



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 03:05 AM UTC

PDB ID : 4V40 / pdb_00004v40
Title : BETA-GALACTOSIDASE
Authors : Jacobson, R.H.; Zhang, X.; Dubose, R.F.; Matthews, B.W.
Deposited on : 1994-07-18
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
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

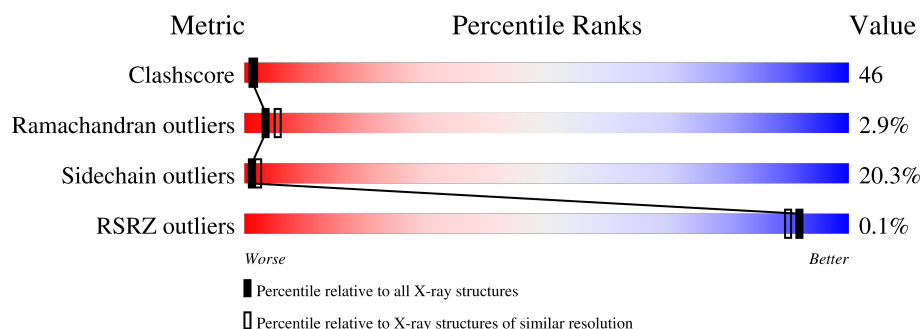
1 Overall quality at a glance

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.



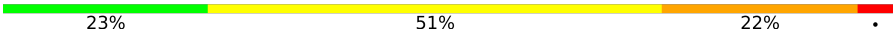
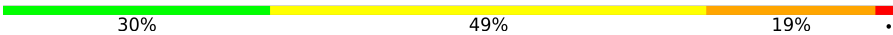
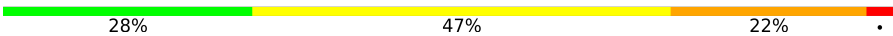
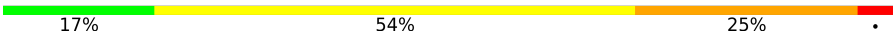
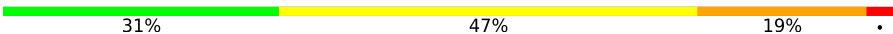
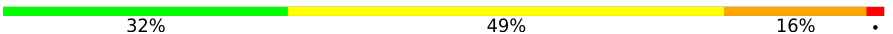
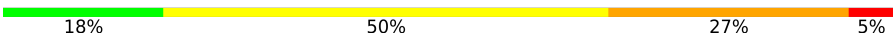
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	
1	B	1023	
1	C	1023	
1	D	1023	
1	E	1023	
1	F	1023	
1	G	1023	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	1023	
1	I	1023	
1	J	1023	
1	K	1023	
1	L	1023	
1	M	1023	
1	N	1023	
1	O	1023	
1	P	1023	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 132654 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	0	0
			8198	5185	1451	1524	38			
1	B	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	C	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	D	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	E	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	F	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	G	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	H	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	I	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	J	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	K	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	L	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	M	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	N	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	O	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	P	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Mg 2	0	0
2	B	2	Total 2	Mg 2	0	0
2	C	2	Total 2	Mg 2	0	0
2	D	2	Total 2	Mg 2	0	0
2	E	2	Total 2	Mg 2	0	0
2	F	2	Total 2	Mg 2	0	0
2	G	2	Total 2	Mg 2	0	0
2	H	2	Total 2	Mg 2	0	0
2	I	2	Total 2	Mg 2	0	0
2	J	2	Total 2	Mg 2	0	0
2	K	2	Total 2	Mg 2	0	0
2	L	2	Total 2	Mg 2	0	0
2	M	1	Total 1	Mg 1	0	0
2	N	2	Total 2	Mg 2	0	0
2	O	2	Total 2	Mg 2	0	0
2	P	2	Total 2	Mg 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	88	Total 88	O 88	0	0
3	B	96	Total 96	O 96	0	0
3	C	91	Total 91	O 91	0	0

Continued on next page...

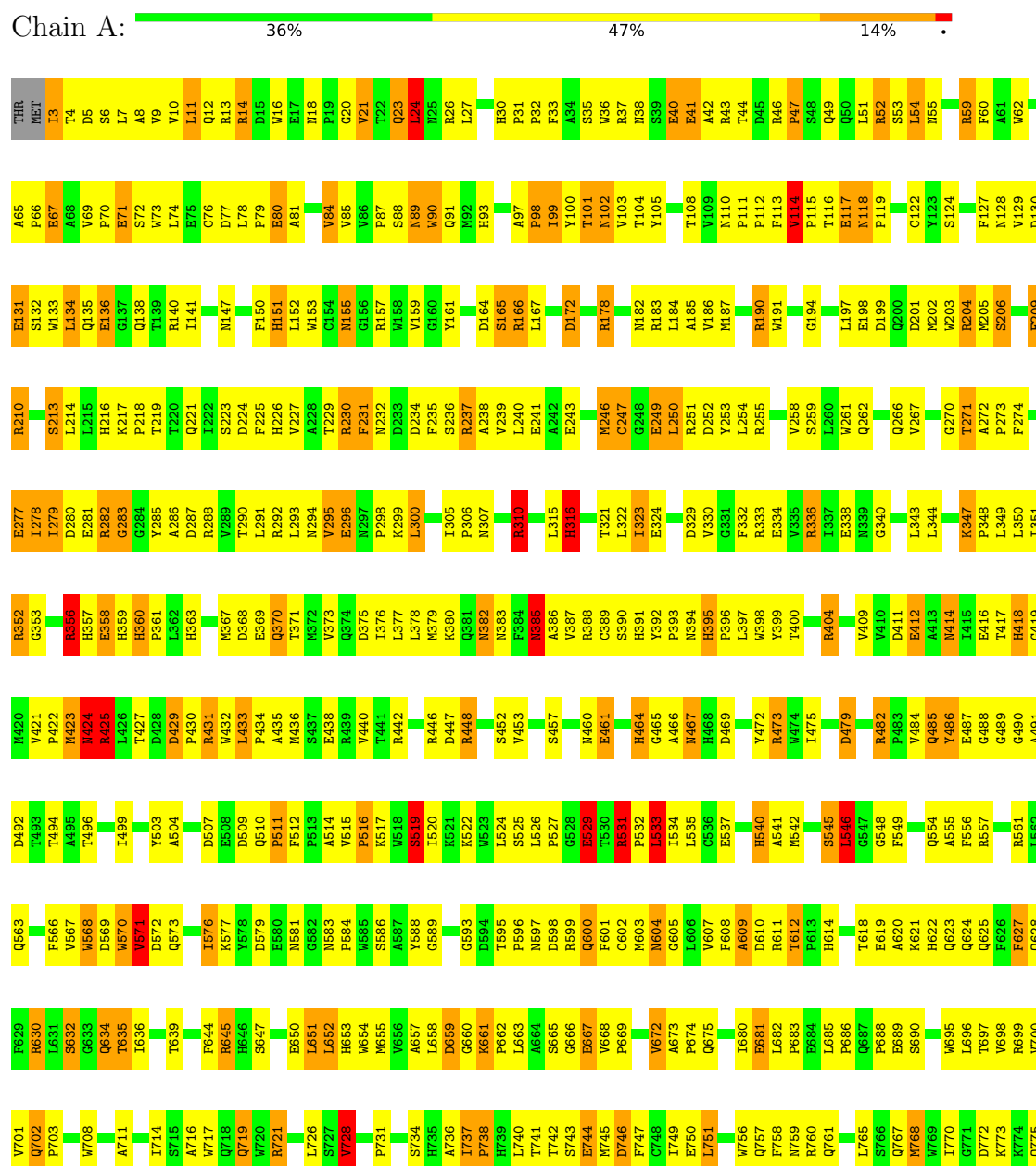
Continued from previous page...

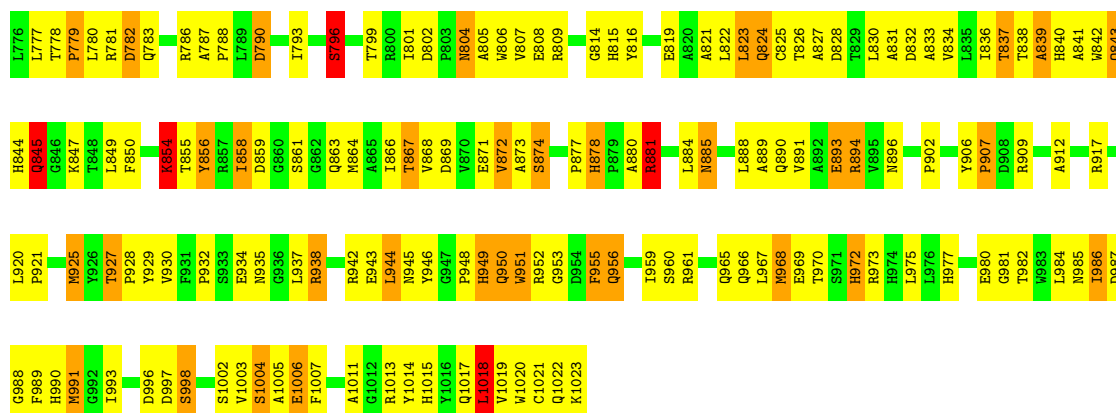
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	97	Total 97	O 97	0	0
3	E	94	Total 94	O 94	0	0
3	F	91	Total 91	O 91	0	0
3	G	95	Total 95	O 95	0	0
3	H	92	Total 92	O 92	0	0
3	I	90	Total 90	O 90	0	0
3	J	97	Total 97	O 97	0	0
3	K	87	Total 87	O 87	0	0
3	L	84	Total 84	O 84	0	0
3	M	79	Total 79	O 79	0	0
3	N	94	Total 94	O 94	0	0
3	O	95	Total 95	O 95	0	0
3	P	85	Total 85	O 85	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.

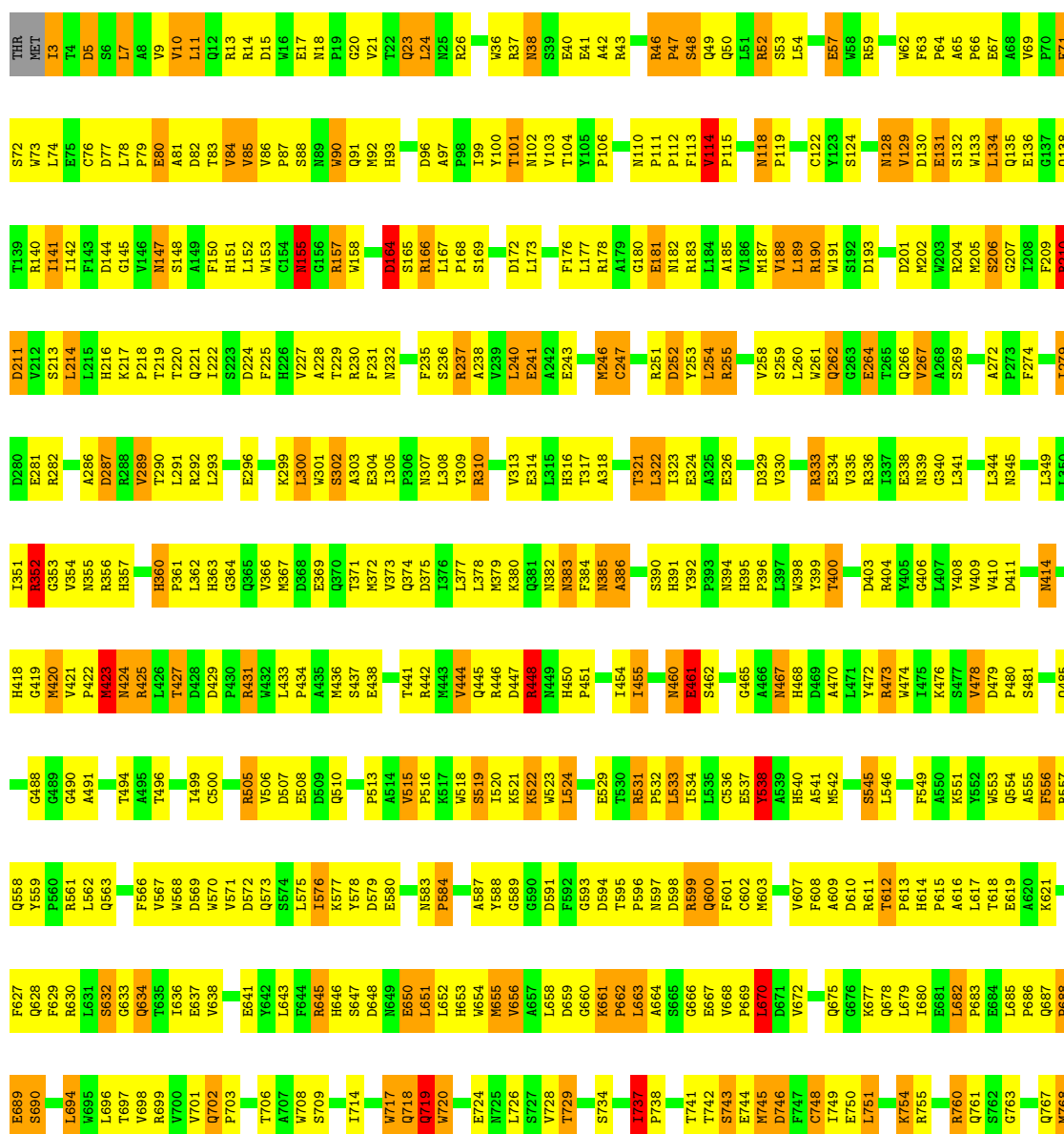
• Molecule 1: BETA-GALACTOSIDASE

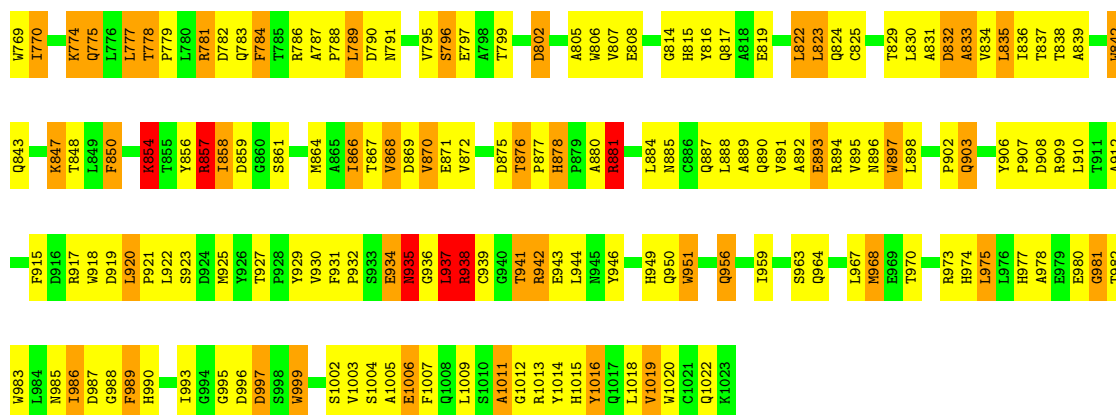




• Molecule 1: BETA-GALACTOSIDASE

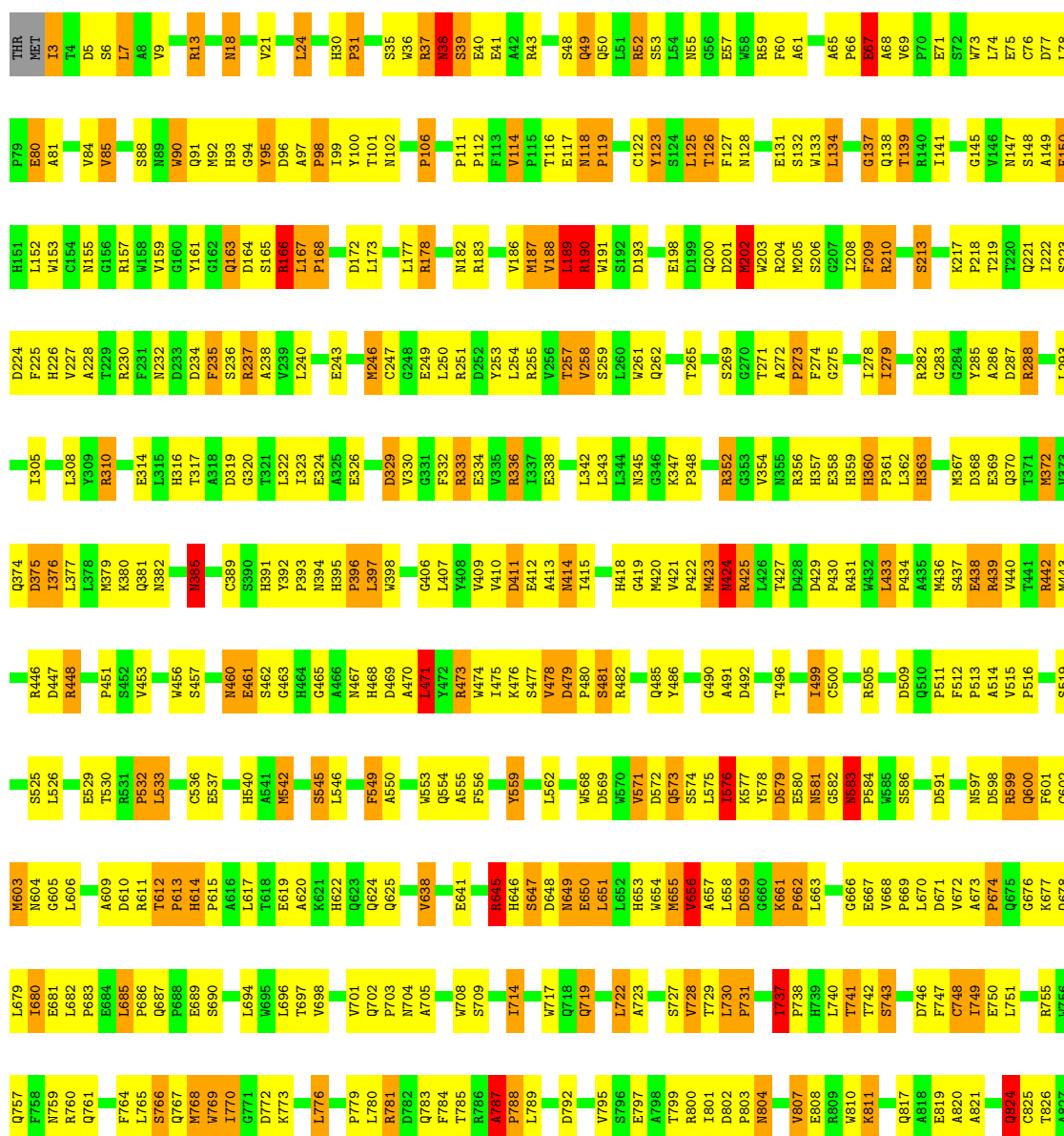
Chain B: 36% 47% 15% .



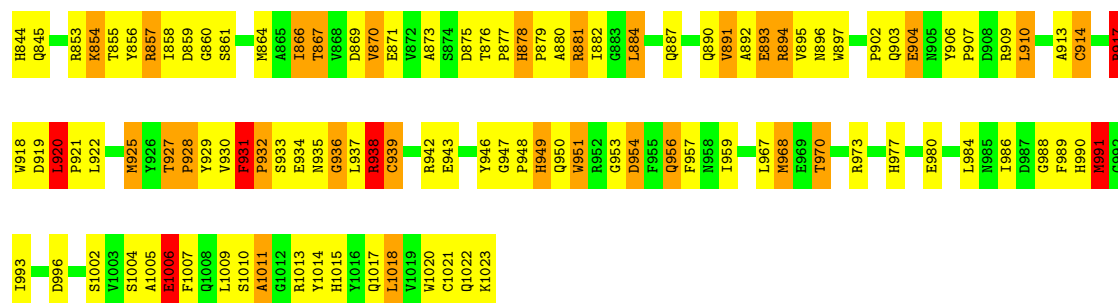


• Molecule 1: BETA-GALACTOSIDASE

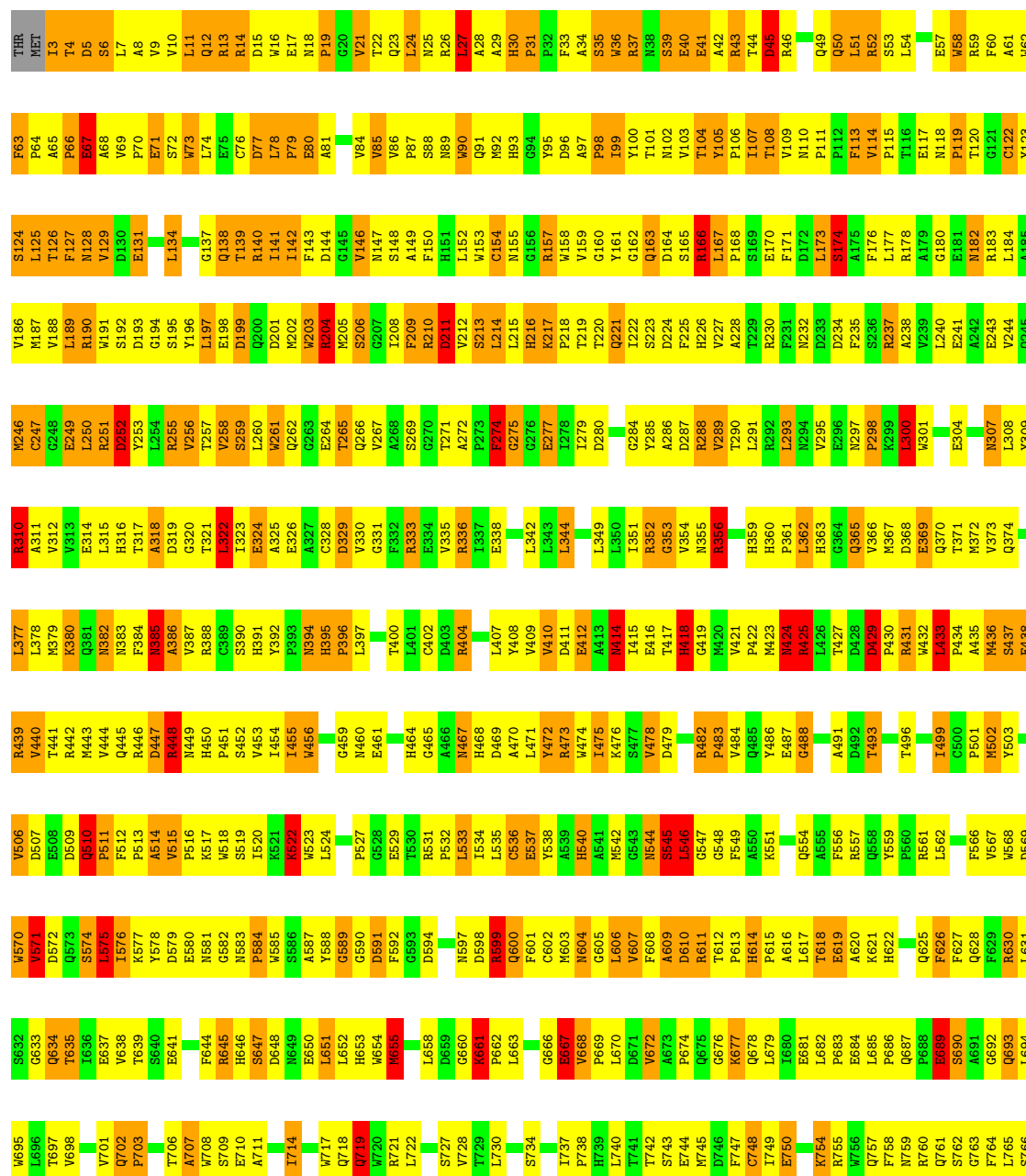
Chain C: 42% 42% 14% •

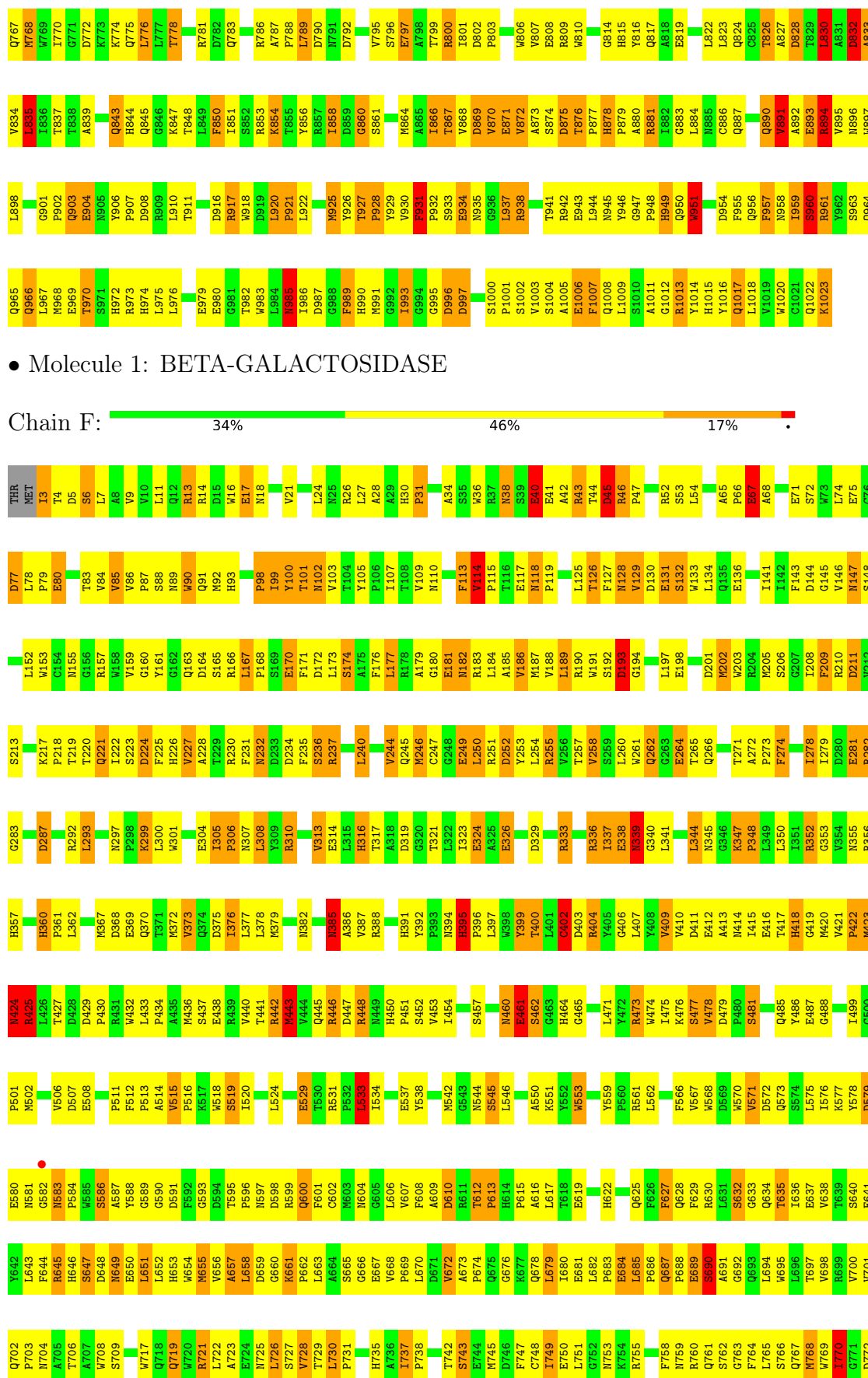


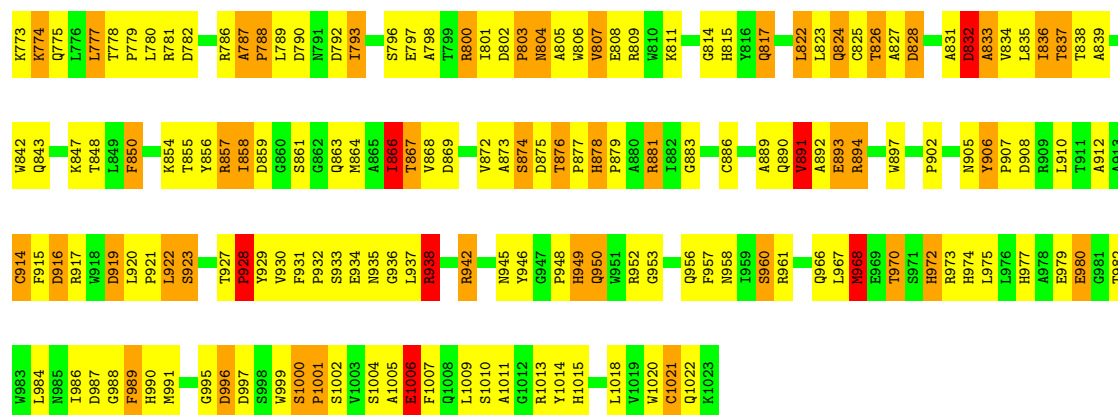




• Molecule 1: BETA-GALACTOSIDASE

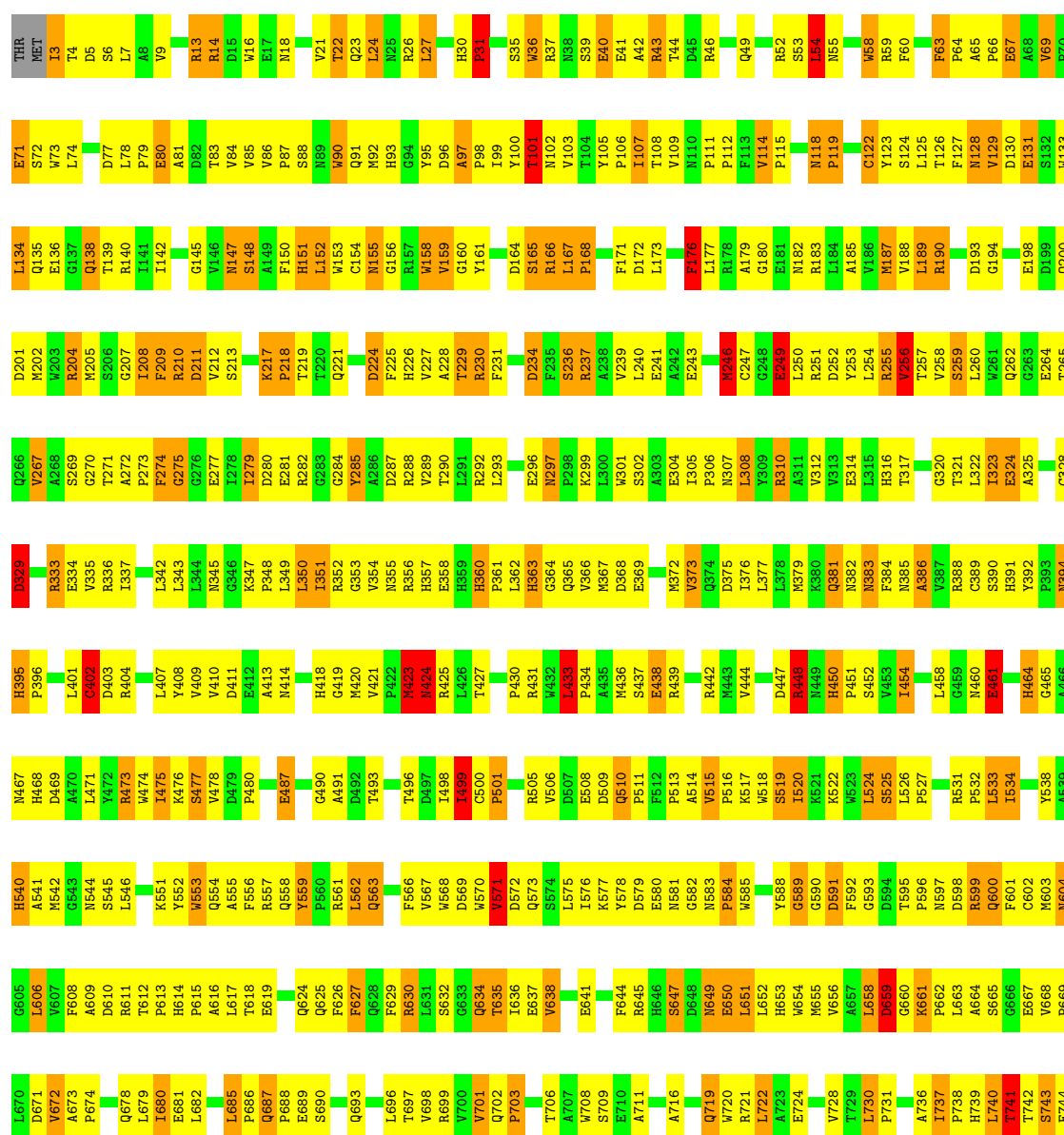


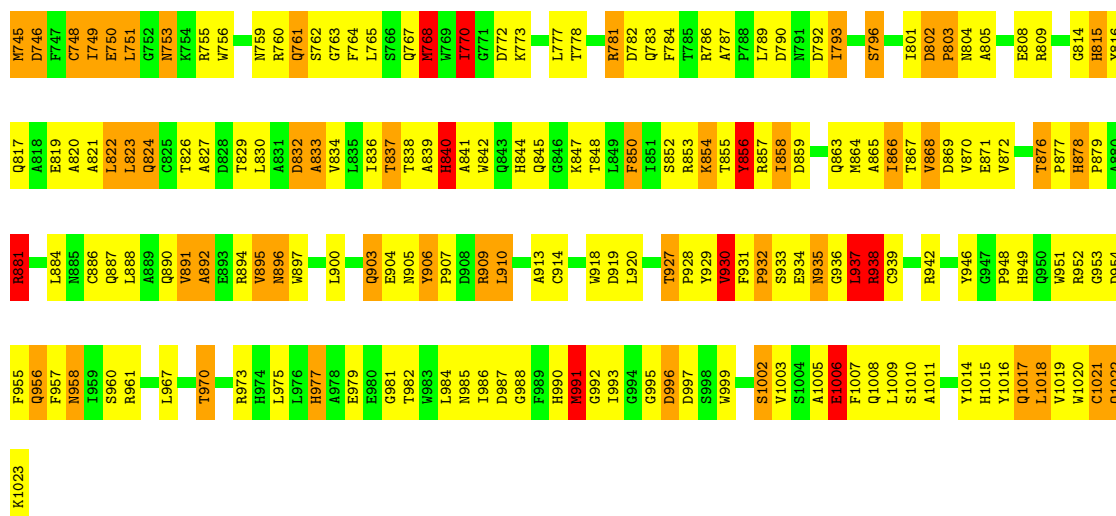




• Molecule 1: BETA-GALACTOSIDASE

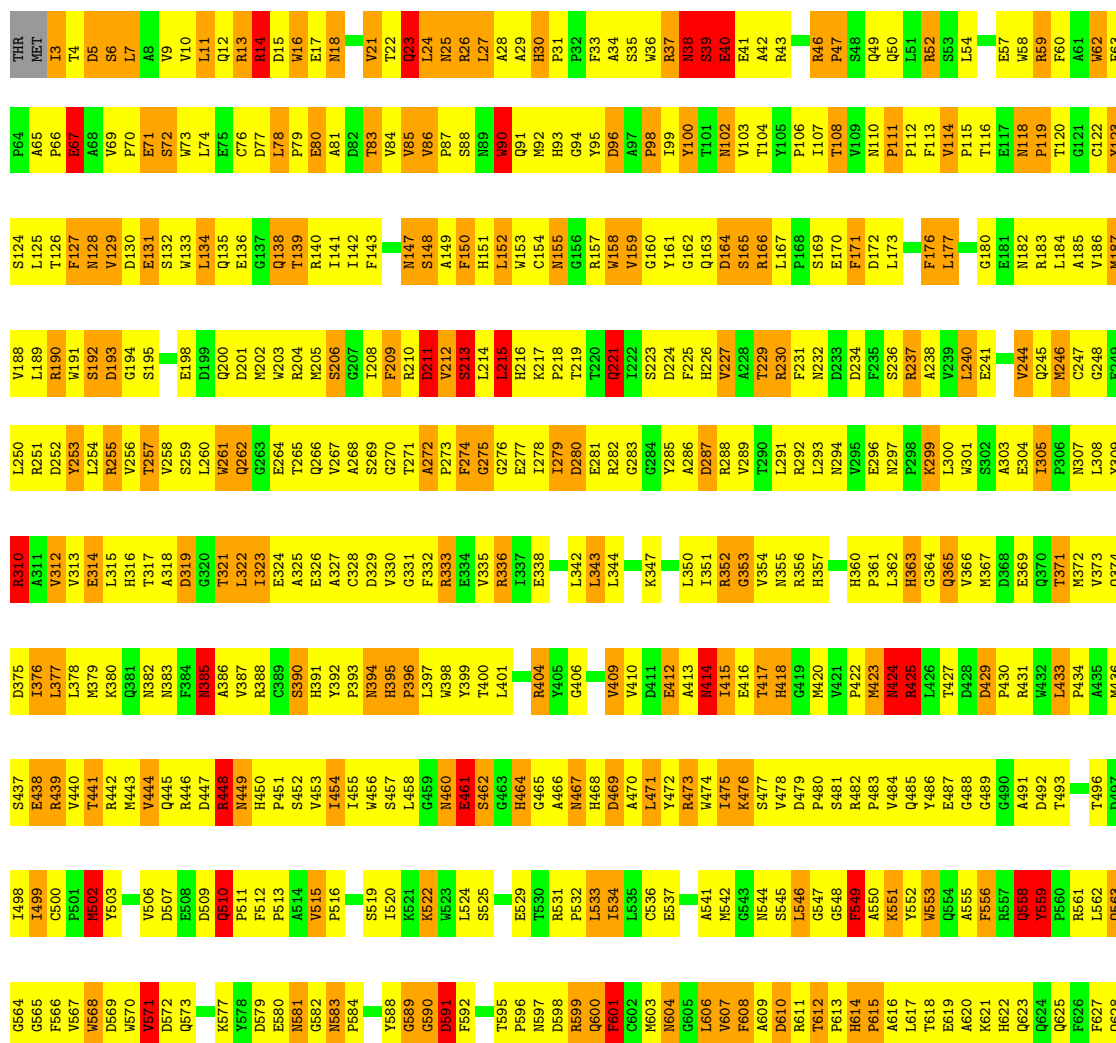
Chain G: 32% 48% 17% .

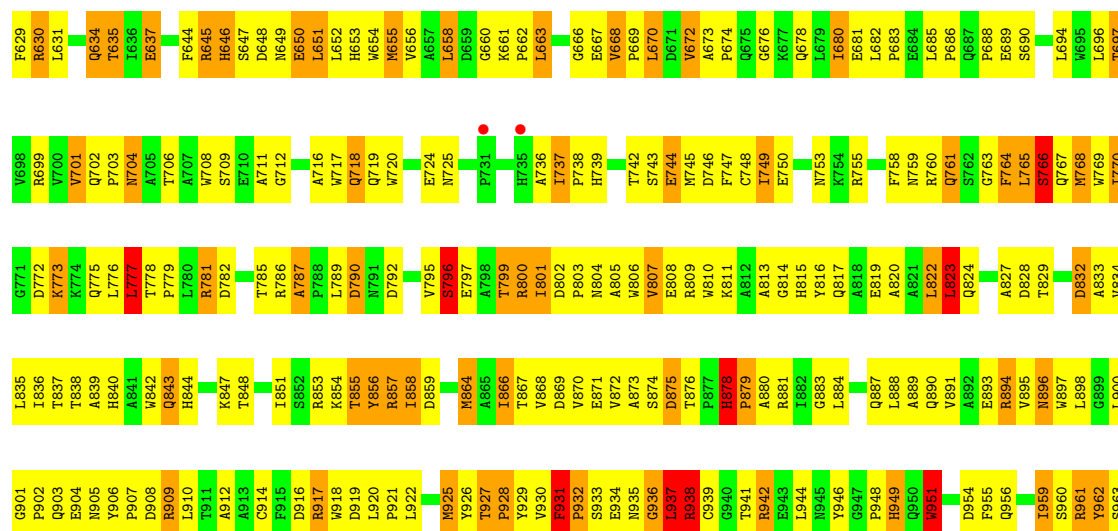




Molecule 1: BETA-GALACTOSIDASE

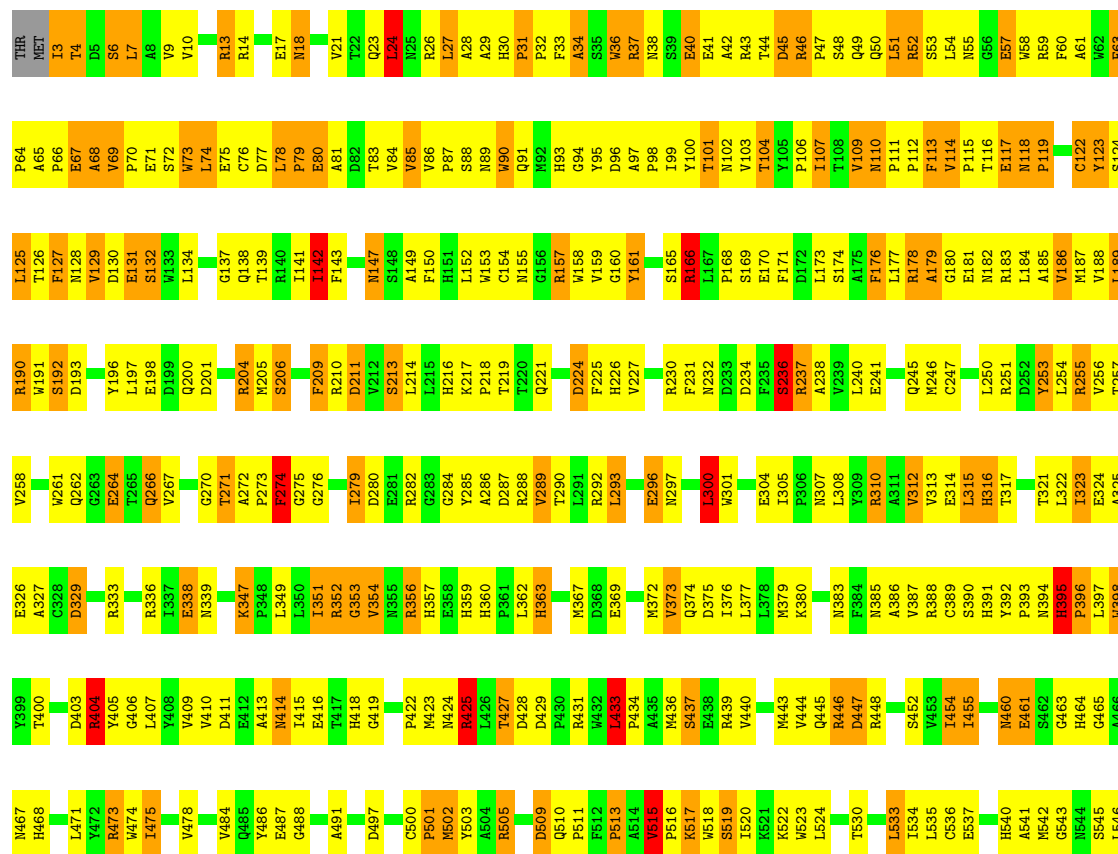
Chain H: 23% 51% 22% .

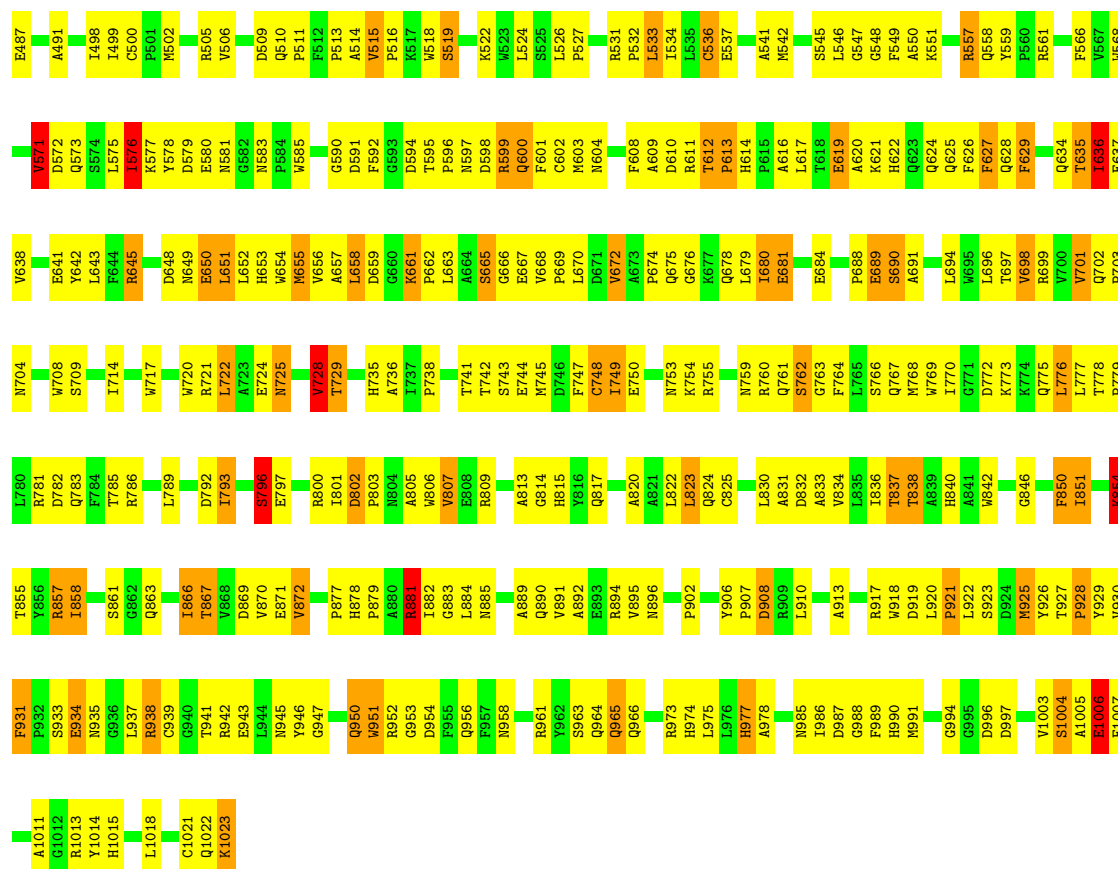




• Molecule 1: BETA-GALACTOSIDASE

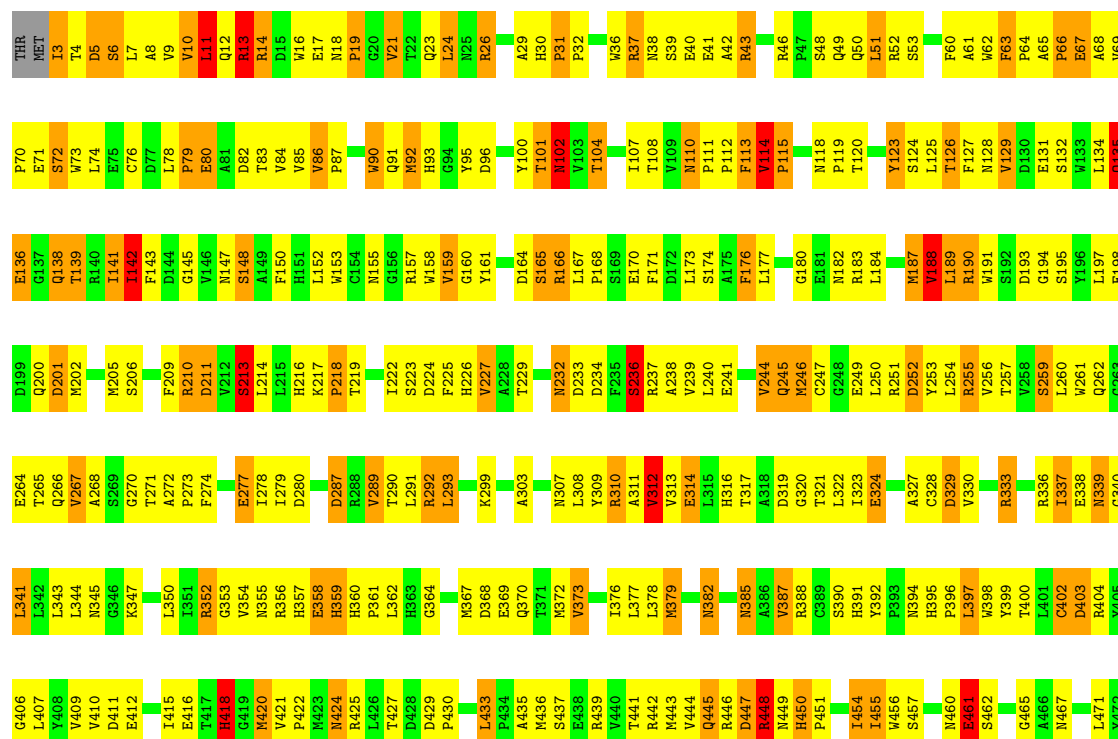
Chain I: 33% 46% 19%

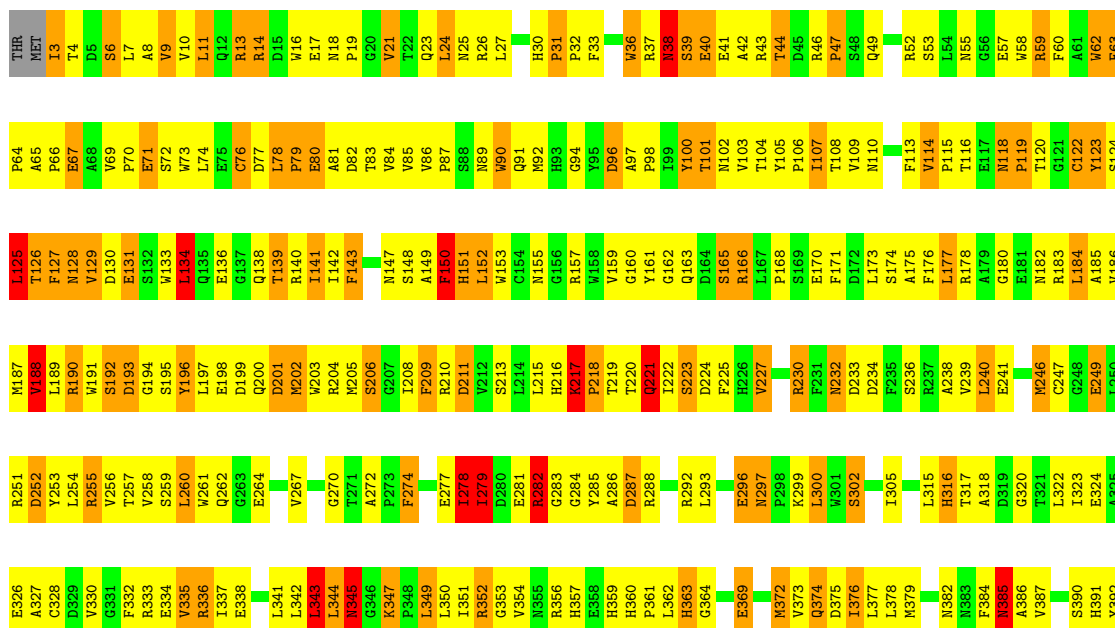




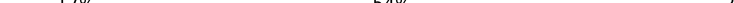
● Molecule 1: BETA-GALACTOSIDASE

Chain K: 30% 49% 19%







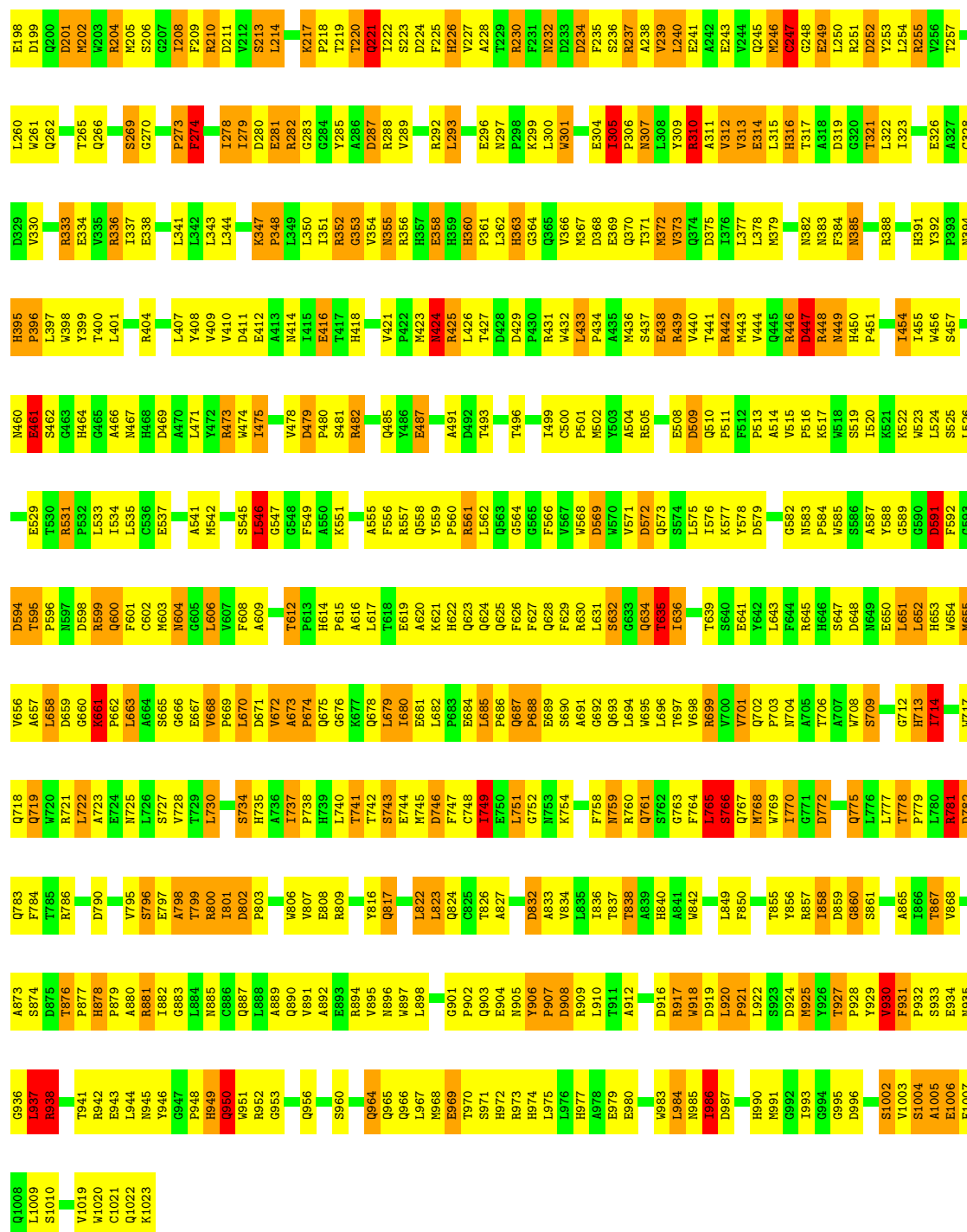
Chain M:  17% 54% 25% .





Chain N: 31% 47% 19% .

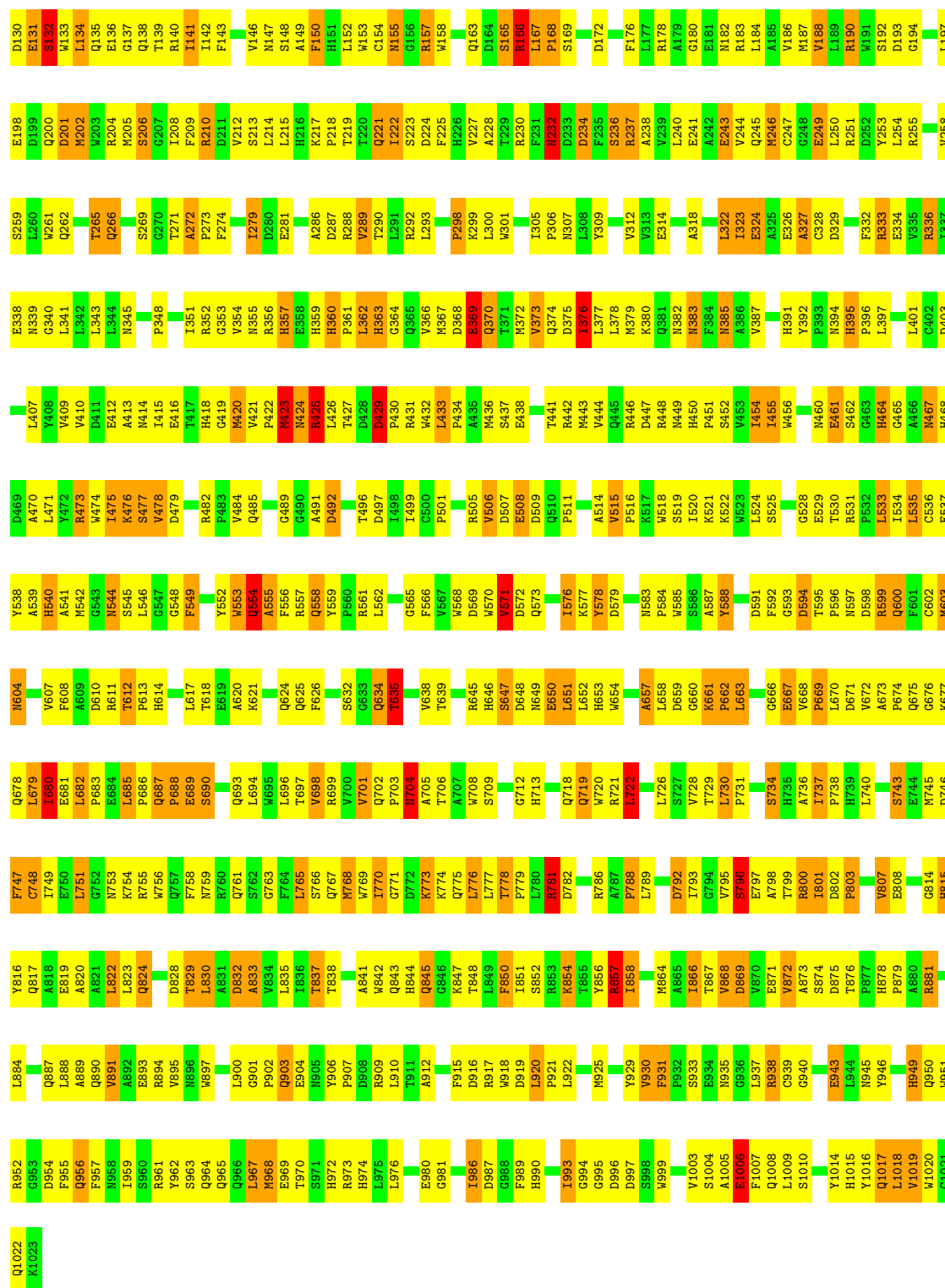




• Molecule 1: BETA-GALACTOSIDASE

Chain O:





● Molecule 1: BETA-GALACTOSIDASE

Chain P: 18% 50% 27% 5%

THR	MEI	I3	T4	D5	S6	L7	A8	V9	L10	L11	Q12	R13	R14	D15	V16	E17	N18	P19	G20	H21	T22	Q23	L24	N25	R26	L27	A28	A29	H30	P31	P32	F33	A34	H35	G36	G37	R38	S39	E40	E41	A42	R43	T44	D45	R46	P47	S48	Q49	Q50	L51	R52	S53	L54	N55	G56	E57	W58	R59	P60
-----	-----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



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)	8.00 – 2.50 8.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.50) 69.8 (8.00-2.50)	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 5D, TNT V. 5-D	Depositor
R, R_{free}	0.174 , (Not available) 0.168 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	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)	0.34 , 110.1	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	0.95	EDS
Total number of atoms	132654	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: 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	18/8440 (0.2%)	1.80	145/11516 (1.3%)
1	B	1.47	24/8440 (0.3%)	1.76	133/11516 (1.2%)
1	C	1.51	46/8440 (0.5%)	1.76	135/11516 (1.2%)
1	D	1.46	26/8440 (0.3%)	1.78	154/11516 (1.3%)
1	E	1.46	26/8440 (0.3%)	1.84	178/11516 (1.5%)
1	F	1.51	26/8440 (0.3%)	1.82	170/11516 (1.5%)
1	G	1.46	24/8440 (0.3%)	1.79	158/11516 (1.4%)
1	H	1.45	30/8440 (0.4%)	1.84	178/11516 (1.5%)
1	I	1.42	20/8440 (0.2%)	1.81	153/11516 (1.3%)
1	J	1.41	18/8440 (0.2%)	1.74	116/11516 (1.0%)
1	K	1.34	14/8440 (0.2%)	1.71	123/11516 (1.1%)
1	L	1.39	18/8440 (0.2%)	1.83	191/11516 (1.7%)
1	M	1.44	24/8440 (0.3%)	1.87	177/11516 (1.5%)
1	N	1.42	27/8440 (0.3%)	1.76	137/11516 (1.2%)
1	O	1.35	11/8440 (0.1%)	1.74	120/11516 (1.0%)
1	P	1.46	29/8440 (0.3%)	1.91	226/11516 (2.0%)
All	All	1.44	381/135040 (0.3%)	1.80	2494/184256 (1.4%)

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	1	0
1	B	1	0
1	D	2	1
1	E	1	0
1	F	2	0
1	G	2	0
1	H	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	1	0
1	J	1	0
1	L	1	0
1	M	2	0
1	P	2	0
All	All	17	1

The worst 5 of 381 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	480	PRO	N-CA	-10.12	1.40	1.47
1	E	111	PRO	CA-C	10.00	1.57	1.51
1	C	222	ILE	CA-CB	-8.20	1.44	1.54
1	N	479	ASP	C-N	-8.11	1.25	1.34
1	P	330	VAL	C-N	8.08	1.38	1.33

The worst 5 of 2494 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	ARG	CA-C-N	-13.58	110.38	122.47
1	A	352	ARG	C-N-CA	-13.58	110.38	122.47
1	H	363	HIS	CA-CB-CG	-12.89	100.91	113.80
1	C	363	HIS	CA-CB-CG	-11.81	101.98	113.80
1	P	424	ASN	CA-CB-CG	-11.69	100.91	112.60

5 of 17 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	90	TRP	CA
1	B	718	GLN	CA
1	D	95	TYR	CA
1	D	914	CYS	CA
1	E	118	ASN	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	473	ARG	Sidechain

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	8198	0	7796	579	0
1	B	8198	0	7796	586	0
1	C	8198	0	7796	466	0
1	D	8198	0	7796	581	0
1	E	8198	0	7795	937	0
1	F	8198	0	7796	624	0
1	G	8198	0	7796	686	0
1	H	8198	0	7796	930	0
1	I	8198	0	7796	656	0
1	J	8198	0	7795	540	0
1	K	8198	0	7796	818	0
1	L	8198	0	7796	841	0
1	M	8198	0	7796	1121	0
1	N	8198	0	7795	676	0
1	O	8198	0	7796	700	0
1	P	8198	0	7796	1203	0
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	1	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	88	0	0	7	0
3	B	96	0	0	15	0
3	C	91	0	0	9	0
3	D	97	0	0	14	0
3	E	94	0	0	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	91	0	0	9	0
3	G	95	0	0	13	0
3	H	92	0	0	19	0
3	I	90	0	0	16	0
3	J	97	0	0	9	0
3	K	87	0	0	9	0
3	L	84	0	0	12	0
3	M	79	0	0	18	0
3	N	94	0	0	19	0
3	O	95	0	0	12	0
3	P	85	0	0	21	0
All	All	132654	0	124733	11736	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 46.

The worst 5 of 11736 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:A:427:THR:HA	1:A:436:MET:HE1	1.25	1.19
1:E:7:LEU:HD13	1:E:74:LEU:HD11	1.23	1.17
1:D:572:ASP:HB3	1:D:603:MET:HG2	1.25	1.16
1:A:770:ILE:HD11	1:A:1022:GLN:HG2	1.18	1.15
1:M:205:MET:HE3	1:M:365:GLN:HG3	1.28	1.14

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1019/1023 (100%)	909 (89%)	92 (9%)	18 (2%)	6 12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1019/1023 (100%)	914 (90%)	85 (8%)	20 (2%)	6	10
1	C	1019/1023 (100%)	919 (90%)	81 (8%)	19 (2%)	6	11
1	D	1019/1023 (100%)	910 (89%)	98 (10%)	11 (1%)	11	22
1	E	1019/1023 (100%)	842 (83%)	135 (13%)	42 (4%)	2	3
1	F	1019/1023 (100%)	892 (88%)	101 (10%)	26 (3%)	4	7
1	G	1019/1023 (100%)	893 (88%)	101 (10%)	25 (2%)	4	7
1	H	1019/1023 (100%)	845 (83%)	140 (14%)	34 (3%)	3	4
1	I	1019/1023 (100%)	884 (87%)	111 (11%)	24 (2%)	4	8
1	J	1019/1023 (100%)	887 (87%)	118 (12%)	14 (1%)	9	17
1	K	1019/1023 (100%)	855 (84%)	131 (13%)	33 (3%)	3	4
1	L	1019/1023 (100%)	838 (82%)	146 (14%)	35 (3%)	3	4
1	M	1019/1023 (100%)	836 (82%)	127 (12%)	56 (6%)	1	1
1	N	1019/1023 (100%)	875 (86%)	117 (12%)	27 (3%)	4	7
1	O	1019/1023 (100%)	889 (87%)	102 (10%)	28 (3%)	4	6
1	P	1019/1023 (100%)	797 (78%)	164 (16%)	58 (6%)	1	1
All	All	16304/16368 (100%)	13985 (86%)	1849 (11%)	470 (3%)	3	5

5 of 470 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	ASP
1	A	277	GLU
1	A	389	CYS
1	A	541	ALA
1	A	659	ASP

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	873/875 (100%)	716 (82%)	157 (18%)	2	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	873/875 (100%)	700 (80%)	173 (20%)	1	2
1	C	873/875 (100%)	737 (84%)	136 (16%)	2	5
1	D	873/875 (100%)	703 (80%)	170 (20%)	1	2
1	E	873/875 (100%)	669 (77%)	204 (23%)	1	1
1	F	873/875 (100%)	717 (82%)	156 (18%)	2	3
1	G	873/875 (100%)	705 (81%)	168 (19%)	1	2
1	H	873/875 (100%)	671 (77%)	202 (23%)	1	1
1	I	873/875 (100%)	705 (81%)	168 (19%)	1	2
1	J	873/875 (100%)	729 (84%)	144 (16%)	2	4
1	K	873/875 (100%)	696 (80%)	177 (20%)	1	2
1	L	873/875 (100%)	681 (78%)	192 (22%)	1	2
1	M	873/875 (100%)	653 (75%)	220 (25%)	0	1
1	N	873/875 (100%)	696 (80%)	177 (20%)	1	2
1	O	873/875 (100%)	704 (81%)	169 (19%)	1	2
1	P	873/875 (100%)	644 (74%)	229 (26%)	0	1
All	All	13968/14000 (100%)	11126 (80%)	2842 (20%)	1	2

5 of 2842 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	1018	LEU
1	N	134	LEU
1	L	211	ASP
1	K	1006	GLU
1	M	116	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 430 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	383	ASN
1	L	102	ASN
1	P	93	HIS
1	I	624	GLN
1	J	990	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 31 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	1021/1023 (99%)	-1.05	0 100 100	2, 24, 54, 79	0
1	B	1021/1023 (99%)	-1.04	0 100 100	2, 23, 54, 81	0
1	C	1021/1023 (99%)	-1.11	0 100 100	4, 21, 52, 80	0
1	D	1021/1023 (99%)	-1.03	0 100 100	4, 25, 56, 81	0
1	E	1021/1023 (99%)	-0.72	0 100 100	8, 34, 61, 86	0
1	F	1021/1023 (99%)	-1.02	1 (0%) 92 90	2, 23, 55, 78	0
1	G	1021/1023 (99%)	-0.93	0 100 100	3, 27, 58, 82	0
1	H	1021/1023 (99%)	-0.75	2 (0%) 91 89	6, 33, 61, 89	0
1	I	1021/1023 (99%)	-0.90	1 (0%) 92 90	4, 30, 59, 80	0
1	J	1021/1023 (99%)	-0.98	1 (0%) 92 90	8, 28, 56, 85	0
1	K	1021/1023 (99%)	-0.80	1 (0%) 92 90	10, 35, 64, 92	0
1	L	1021/1023 (99%)	-0.76	0 100 100	6, 35, 63, 84	0
1	M	1021/1023 (99%)	-0.53	1 (0%) 92 90	12, 39, 65, 80	0
1	N	1021/1023 (99%)	-0.88	0 100 100	9, 30, 59, 89	0
1	O	1021/1023 (99%)	-0.91	0 100 100	11, 31, 60, 81	0
1	P	1021/1023 (99%)	-0.35	3 (0%) 90 87	14, 43, 69, 89	0
All	All	16336/16368 (99%)	-0.86	10 (0%) 92 90	2, 30, 60, 92	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	180	GLY	3.1
1	P	81	ALA	2.6
1	M	180	GLY	2.5
1	F	582	GLY	2.4
1	I	581	ASN	2.4

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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	E	1102	1/1	0.86	0.05	32,32,32,32	0
2	MG	J	1101	1/1	0.86	0.04	34,34,34,34	0
2	MG	K	1102	1/1	0.89	0.03	25,25,25,25	0
2	MG	P	1101	1/1	0.90	0.05	49,49,49,49	0
2	MG	B	1102	1/1	0.91	0.09	23,23,23,23	0
2	MG	M	1101	1/1	0.91	0.04	56,56,56,56	0
2	MG	J	1102	1/1	0.91	0.07	29,29,29,29	0
2	MG	F	1101	1/1	0.92	0.06	35,35,35,35	0
2	MG	I	1101	1/1	0.94	0.05	33,33,33,33	0
2	MG	L	1101	1/1	0.95	0.07	31,31,31,31	0
2	MG	A	1102	1/1	0.95	0.07	37,37,37,37	0
2	MG	H	1101	1/1	0.95	0.05	27,27,27,27	0
2	MG	L	1102	1/1	0.96	0.06	28,28,28,28	0
2	MG	H	1102	1/1	0.96	0.09	22,22,22,22	0
2	MG	N	1101	1/1	0.96	0.05	32,32,32,32	0
2	MG	C	1102	1/1	0.96	0.04	28,28,28,28	0
2	MG	E	1101	1/1	0.97	0.04	39,39,39,39	0
2	MG	K	1101	1/1	0.97	0.04	34,34,34,34	0
2	MG	I	1102	1/1	0.97	0.03	33,33,33,33	0
2	MG	G	1102	1/1	0.97	0.06	18,18,18,18	0
2	MG	F	1102	1/1	0.98	0.06	26,26,26,26	0
2	MG	G	1101	1/1	0.98	0.07	32,32,32,32	0
2	MG	A	1101	1/1	0.98	0.06	37,37,37,37	0
2	MG	O	1101	1/1	0.98	0.09	40,40,40,40	0
2	MG	O	1102	1/1	0.98	0.05	15,15,15,15	0
2	MG	C	1101	1/1	0.98	0.04	23,23,23,23	0
2	MG	P	1102	1/1	0.98	0.07	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	1101	1/1	0.99	0.05	25,25,25,25	0
2	MG	D	1101	1/1	0.99	0.04	28,28,28,28	0
2	MG	D	1102	1/1	0.99	0.11	42,42,42,42	0
2	MG	N	1102	1/1	0.99	0.06	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.