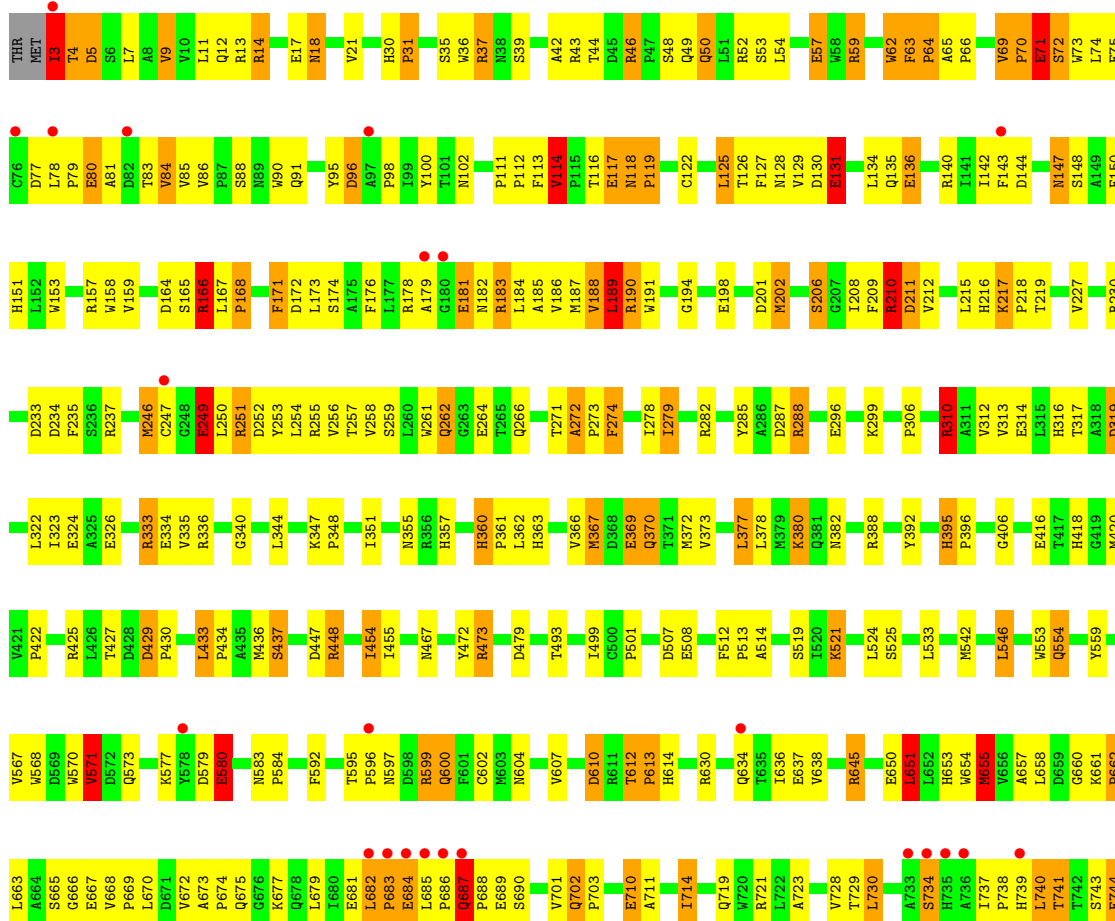
• Molecule 1: BETA-GALACTOSIDASE

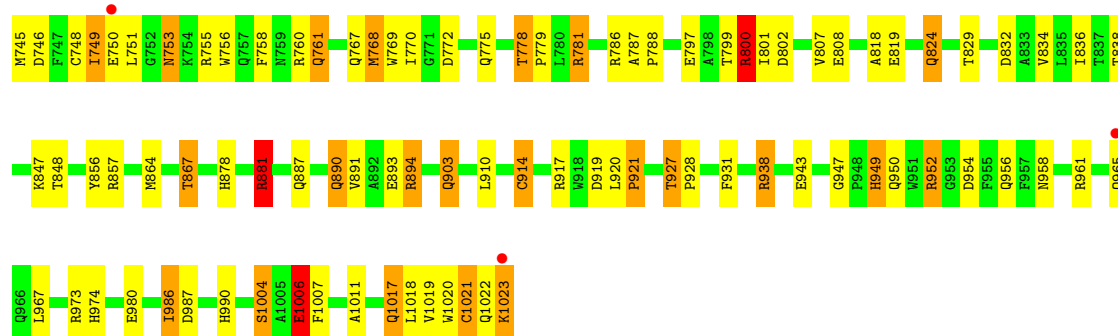




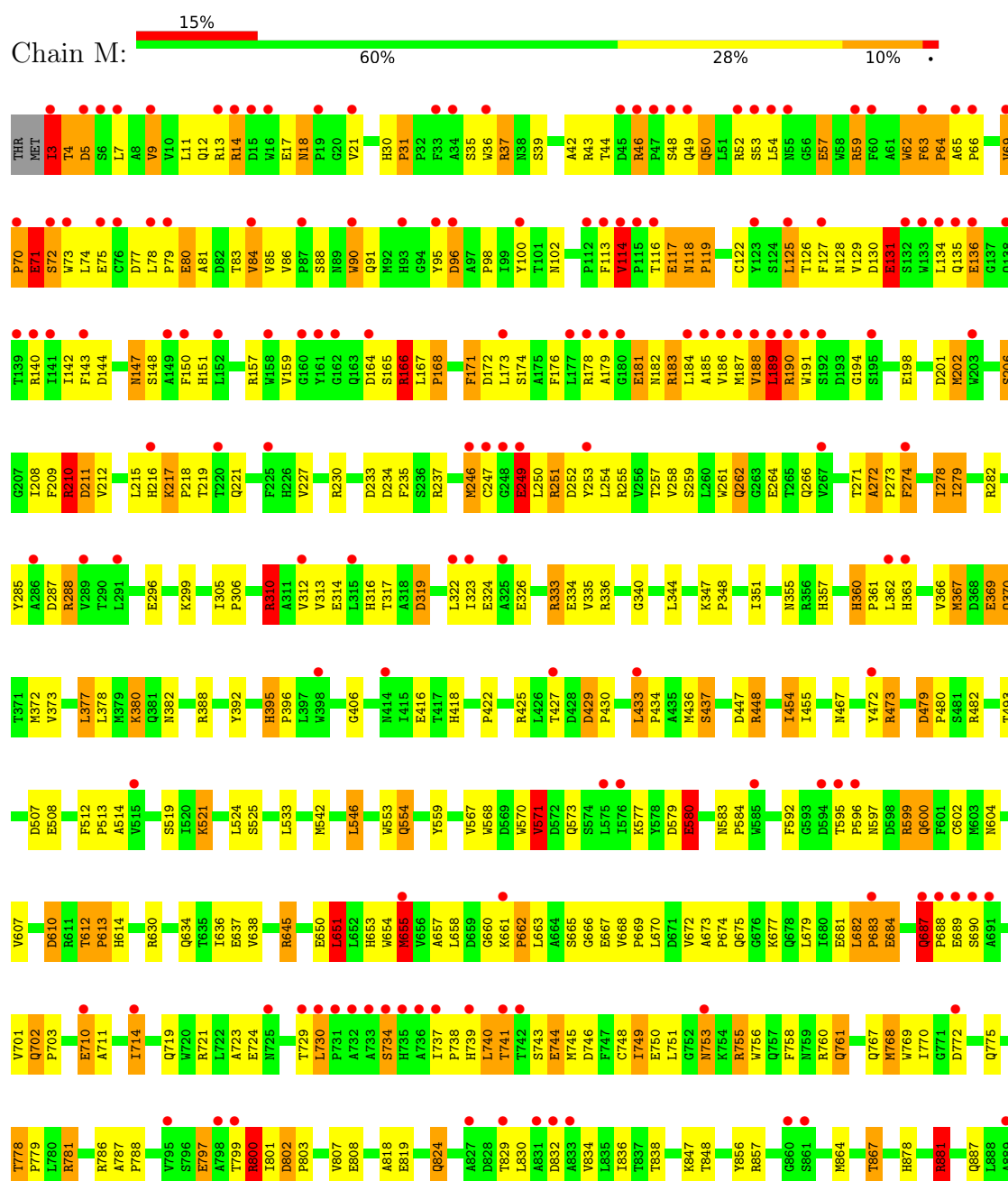
• Molecule 1: BETA-GALACTOSIDASE

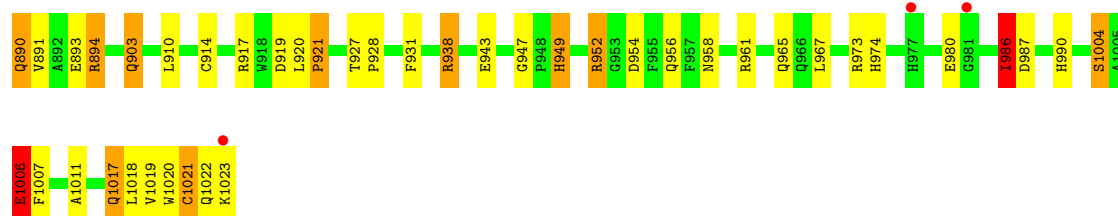




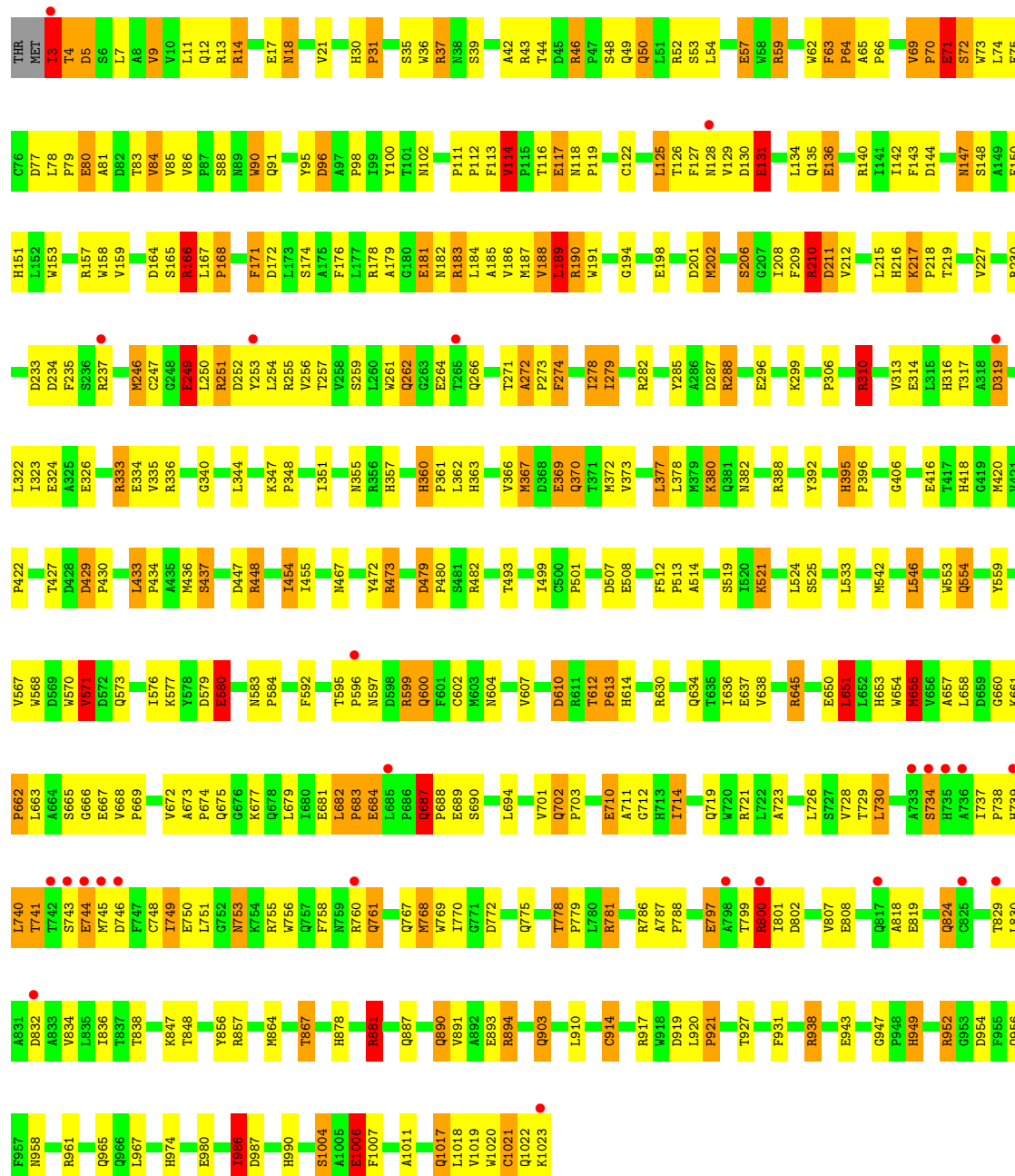


• Molecule 1: BETA-GALACTOSIDASE

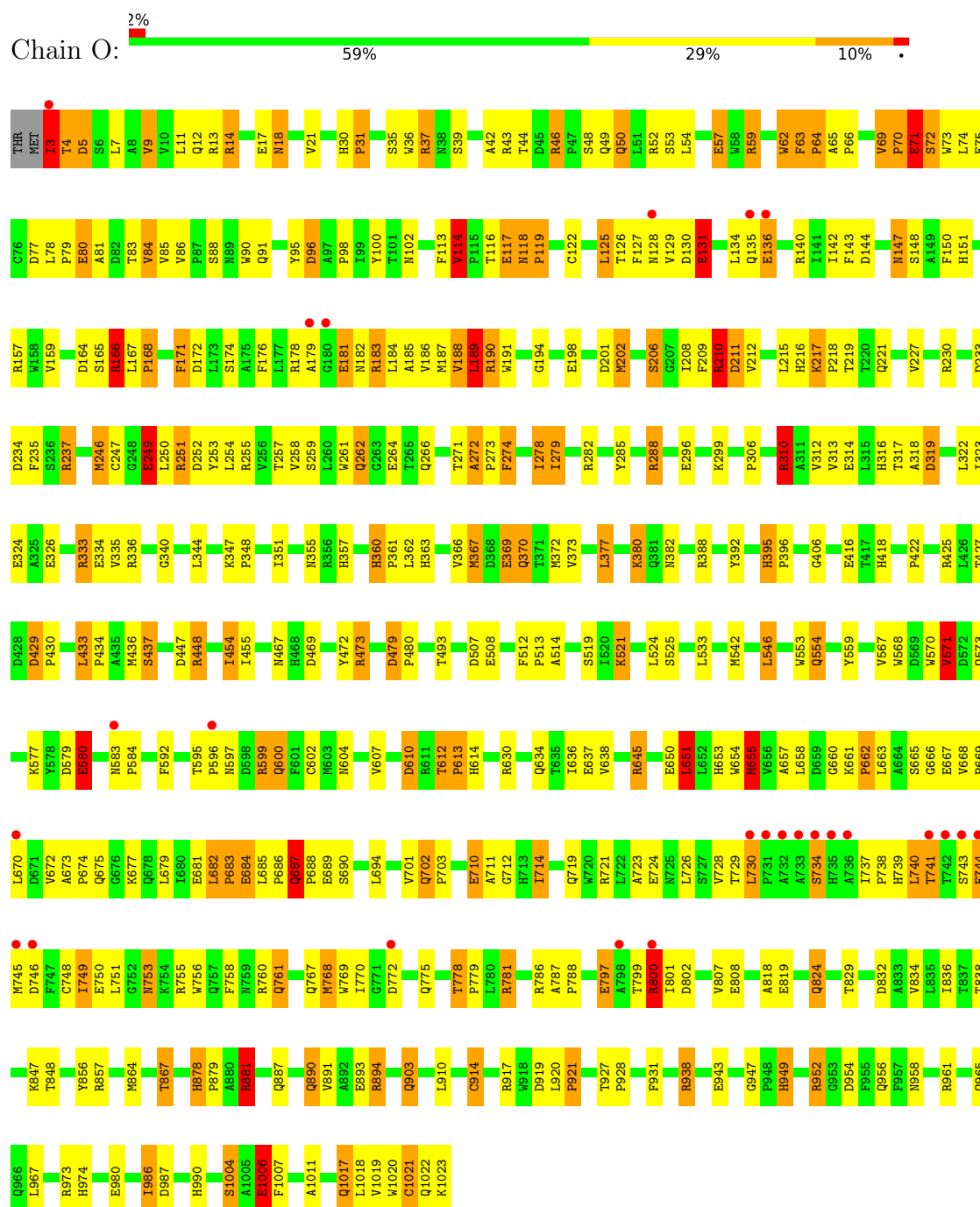


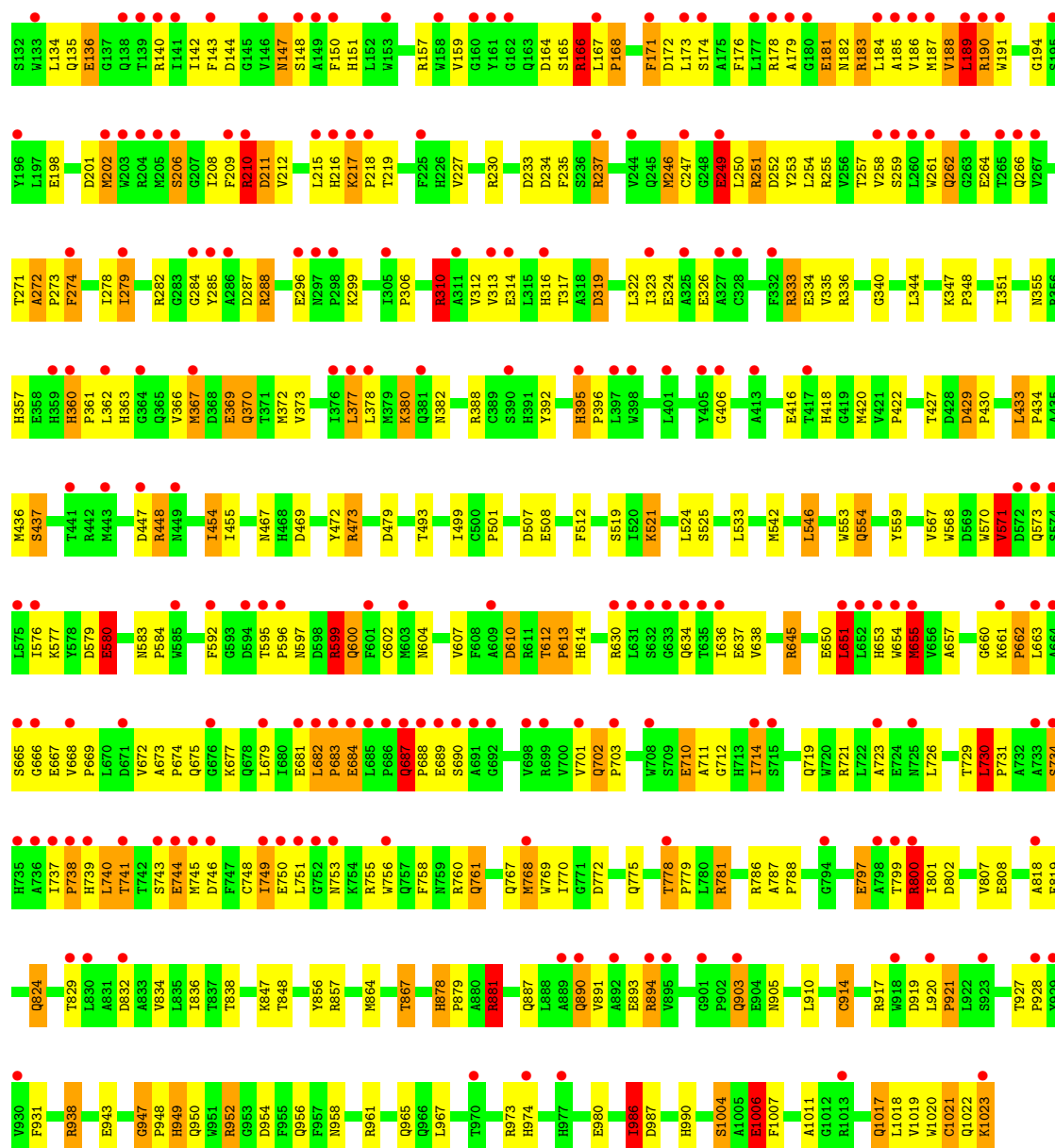


• Molecule 1: BETA-GALACTOSIDASE



• Molecule 1: BETA-GALACTOSIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.90Å 207.50Å 509.90Å 90.00° 94.70° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50 200.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	71.0 ((Not available)-2.50) 72.7 (200.00-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.00Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.199 , 0.207 0.184 , 0.191	Depositor DCC
R_{free} test set	1680 reflections (0.28%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 100.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	138704	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.98% 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: CME, MG

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	1.47	37/8472 (0.4%)	1.85	177/11553 (1.5%)
1	B	1.47	37/8472 (0.4%)	1.85	179/11553 (1.5%)
1	C	1.47	39/8472 (0.5%)	1.85	180/11553 (1.6%)
1	D	1.47	36/8472 (0.4%)	1.85	182/11553 (1.6%)
1	E	1.47	37/8472 (0.4%)	1.85	179/11553 (1.5%)
1	F	1.47	37/8472 (0.4%)	1.85	180/11553 (1.6%)
1	G	1.47	37/8472 (0.4%)	1.85	180/11553 (1.6%)
1	H	1.47	36/8472 (0.4%)	1.85	182/11553 (1.6%)
1	I	1.47	38/8472 (0.4%)	1.85	180/11553 (1.6%)
1	J	1.47	38/8472 (0.4%)	1.85	180/11553 (1.6%)
1	K	1.47	36/8472 (0.4%)	1.85	180/11553 (1.6%)
1	L	1.47	36/8472 (0.4%)	1.85	178/11553 (1.5%)
1	M	1.47	37/8472 (0.4%)	1.85	179/11553 (1.5%)
1	N	1.47	35/8472 (0.4%)	1.85	180/11553 (1.6%)
1	O	1.47	37/8472 (0.4%)	1.85	182/11553 (1.6%)
1	P	1.47	37/8472 (0.4%)	1.85	178/11553 (1.5%)
All	All	1.47	590/135552 (0.4%)	1.85	2876/184848 (1.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	0
1	B	2	0
1	C	2	0
1	D	2	0
1	E	2	0
1	F	2	0
1	G	2	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	2	0
1	I	2	0
1	J	2	0
1	K	2	0
1	L	2	0
1	M	2	0
1	N	2	0
1	O	2	0
1	P	2	0
All	All	32	0

The worst 5 of 590 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	118	ASN	N-CA	-9.04	1.38	1.46
1	K	118	ASN	N-CA	-9.02	1.38	1.46
1	C	118	ASN	N-CA	-9.00	1.38	1.46
1	B	118	ASN	N-CA	-8.98	1.38	1.46
1	M	118	ASN	N-CA	-8.98	1.38	1.46

The worst 5 of 2876 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	571	VAL	CB-CA-C	-10.10	95.27	110.82
1	L	571	VAL	CB-CA-C	-10.10	95.27	110.82
1	F	571	VAL	CB-CA-C	-10.09	95.28	110.82
1	E	571	VAL	CB-CA-C	-10.09	95.28	110.82
1	M	571	VAL	CB-CA-C	-10.08	95.29	110.82

5 of 32 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	166	ARG	CA
1	A	249	GLU	CA
1	B	166	ARG	CA
1	B	249	GLU	CA
1	C	166	ARG	CA

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	8232	0	7817	279	3
1	B	8232	0	7817	274	4
1	C	8232	0	7817	272	1
1	D	8232	0	7817	286	0
1	E	8232	0	7817	278	0
1	F	8232	0	7817	283	0
1	G	8232	0	7817	277	0
1	H	8232	0	7817	274	0
1	I	8232	0	7817	282	1
1	J	8232	0	7817	284	0
1	K	8232	0	7817	284	0
1	L	8232	0	7817	274	0
1	M	8232	0	7817	284	0
1	N	8232	0	7817	278	0
1	O	8232	0	7817	279	0
1	P	8232	0	7817	282	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
3	A	434	0	0	13	0
3	B	436	0	0	13	0
3	C	433	0	0	13	0
3	D	437	0	0	13	0
3	E	435	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	436	0	0	13	0
3	G	434	0	0	13	0
3	H	435	0	0	13	0
3	I	434	0	0	13	0
3	J	436	0	0	13	0
3	K	435	0	0	13	0
3	L	435	0	0	13	0
3	M	434	0	0	13	0
3	N	436	0	0	13	0
3	O	433	0	0	13	0
3	P	437	0	0	13	0
All	All	138704	0	125072	4364	5

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 17.

The worst 5 of 4364 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:H:427:THR:HA	1:H:436:MET:HE1	1.17	1.17
1:I:427:THR:HA	1:I:436:MET:HE1	1.17	1.17
1:P:427:THR:HA	1:P:436:MET:HE1	1.17	1.16
1:O:427:THR:HA	1:O:436:MET:HE1	1.17	1.16
1:B:427:THR:HA	1:B:436:MET:HE1	1.17	1.15

All (5) 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:CB[2_555]	1.77	0.43
1:A:580:GLU:O	1:B:578:TYR:CG[2_555]	1.85	0.35
1:A:580:GLU:O	1:B:578:TYR:CD1[2_555]	2.10	0.10
1:B:739:HIS:NE2	1:P:738:PRO:O[1_354]	2.10	0.10
1:C:739:HIS:ND1	1:I:734:SER:O[1_655]	2.15	0.05

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	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	B	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	C	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	D	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	E	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	F	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	G	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	H	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	I	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	J	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	K	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	L	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	M	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	N	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	O	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	P	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
All	All	16336/16368 (100%)	15616 (96%)	672 (4%)	48 (0%)	36	55

5 of 48 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	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	B	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	C	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	D	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	E	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	F	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	G	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	H	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	I	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	J	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	K	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	L	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	M	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	N	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	O	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	P	875/872 (100%)	767 (88%)	108 (12%)	4	10
All	All	14000/13952 (100%)	12272 (88%)	1728 (12%)	4	10

5 of 1728 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	599	ARG
1	K	651	LEU
1	O	797	GLU
1	I	800	ARG
1	I	580	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 346 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	739	HIS
1	N	316	HIS
1	K	1017	GLN
1	M	102	ASN
1	N	950	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	A	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)
1	CME	C	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.98	0
1	CME	D	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.40	1 (16%)
1	CME	G	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	P	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	G	914	1	8,9,10	0.84	0	6,9,11	1.72	1 (16%)
1	CME	J	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)
1	CME	O	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	K	1021	1	8,9,10	1.29	1 (12%)	6,9,11	3.40	1 (16%)
1	CME	M	748	1	8,9,10	0.92	1 (12%)	6,9,11	0.99	0
1	CME	C	1021	1	8,9,10	1.31	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	G	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	J	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	D	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	F	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	H	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CME	F	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)
1	CME	N	748	1	8,9,10	0.92	1 (12%)	6,9,11	0.99	0
1	CME	C	914	1	8,9,10	0.84	0	6,9,11	1.72	1 (16%)
1	CME	I	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)
1	CME	J	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	O	1021	1	8,9,10	1.31	1 (12%)	6,9,11	3.38	1 (16%)
1	CME	A	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	O	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)
1	CME	P	914	1	8,9,10	0.84	0	6,9,11	1.72	1 (16%)
1	CME	H	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	B	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	I	748	1	8,9,10	0.92	1 (12%)	6,9,11	0.99	0
1	CME	N	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	H	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	A	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	B	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	B	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)
1	CME	F	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	L	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	L	914	1	8,9,10	0.85	0	6,9,11	1.73	1 (16%)
1	CME	I	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	E	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	E	914	1	8,9,10	0.84	0	6,9,11	1.72	1 (16%)
1	CME	D	914	1	8,9,10	0.84	0	6,9,11	1.72	1 (16%)
1	CME	K	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.98	0
1	CME	E	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	K	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)
1	CME	L	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	M	914	1	8,9,10	0.86	0	6,9,11	1.72	1 (16%)
1	CME	P	748	1	8,9,10	0.92	1 (12%)	6,9,11	0.99	0
1	CME	N	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)
1	CME	M	1021	1	8,9,10	1.31	1 (12%)	6,9,11	3.39	1 (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
1	CME	A	914	1	-	3/5/8/10	-
1	CME	C	748	1	-	3/5/8/10	-
1	CME	D	1021	1	-	4/5/8/10	-
1	CME	G	748	1	-	3/5/8/10	-
1	CME	P	1021	1	-	4/5/8/10	-
1	CME	G	914	1	-	3/5/8/10	-
1	CME	J	914	1	-	3/5/8/10	-
1	CME	O	748	1	-	3/5/8/10	-
1	CME	K	1021	1	-	4/5/8/10	-
1	CME	M	748	1	-	3/5/8/10	-
1	CME	C	1021	1	-	4/5/8/10	-
1	CME	G	1021	1	-	4/5/8/10	-
1	CME	J	748	1	-	3/5/8/10	-
1	CME	D	748	1	-	3/5/8/10	-
1	CME	F	748	1	-	3/5/8/10	-
1	CME	H	914	1	-	3/5/8/10	-
1	CME	F	914	1	-	3/5/8/10	-
1	CME	N	748	1	-	3/5/8/10	-
1	CME	C	914	1	-	3/5/8/10	-
1	CME	I	914	1	-	3/5/8/10	-
1	CME	J	1021	1	-	4/5/8/10	-
1	CME	O	1021	1	-	4/5/8/10	-
1	CME	A	748	1	-	3/5/8/10	-
1	CME	O	914	1	-	3/5/8/10	-
1	CME	P	914	1	-	3/5/8/10	-
1	CME	H	748	1	-	3/5/8/10	-
1	CME	B	1021	1	-	4/5/8/10	-
1	CME	I	748	1	-	3/5/8/10	-
1	CME	N	1021	1	-	4/5/8/10	-
1	CME	H	1021	1	-	4/5/8/10	-
1	CME	A	1021	1	-	4/5/8/10	-
1	CME	B	748	1	-	3/5/8/10	-
1	CME	B	914	1	-	3/5/8/10	-

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	748	CME	CA-N	-2.50	1.41	1.48
1	H	748	CME	CA-N	-2.50	1.41	1.48
1	K	748	CME	CA-N	-2.50	1.41	1.48
1	F	748	CME	CA-N	-2.49	1.41	1.48
1	G	748	CME	CA-N	-2.49	1.41	1.48

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1021	CME	CB-SG-SD	-8.04	83.06	103.86
1	K	1021	CME	CB-SG-SD	-8.03	83.07	103.86
1	P	1021	CME	CB-SG-SD	-8.03	83.08	103.86
1	N	1021	CME	CB-SG-SD	-8.03	83.09	103.86
1	I	1021	CME	CB-SG-SD	-8.02	83.10	103.86

There are no chirality outliers.

5 of 160 torsion outliers are listed below:

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

There are no ring outliers.

32 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	914	CME	1	0
1	D	1021	CME	3	0
1	P	1021	CME	3	0
1	G	914	CME	1	0
1	J	914	CME	1	0
1	K	1021	CME	3	0
1	C	1021	CME	3	0
1	G	1021	CME	3	0
1	D	748	CME	1	0
1	H	914	CME	1	0
1	C	914	CME	1	0
1	I	914	CME	1	0
1	J	1021	CME	3	0
1	O	1021	CME	3	0
1	A	748	CME	1	0
1	O	914	CME	1	0
1	P	914	CME	1	0
1	B	1021	CME	3	0
1	N	1021	CME	3	0
1	H	1021	CME	3	0
1	A	1021	CME	3	0
1	B	914	CME	1	0
1	F	1021	CME	3	0
1	L	914	CME	1	0
1	I	1021	CME	3	0
1	D	914	CME	1	0
1	K	748	CME	1	0
1	E	1021	CME	3	0
1	K	914	CME	1	0
1	L	1021	CME	3	0
1	N	914	CME	1	0
1	M	1021	CME	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 32 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	1018/1023 (99%)	-0.13	37 (3%)	46	41	3, 21, 66, 100	6 (0%)
1	B	1018/1023 (99%)	-0.11	36 (3%)	47	42	3, 21, 66, 100	6 (0%)
1	C	1018/1023 (99%)	-0.08	32 (3%)	51	47	2, 19, 63, 98	6 (0%)
1	D	1018/1023 (99%)	0.04	38 (3%)	45	40	5, 23, 67, 100	6 (0%)
1	E	1018/1023 (99%)	0.46	53 (5%)	33	29	15, 33, 74, 100	6 (0%)
1	F	1018/1023 (99%)	-0.18	31 (3%)	52	48	3, 21, 66, 100	6 (0%)
1	G	1018/1023 (99%)	-0.09	24 (2%)	59	55	7, 25, 68, 100	6 (0%)
1	H	1018/1023 (99%)	0.25	36 (3%)	47	42	14, 32, 73, 100	6 (0%)
1	I	1018/1023 (99%)	0.06	24 (2%)	59	55	10, 28, 70, 100	6 (0%)
1	J	1018/1023 (99%)	-0.07	31 (3%)	52	48	8, 26, 69, 100	6 (0%)
1	K	1018/1023 (99%)	0.09	14 (1%)	73	70	17, 35, 76, 100	6 (0%)
1	L	1018/1023 (99%)	0.20	26 (2%)	57	52	16, 34, 75, 100	6 (0%)
1	M	1018/1023 (99%)	1.07	156 (15%)	5	4	22, 40, 79, 100	6 (0%)
1	N	1018/1023 (99%)	0.06	26 (2%)	57	52	11, 29, 71, 100	6 (0%)
1	O	1018/1023 (99%)	0.04	25 (2%)	58	54	12, 30, 72, 100	6 (0%)
1	P	1018/1023 (99%)	1.49	262 (25%)	1	1	29, 47, 83, 100	6 (0%)
All	All	16288/16368 (99%)	0.19	851 (5%)	33	29	2, 30, 72, 100	96 (0%)

The worst 5 of 851 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	582	GLY	8.3
1	D	734	SER	7.3
1	A	581	ASN	7.0
1	B	582	GLY	6.4
1	P	739	HIS	6.1

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	748	10/11	0.83	0.17	44,54,100,100	0
1	CME	P	914	10/11	0.85	0.16	34,40,100,100	0
1	CME	C	748	10/11	0.88	0.16	16,26,97,97	0
1	CME	L	748	10/11	0.88	0.17	31,41,100,100	0
1	CME	H	748	10/11	0.89	0.15	29,39,100,100	0
1	CME	N	1021	10/11	0.90	0.14	9,33,100,100	0
1	CME	B	748	10/11	0.90	0.14	18,28,99,99	0
1	CME	M	1021	10/11	0.90	0.14	21,44,100,100	0
1	CME	P	1021	10/11	0.90	0.14	28,51,100,100	0
1	CME	F	1021	10/11	0.91	0.13	2,25,100,100	0
1	CME	I	1021	10/11	0.92	0.13	9,32,100,100	0
1	CME	J	1021	10/11	0.92	0.12	7,30,100,100	0
1	CME	O	1021	10/11	0.92	0.12	11,34,100,100	0
1	CME	K	748	10/11	0.92	0.13	32,42,100,100	0
1	CME	H	1021	10/11	0.92	0.13	13,36,100,100	0
1	CME	M	914	10/11	0.92	0.15	27,33,100,100	0
1	CME	L	1021	10/11	0.93	0.11	15,38,100,100	0
1	CME	E	1021	10/11	0.93	0.13	14,37,100,100	0
1	CME	C	1021	10/11	0.93	0.13	1,23,97,97	0
1	CME	J	748	10/11	0.93	0.11	23,33,100,100	0
1	CME	G	748	10/11	0.93	0.11	22,32,100,100	0
1	CME	G	1021	10/11	0.93	0.10	6,29,100,100	0
1	CME	K	1021	10/11	0.93	0.11	16,39,100,100	0
1	CME	D	748	10/11	0.93	0.15	21,30,100,100	0
1	CME	E	748	10/11	0.94	0.13	30,40,100,100	0
1	CME	A	1021	10/11	0.94	0.12	2,25,100,100	0
1	CME	O	748	10/11	0.94	0.13	27,37,100,100	0
1	CME	F	748	10/11	0.94	0.12	18,28,100,100	0
1	CME	I	748	10/11	0.94	0.11	25,35,100,100	0
1	CME	A	748	10/11	0.94	0.12	18,28,100,100	0
1	CME	B	1021	10/11	0.94	0.11	2,25,99,99	0
1	CME	O	914	10/11	0.95	0.10	17,23,100,100	0
1	CME	D	1021	10/11	0.95	0.13	4,27,100,100	0
1	CME	N	748	10/11	0.95	0.10	26,35,100,100	0
1	CME	M	748	10/11	0.95	0.11	37,47,100,100	0
1	CME	H	914	10/11	0.95	0.12	19,25,100,100	0
1	CME	K	914	10/11	0.96	0.10	22,28,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CME	G	914	10/11	0.96	0.10	12,18,100,100	0
1	CME	I	914	10/11	0.96	0.10	15,21,100,100	0
1	CME	L	914	10/11	0.96	0.10	21,27,100,100	0
1	CME	E	914	10/11	0.97	0.10	20,26,100,100	0
1	CME	A	914	10/11	0.97	0.10	8,14,100,100	0
1	CME	N	914	10/11	0.97	0.10	16,22,100,100	0
1	CME	J	914	10/11	0.97	0.10	13,19,100,100	0
1	CME	B	914	10/11	0.97	0.10	8,14,99,99	0
1	CME	C	914	10/11	0.98	0.09	6,12,97,97	0
1	CME	F	914	10/11	0.98	0.08	8,14,100,100	0
1	CME	D	914	10/11	0.98	0.09	10,16,100,100	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	C	3002	1/1	0.89	0.09	16,16,16,16	0
2	MG	P	3002	1/1	0.91	0.07	44,44,44,44	0
2	MG	M	3002	1/1	0.92	0.14	37,37,37,37	0
2	MG	I	3001	1/1	0.93	0.07	25,25,25,25	0
2	MG	M	3001	1/1	0.93	0.12	37,37,37,37	0
2	MG	L	3002	1/1	0.94	0.07	31,31,31,31	0
2	MG	P	3001	1/1	0.94	0.12	44,44,44,44	0
2	MG	E	3002	1/1	0.94	0.09	30,30,30,30	0
2	MG	D	3002	1/1	0.95	0.07	21,21,21,21	0
2	MG	I	3002	1/1	0.95	0.08	25,25,25,25	0
2	MG	L	3001	1/1	0.95	0.05	31,31,31,31	0
2	MG	H	3002	1/1	0.95	0.08	30,30,30,30	0
2	MG	B	3002	1/1	0.96	0.06	18,18,18,18	0
2	MG	K	3002	1/1	0.96	0.05	32,32,32,32	0
2	MG	J	3002	1/1	0.97	0.09	23,23,23,23	0
2	MG	A	3002	1/1	0.97	0.09	18,18,18,18	0
2	MG	F	3002	1/1	0.97	0.10	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	G	3002	1/1	0.97	0.04	22,22,22,22	0
2	MG	A	3001	1/1	0.98	0.11	18,18,18,18	0
2	MG	B	3001	1/1	0.98	0.03	18,18,18,18	0
2	MG	N	3001	1/1	0.98	0.04	26,26,26,26	0
2	MG	N	3002	1/1	0.98	0.09	26,26,26,26	0
2	MG	H	3001	1/1	0.98	0.03	29,29,29,29	0
2	MG	J	3001	1/1	0.98	0.07	23,23,23,23	0
2	MG	E	3001	1/1	0.99	0.07	30,30,30,30	0
2	MG	D	3001	1/1	0.99	0.03	20,20,20,20	0
2	MG	K	3001	1/1	0.99	0.08	32,32,32,32	0
2	MG	F	3001	1/1	0.99	0.03	18,18,18,18	0
2	MG	O	3001	1/1	0.99	0.04	27,27,27,27	0
2	MG	O	3002	1/1	0.99	0.07	27,27,27,27	0
2	MG	C	3001	1/1	0.99	0.03	16,16,16,16	0
2	MG	G	3001	1/1	0.99	0.03	22,22,22,22	0

6.5 Other polymers ⓘ

There are no such residues in this entry.