



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 07:21 am BST

PDB ID : 4V40
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

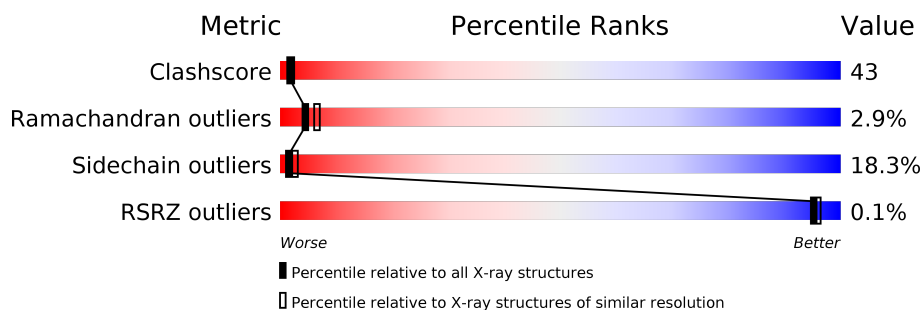
1 Overall quality at a glance

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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1023	<div> <div style="width: 39%; background-color: green;"></div> <div style="width: 45%; background-color: yellow;"></div> <div style="width: 14%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> </div> <div>39% 45% 14% .</div>
1	B	1023	<div> <div style="width: 38%; background-color: green;"></div> <div style="width: 43%; background-color: yellow;"></div> <div style="width: 16%; background-color: orange;"></div> <div style="width: 3%; background-color: red;"></div> </div> <div>38% 43% 16% .</div>
1	C	1023	<div> <div style="width: 44%; background-color: green;"></div> <div style="width: 41%; background-color: yellow;"></div> <div style="width: 12%; background-color: orange;"></div> <div style="width: 3%; background-color: red;"></div> </div> <div>44% 41% 12% .</div>
1	D	1023	<div> <div style="width: 38%; background-color: green;"></div> <div style="width: 46%; background-color: yellow;"></div> <div style="width: 14%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> </div> <div>38% 46% 14% .</div>
1	E	1023	<div> <div style="width: 26%; background-color: green;"></div> <div style="width: 49%; background-color: yellow;"></div> <div style="width: 21%; background-color: orange;"></div> <div style="width: 4%; background-color: red;"></div> </div> <div>26% 49% 21% .</div>
1	F	1023	<div> <div style="width: 37%; background-color: green;"></div> <div style="width: 46%; background-color: yellow;"></div> <div style="width: 13%; background-color: orange;"></div> <div style="width: 4%; background-color: red;"></div> </div> <div>37% 46% 13% .</div>
1	G	1023	<div> <div style="width: 35%; background-color: green;"></div> <div style="width: 44%; background-color: yellow;"></div> <div style="width: 18%; background-color: orange;"></div> <div style="width: 3%; background-color: red;"></div> </div> <div>35% 44% 18% .</div>

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Mol	Chain	Length	Quality of chain
1	H	1023	 26% 50% 20% .
1	I	1023	 33% 49% 15% .
1	J	1023	 39% 46% 13% .
1	K	1023	 30% 50% 16% .
1	L	1023	 29% 49% 19% .
1	M	1023	 19% 54% 23% .
1	N	1023	 34% 46% 17% .
1	O	1023	 32% 49% 16% .
1	P	1023	 19% 52% 25% .

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 (three-letter code: MG) (formula: Mg).

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

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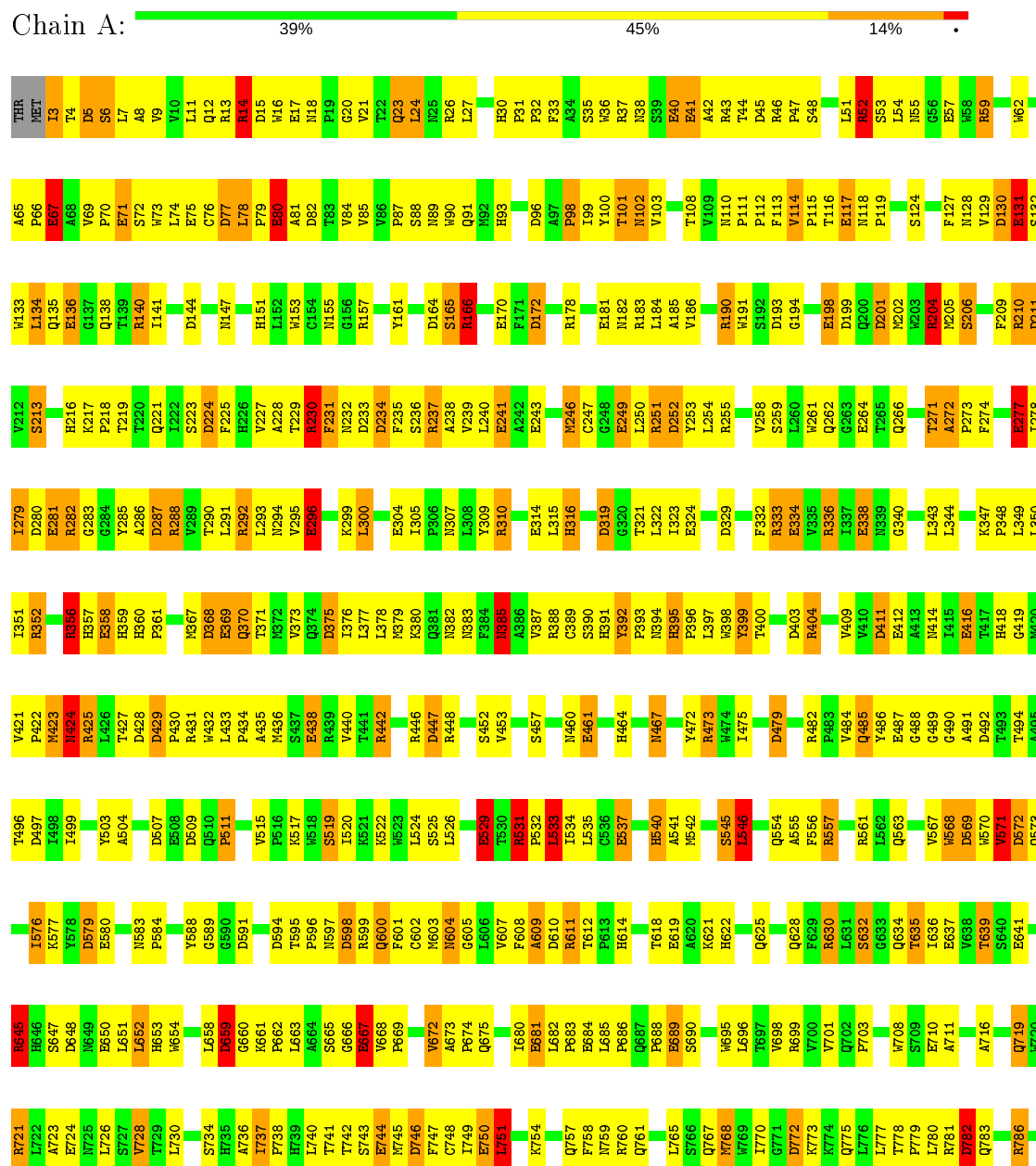
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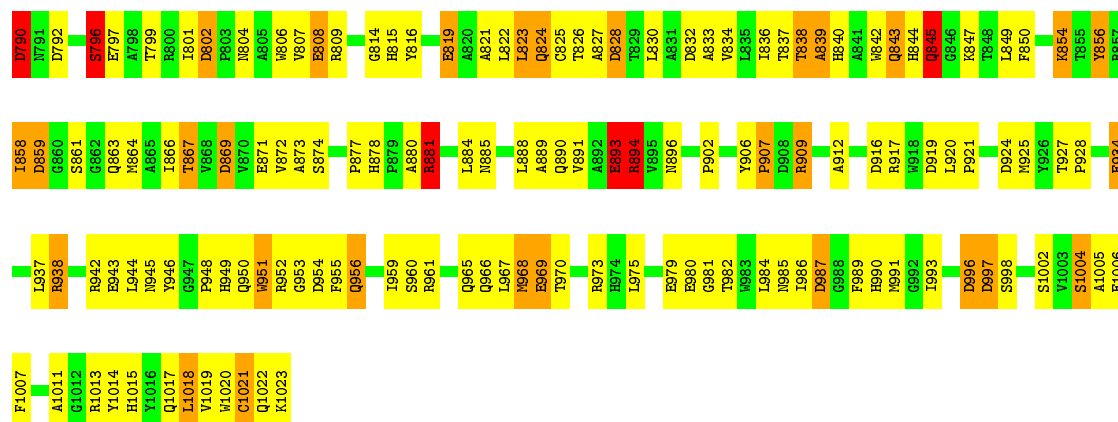
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	97	Total 97	O 97	0	0
3	E	94	Total 94	O 94	0	0
3	F	91	Total 91	O 91	0	0
3	G	95	Total 95	O 95	0	0
3	H	92	Total 92	O 92	0	0
3	I	90	Total 90	O 90	0	0
3	J	97	Total 97	O 97	0	0
3	K	87	Total 87	O 87	0	0
3	L	84	Total 84	O 84	0	0
3	M	79	Total 79	O 79	0	0
3	N	94	Total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

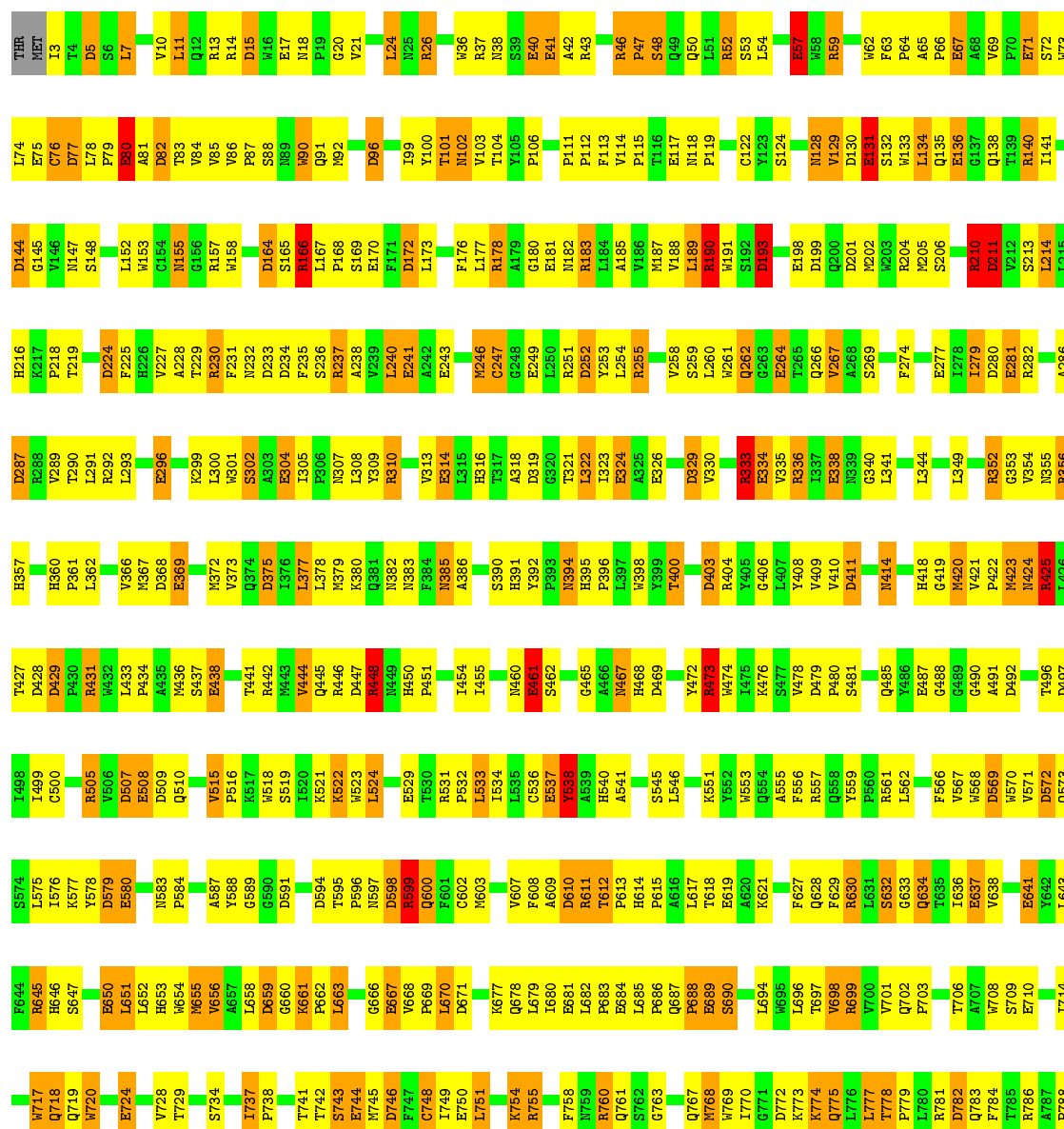
• Molecule 1: BETA-GALACTOSIDASE

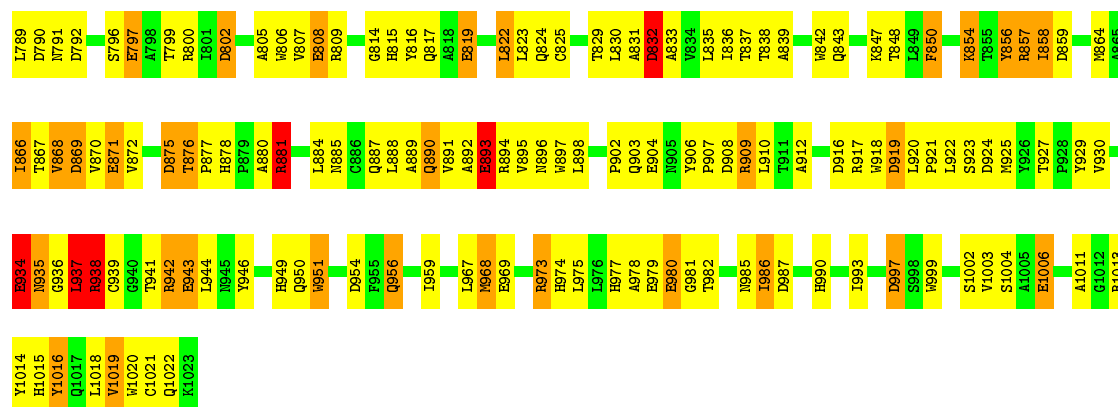




• Molecule 1: BETA-GALACTOSIDASE

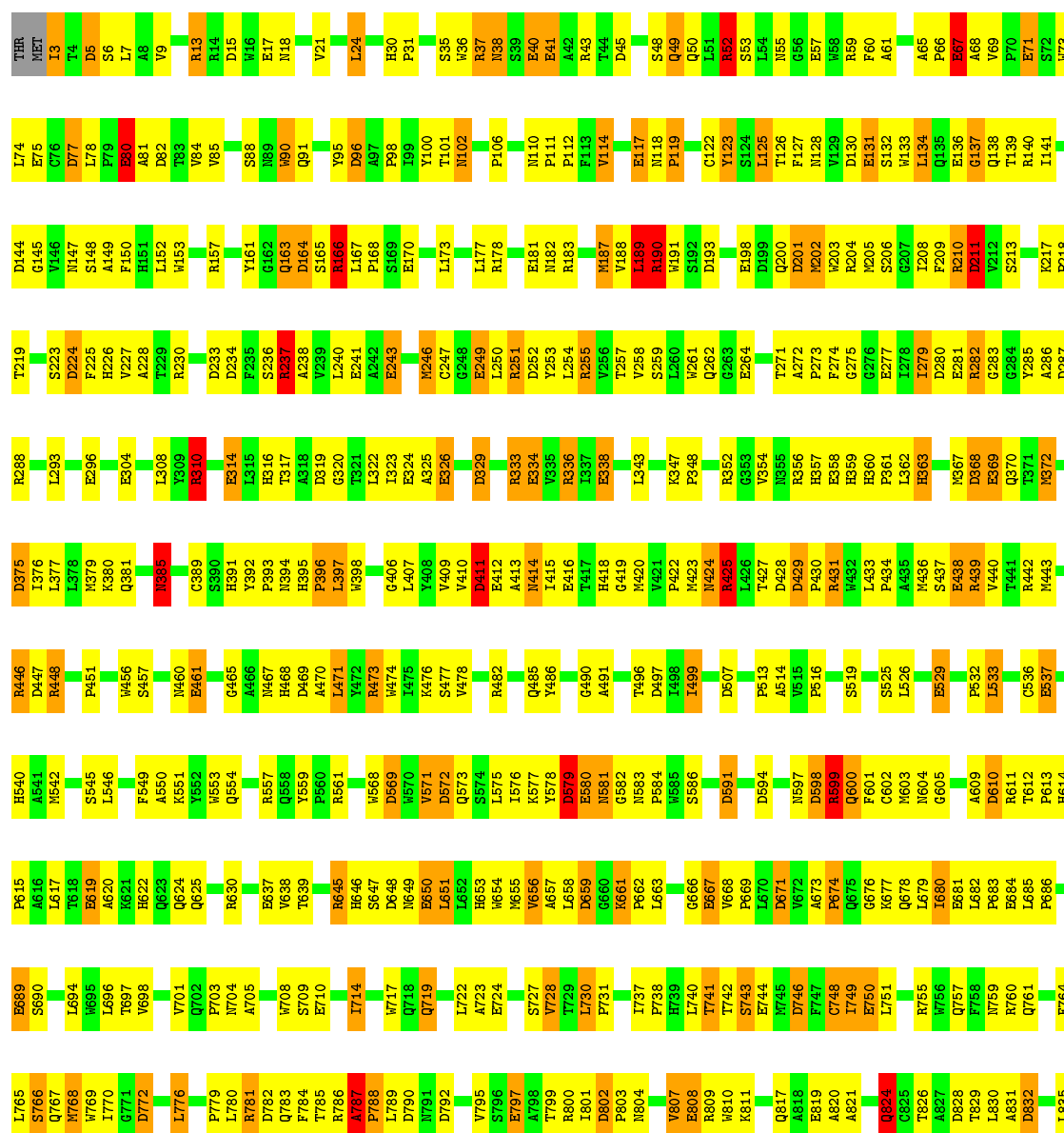
Chain B: 38% 43% 16%

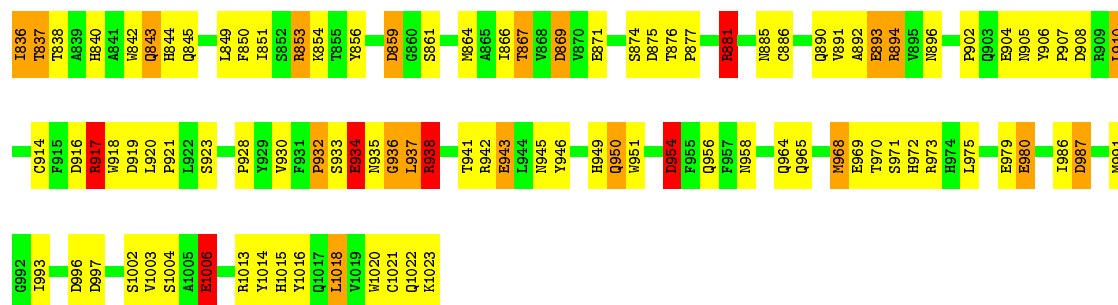




• Molecule 1: BETA-GALACTOSIDASE

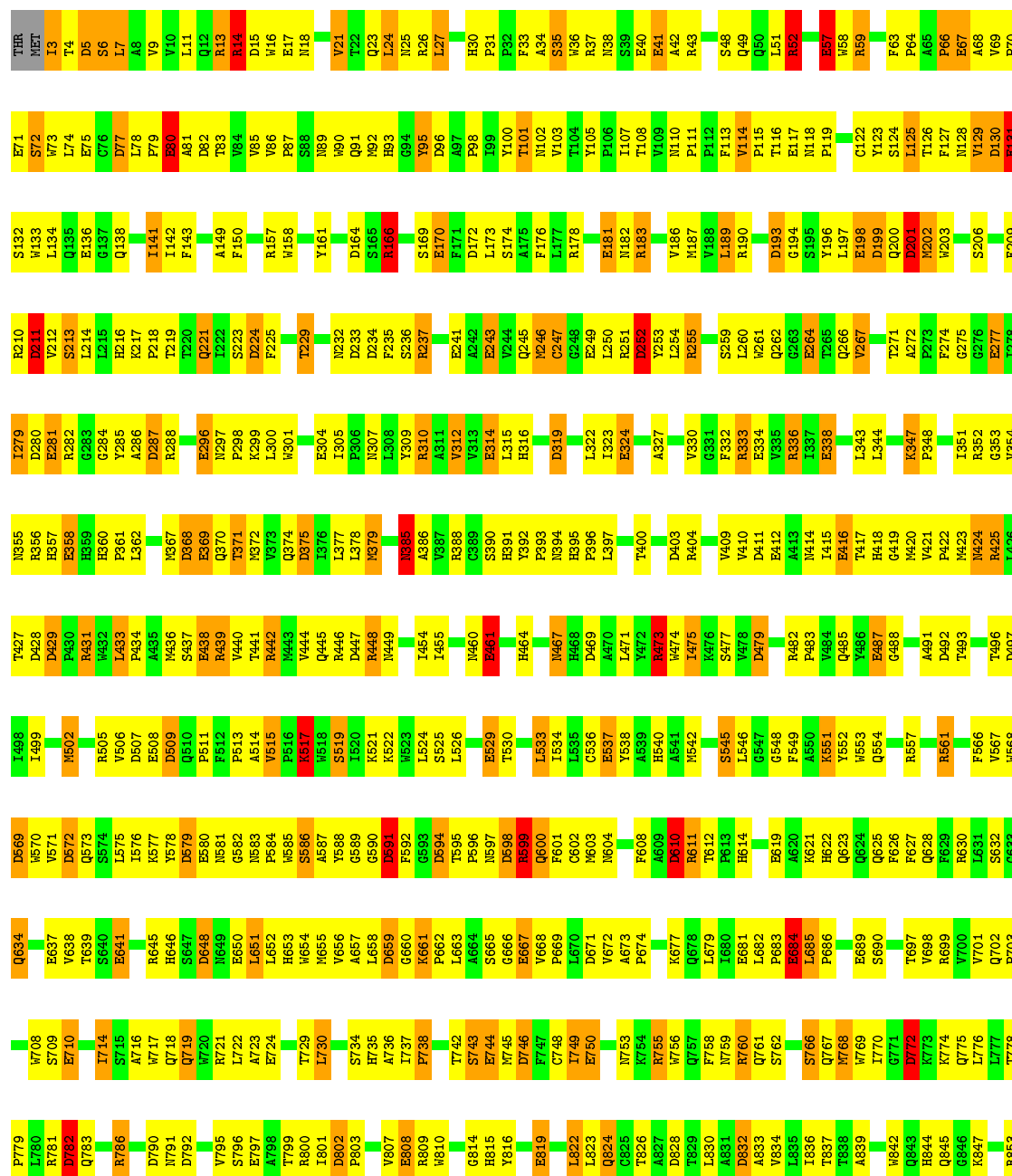
Chain C: 44% 41% 12% .



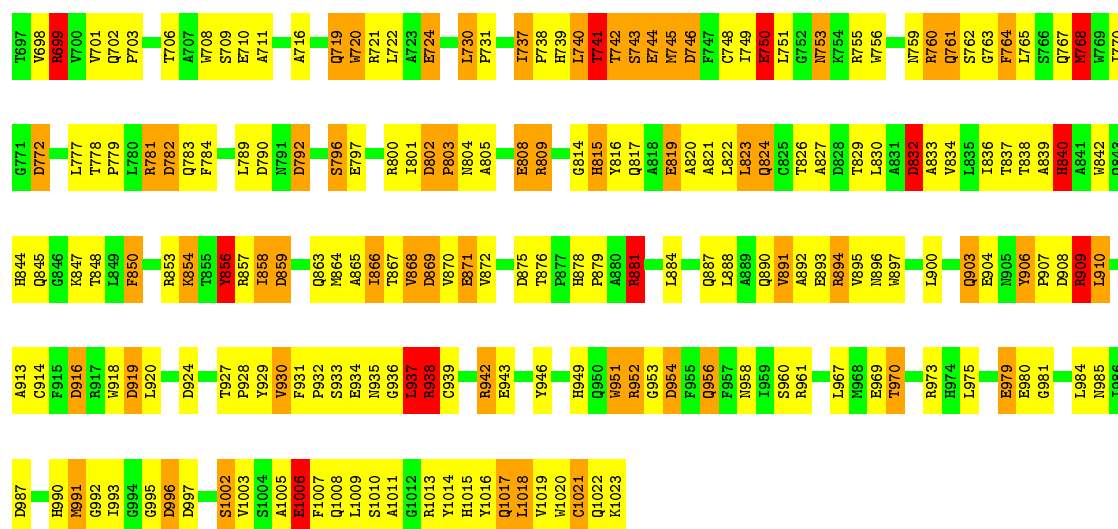


• Molecule 1: BETA-GALACTOSIDASE

Chain D:

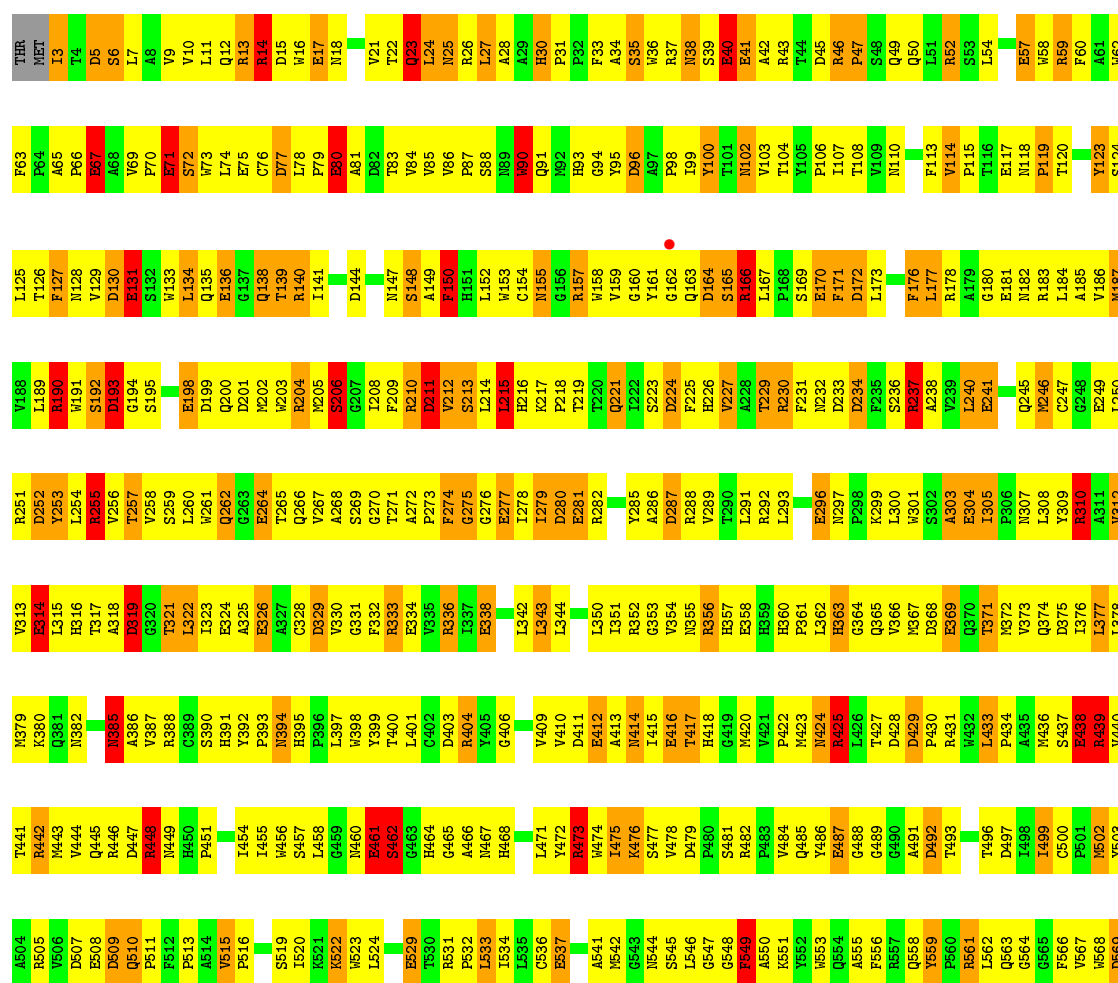


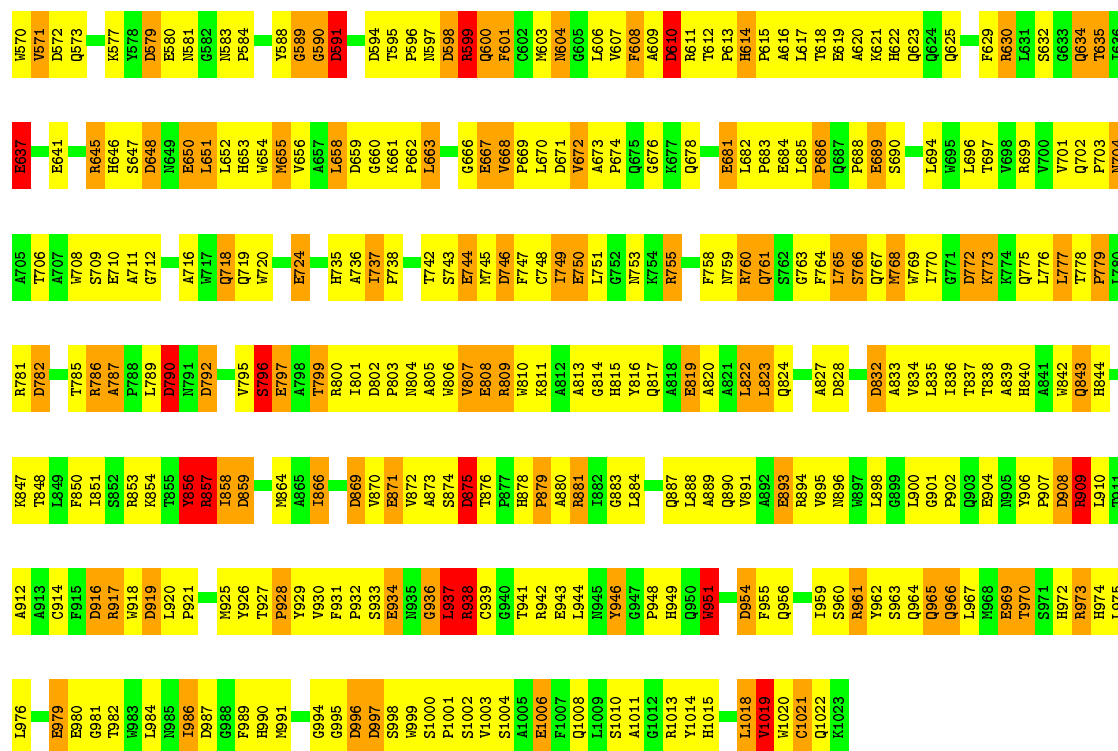




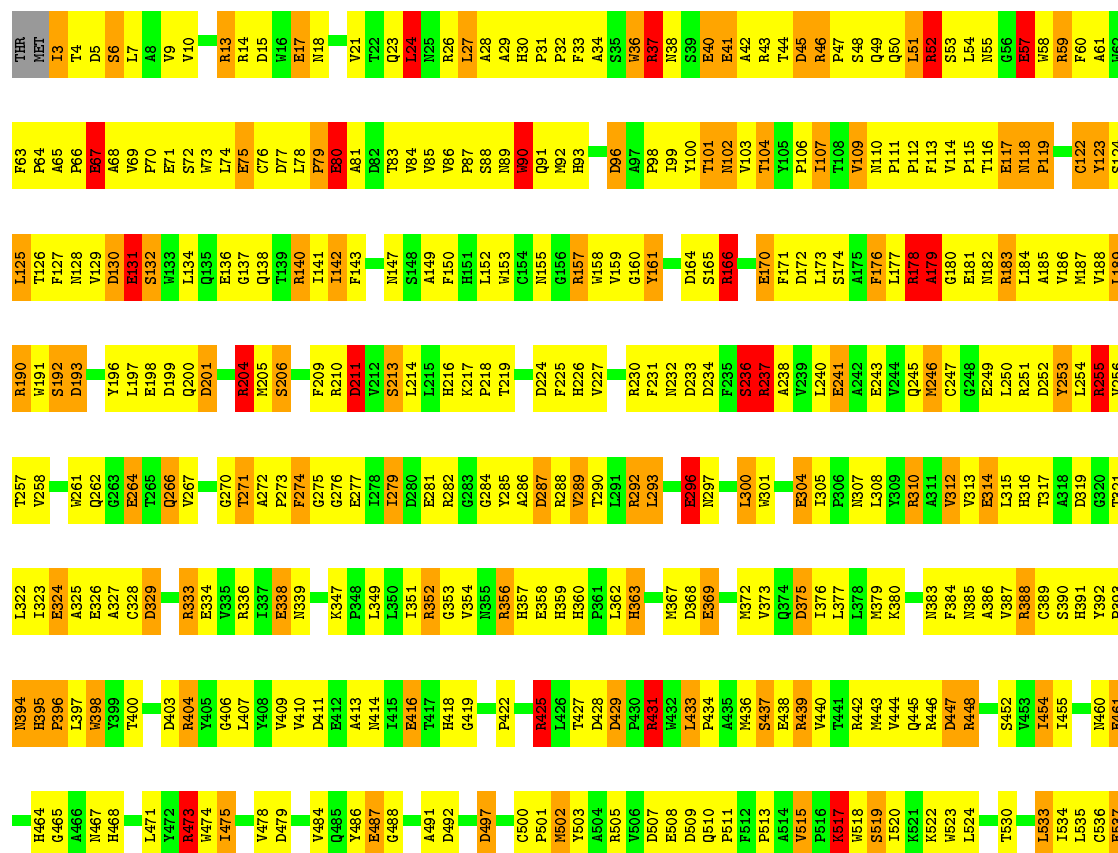
• Molecule 1: BETA-GALACTOSIDASE

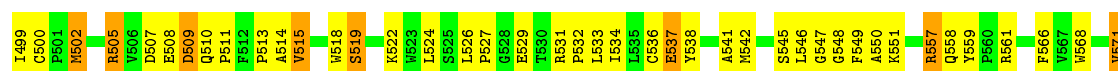
Chain H: 26% 50% 20%





Chain I: 33% 49% 15%

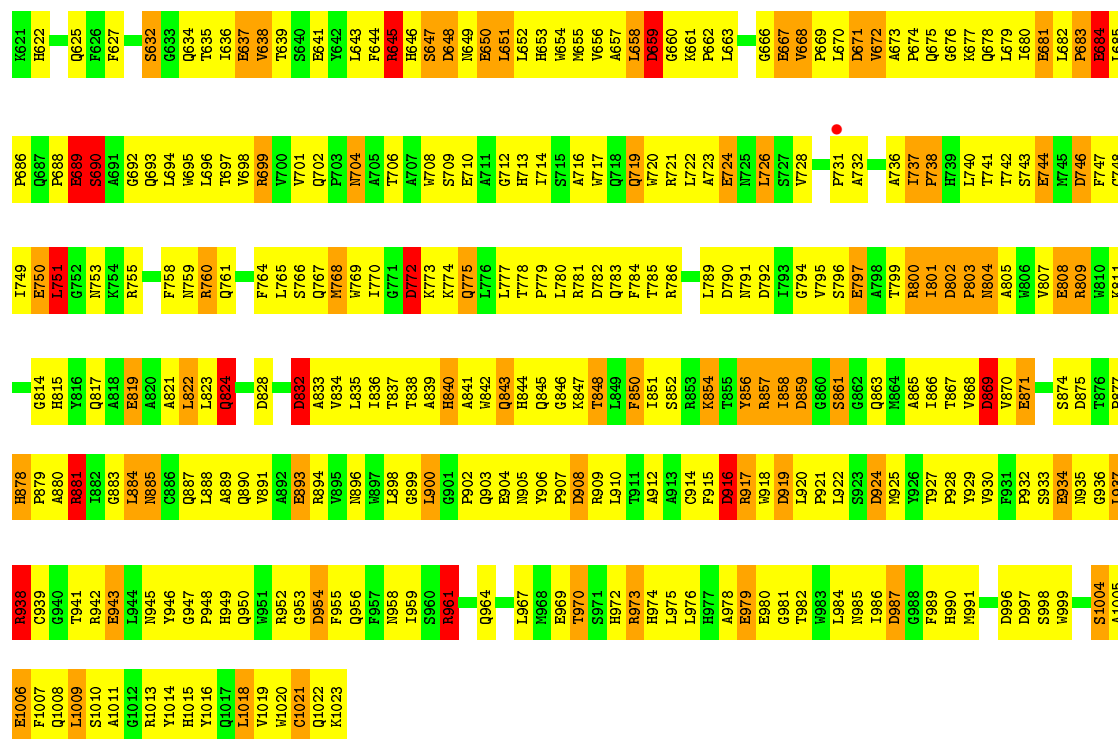




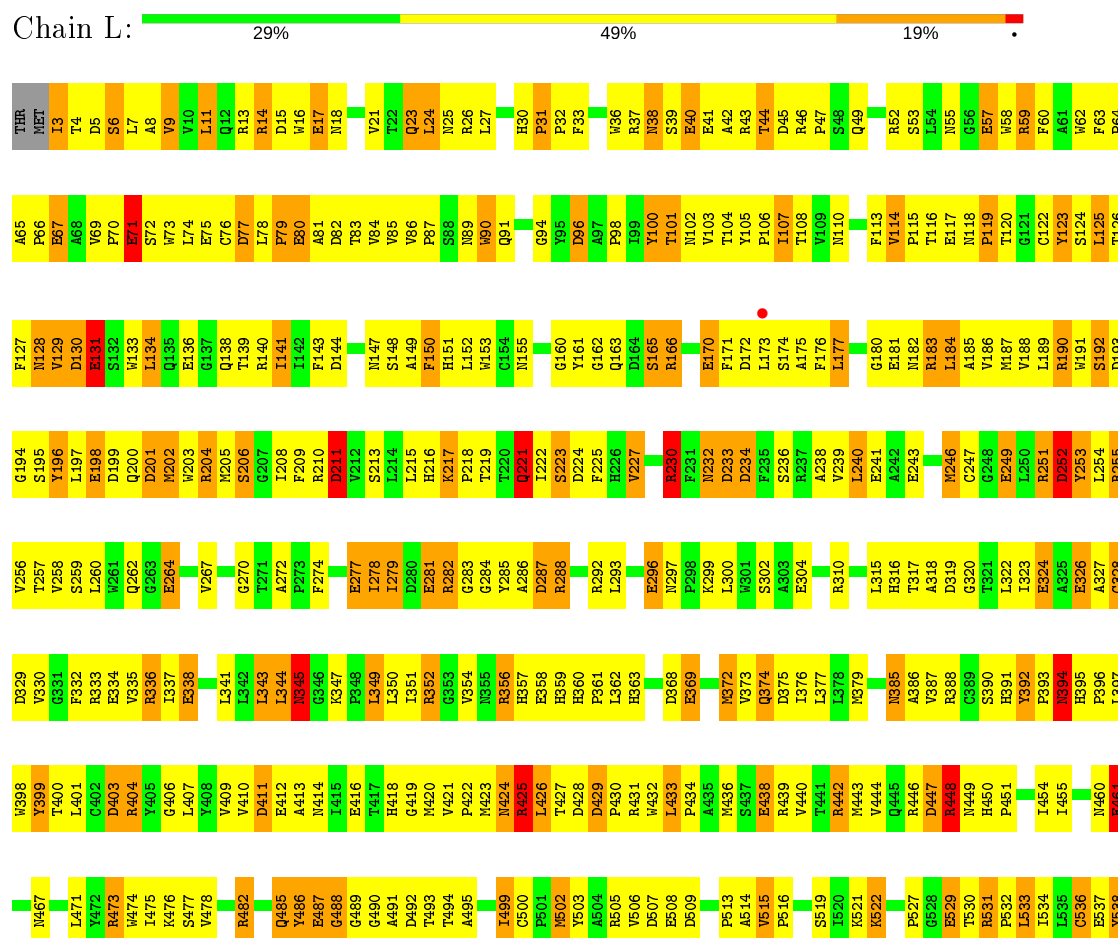


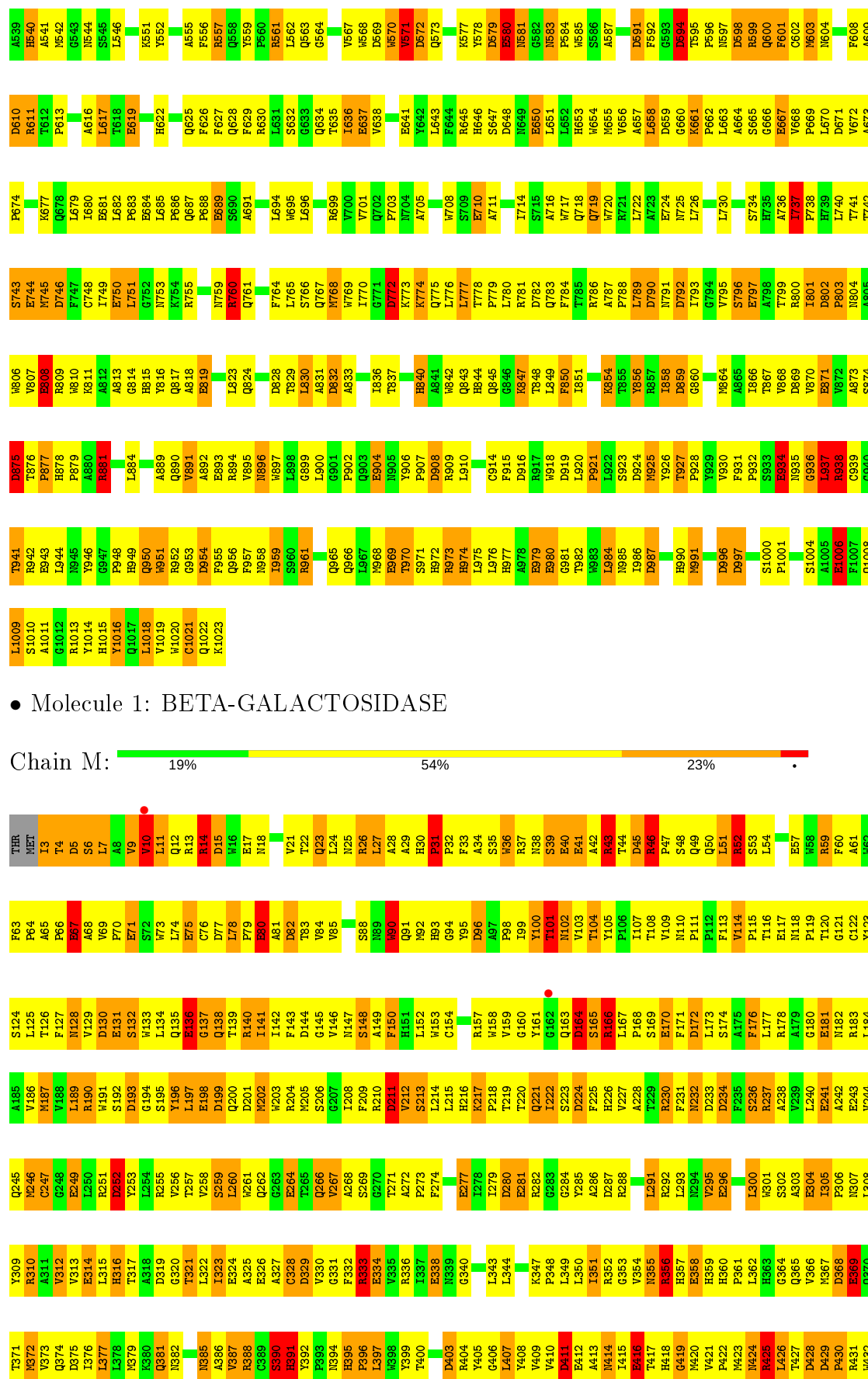
Category	Percentage
Very bad	30%
Bad	50%
Average	16%
Good	4%

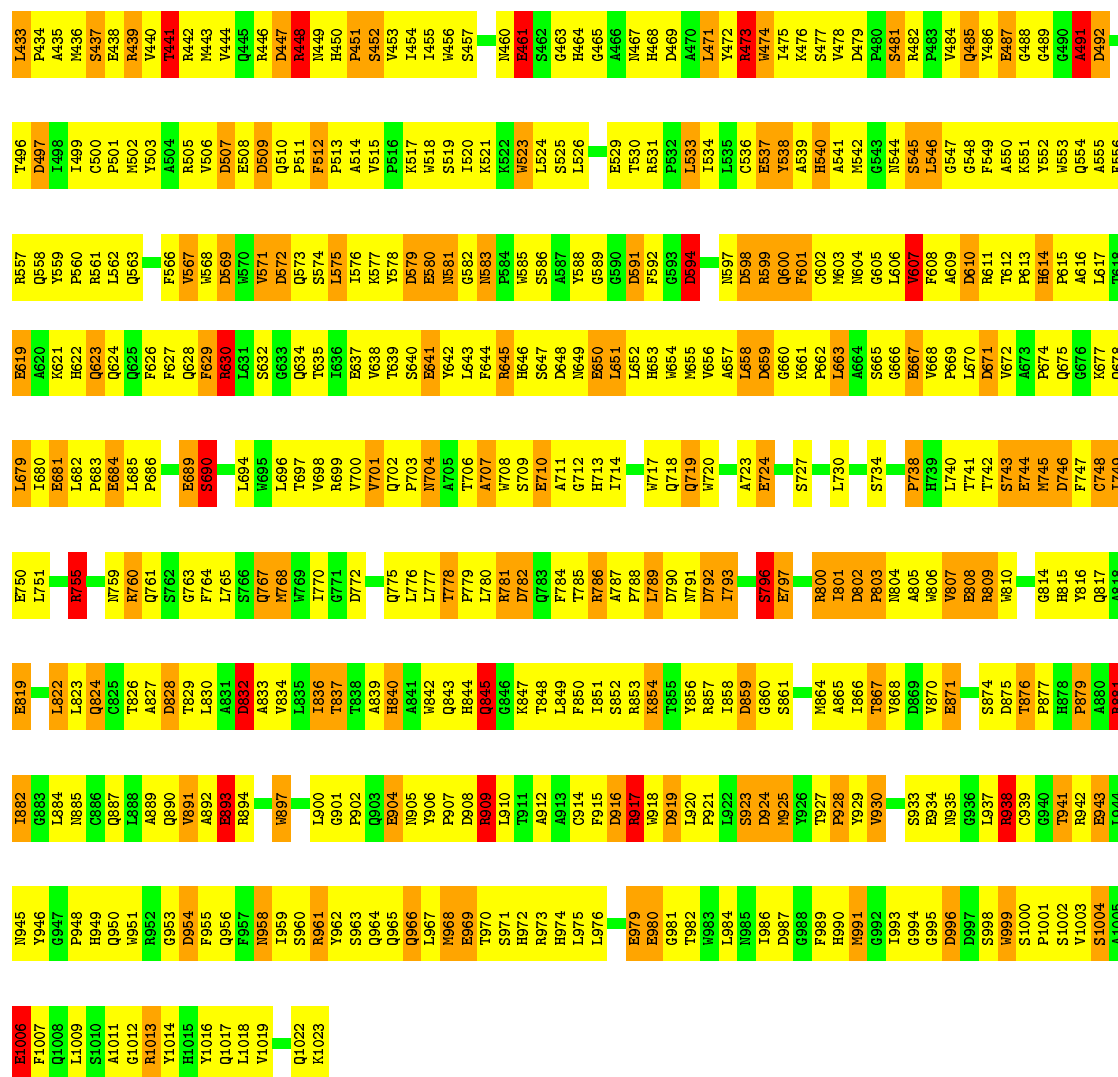




- Molecule 1: BETA-GALACTOSIDASE

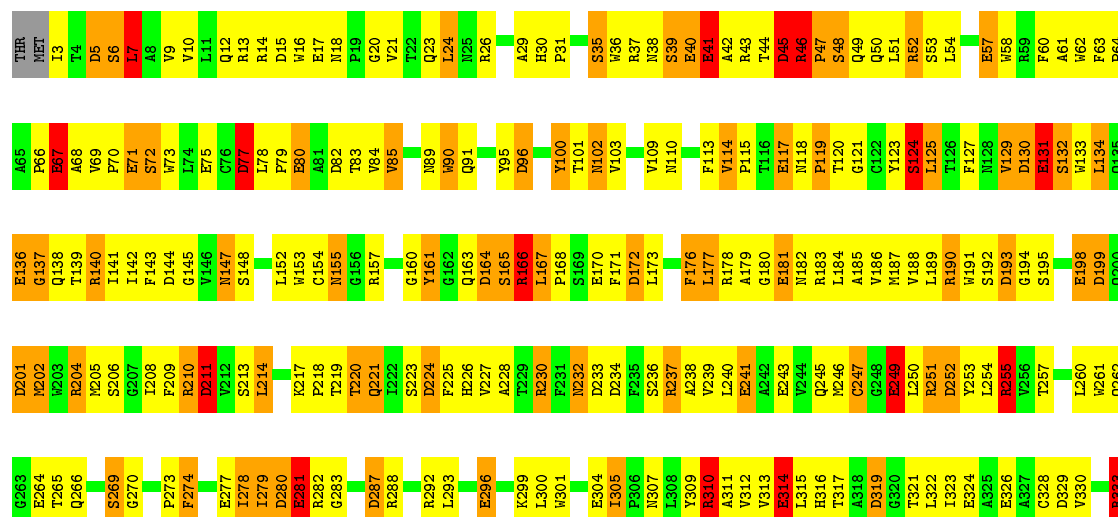


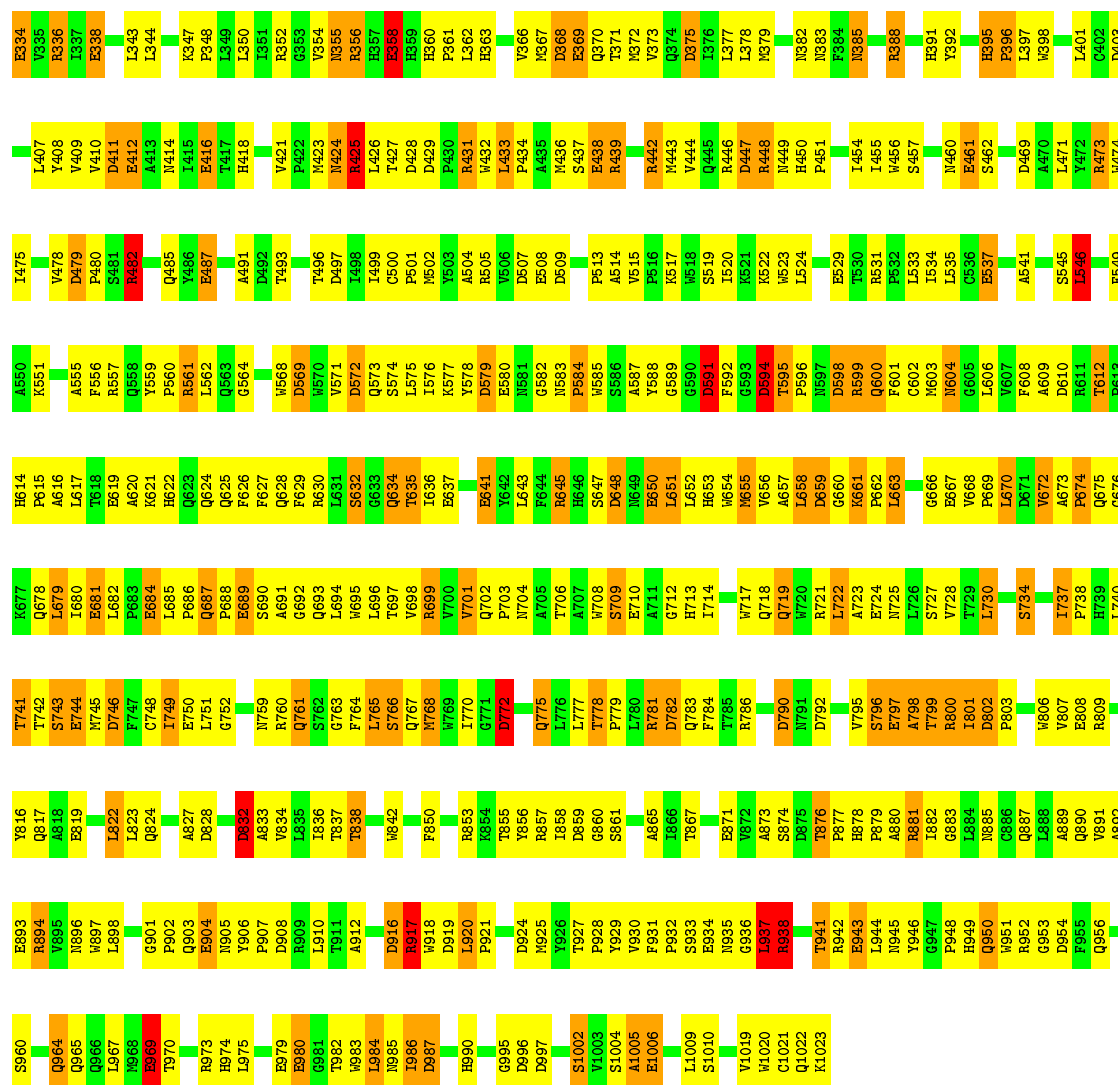




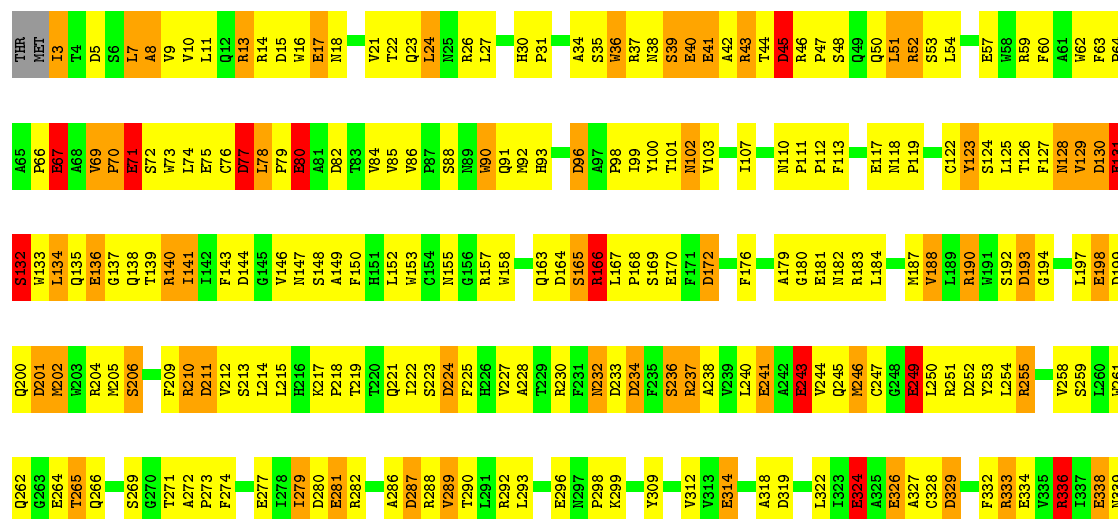
● Molecule 1: BETA-GALACTOSIDASE

Chain N: 34% 46% 17%





• Molecule 1: BETA-GALACTOSIDASE





Category	Percentage
Green	19%
Yellow	52%
Orange	25%



F1007	Q245	N307	D368	P430	G490	Y559	Q623	L685	N753	H815	B881	R942
Q1008	M246	L308	E369	R431	A491	P560	Q624	P686	K754	Y816	L884	E943
L1009	C248	Y309	Q370	W432	D492	R561	Q625	Q687	R755	Q817	L885	E944
S1010	G248	R310		L433	T493	L562	F626	P688		A818	N885	I945
	E249	A311		P434	T494	L563		S689	F758	E819	Q886	Y946
R1013	L250	V312	Q374	A435	A495	F566	F629	S690	N759	L822	Q887	G947
Y1014	R251	V313	D375	W436	T496	F567	R630	L694	R760	L823	L888	P948
H1015	D252	E314	L376	S437	D497	F568	L631	W695	Q761	Q824	A889	P949
L1016	Y253	L315	L377	E438	T498	W568	S632	Q695	F764		Q890	Q950
Q1017	R254	L316	L378	R439	T499	D569	Q633	L696	L765	D828	W891	R951
V1019	R255	T317	L379	W440	C500	Q570	Q634	T697	Q634	T829	A892	R952
W1020	V256	T318	K380	T441	P501	V571	T635	V698	S766	L830	E893	G953
C1021	T257	A318	A318	T442	W502	D572	T636	R689	Q767	L831	R894	P954
Q1022	T258	D819	Q381	R443	Y503	Q573	E637	V700	M768	A831	W895	F955
K1023	S259	G320	N382	W444	A504	S574		V701	W769	D832	N896	Q956
	L260	T321	N383	Q445	R505	L575	R639	Q702	I770	A833	W897	Q957
	L261	L322	F384	R446	V506	L576	S840	P703	G711	W834	L898	R958
	W261	L323	N385	R447	V507	X577	E641	N704	D712	L835	G899	I959
	Q262	E324	A386	D447	E508	Y578	V642	A705	K773	I836	L900	S960
	G263	A325	V387	R448	E509	D579	L643	T706	K774	T837	Q901	R961
	E264	E326	R388	W449			F644	A707	Q775	T838	P902	Y962
	T265	A327	C389	H450	V515	E580		W708	L776	A839	Q903	
	A272	C328	S390	P451	W518	N583	R645	S709	L777	H840	E904	Q965
	Q266	V267	H391	S452	W519	P584	H646	E710	T778	A841	N905	Q966
	A268	V330	Y392	V453	W520	H585	D648	A711	P779	W842	Y906	L967
	S269	G331	P393	T454	E521	S586	R649	G712	L780	Q843	P907	R968
	G270	F332	N394	L455	W522	A587	E650	H713		R844	D908	E969
	T271	R393	H395	W456	K522	L651	L651	I714	D781	Q845	R909	T970
	A272	E334	P396	S457	W523	E590	L652	S715	G783	G846	L910	S971
	P273	V335	L397	L458	W524	D591	H653	A716	F784	K847	T911	H972
	F274	R336	W398	C459	L524	F592	W654	W717	T785	T848	A912	R973
	G275	I337	Y399	W460	S525	G593	W655		R786	L849	A813	H974
	G276	E338	T400	R461	L526	D594	W656	L722	A787	F850	C914	L975
	E277		L401	S462	P527	S595		A723	R788	R853	F915	L976
	L278		D403	Q463	W528	T595	A657	E724	L789	K854	D916	E980
	D280	L342	R404	C465	T530	D597	D659	W725	D790	T855	W918	G981
	E281	L343	E466	W467	W531	N597	L661	S727	D791	Y856	D919	T982
	R282	N345	I467	I467	P532	R599		S728	D792	R857	L920	
	G283	G346	Y408	H468	L533	Q600	P662	V728	I793	L858	P921	N985
	G284	R347	V409	D469	W534	F601	L663	T729	G794	D859	L922	I986
	Y285	P348	V410	A470	L535	C602	A664	W730	S795	G860	S923	G994
	A286	D411	D411	L471	C536	N603	S665		S796	T867	S924	D987
	D287	L350	E412	Y472	E537	W604	Q666	H735	E797	S861	D924	
	R288	A413	R473	R473	W538	L605	E667	A736	A798	Q862	N925	H990
	V289	R352	W474	W474	A539	L606	V668	I737	T799	Q863	Y926	I991
								P738	R800	N864	T927	G992
	L293	G353	E416	I415	H540	F607	P669	H739	I801	A865	P928	I993
	N294	V354	R476	S475	A541	F608	L670	L740	D802	L866	Y929	G994
	W295	N355	T417	S477	W542	A609	D671	T741	P803	T867	V930	G995
	V296	R356	R418	V478	G543	D610	V672	T742	N804	V868	F931	D996
	E297	H357	G419	D479	N544	R611	A673	S743	A805	D869	P932	D997
	I297	E358	W420	P480	S545	T612	P674	E744	W806	V870	P933	S998
	P298	R359	V421	S481	L546	P613		W745	V807	E871	E934	W999
	K299	H360	P422	R482	G547		Q677	D746	E808	S874	N935	S1000
	L300	P361	N423	P483	O548	L617	L679	F747	R809	D875	G936	P1001
	W301	L362	V484	V484	F549	T618	L680	G748	N810	T876	L937	S1002
	S302	H363	R425	Q485	A550	E619	E681	I749	W811	R876	R938	V1003
	A303	G364	L426	Y486	K551	A620	L682	E750	A812	R877	C939	S1004
	E304	Q365	T427	E487	W552	R621	P683	L751	A813	H878	G940	A1005
	I305	V366	D428	G488	W553	H622	E684	G752	G814		T941	E1006

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 92.62 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.50) 39.3 (92.62-2.00)	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) 0.169 , (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)	0.28 , 89.5	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	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	1.16	51/8440 (0.6%)	1.52	139/11516 (1.2%)
1	B	1.17	54/8440 (0.6%)	1.51	130/11516 (1.1%)
1	C	1.18	56/8440 (0.7%)	1.50	132/11516 (1.1%)
1	D	1.16	55/8440 (0.7%)	1.52	148/11516 (1.3%)
1	E	1.16	55/8440 (0.7%)	1.56	145/11516 (1.3%)
1	F	1.18	45/8440 (0.5%)	1.53	144/11516 (1.3%)
1	G	1.16	58/8440 (0.7%)	1.51	151/11516 (1.3%)
1	H	1.16	56/8440 (0.7%)	1.57	150/11516 (1.3%)
1	I	1.13	53/8440 (0.6%)	1.52	140/11516 (1.2%)
1	J	1.12	48/8440 (0.6%)	1.48	134/11516 (1.2%)
1	K	1.09	53/8440 (0.6%)	1.45	115/11516 (1.0%)
1	L	1.13	53/8440 (0.6%)	1.54	134/11516 (1.2%)
1	M	1.16	55/8440 (0.7%)	1.58	142/11516 (1.2%)
1	N	1.14	51/8440 (0.6%)	1.49	127/11516 (1.1%)
1	O	1.11	54/8440 (0.6%)	1.49	141/11516 (1.2%)
1	P	1.17	57/8440 (0.7%)	1.60	151/11516 (1.3%)
All	All	1.15	854/135040 (0.6%)	1.52	2223/184256 (1.2%)

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

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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 854 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	358	GLU	CD-OE2	11.52	1.38	1.25
1	F	75	GLU	CD-OE1	10.30	1.36	1.25
1	K	358	GLU	CD-OE2	9.34	1.35	1.25
1	B	650	GLU	CD-OE1	9.31	1.35	1.25
1	F	326	GLU	CD-OE2	9.01	1.35	1.25

The worst 5 of 2223 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	881	ARG	NE-CZ-NH2	-14.45	113.08	120.30
1	B	166	ARG	NE-CZ-NH2	-14.23	113.19	120.30
1	N	561	ARG	NE-CZ-NH2	-14.06	113.27	120.30
1	L	425	ARG	NE-CZ-NH2	13.74	127.17	120.30
1	L	997	ASP	CB-CG-OD2	-13.64	106.02	118.30

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	540	0
1	B	8198	0	7796	546	0
1	C	8198	0	7796	446	0
1	D	8198	0	7796	551	0
1	E	8198	0	7795	892	0
1	F	8198	0	7796	579	0
1	G	8198	0	7796	641	0
1	H	8198	0	7796	882	0
1	I	8198	0	7796	618	0
1	J	8198	0	7795	507	0
1	K	8198	0	7796	781	0
1	L	8198	0	7796	792	0
1	M	8198	0	7796	1078	0
1	N	8198	0	7795	630	0
1	O	8198	0	7796	659	0
1	P	8198	0	7796	1151	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	14	0
3	C	91	0	0	9	0
3	D	97	0	0	13	0
3	E	94	0	0	20	0

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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	18	0
3	I	90	0	0	15	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	17	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	11096	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 43.

The worst 5 of 11096 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:E:7:LEU:HD13	1:E:74:LEU:HD11	1.23	1.17
1:C:427:THR:HA	1:C:436:MET:HE1	1.21	1.16
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:I:316:HIS:HA	1:I:323:ILE:HD13	1.24	1.13

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%)	8 14

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

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%)	723 (83%)	150 (17%)	2	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	873/875 (100%)	709 (81%)	164 (19%)	1	2
1	C	873/875 (100%)	754 (86%)	119 (14%)	3	7
1	D	873/875 (100%)	729 (84%)	144 (16%)	2	4
1	E	873/875 (100%)	686 (79%)	187 (21%)	1	2
1	F	873/875 (100%)	735 (84%)	138 (16%)	2	4
1	G	873/875 (100%)	717 (82%)	156 (18%)	2	3
1	H	873/875 (100%)	693 (79%)	180 (21%)	1	2
1	I	873/875 (100%)	716 (82%)	157 (18%)	1	3
1	J	873/875 (100%)	755 (86%)	118 (14%)	4	7
1	K	873/875 (100%)	722 (83%)	151 (17%)	2	3
1	L	873/875 (100%)	704 (81%)	169 (19%)	1	2
1	M	873/875 (100%)	677 (78%)	196 (22%)	1	1
1	N	873/875 (100%)	717 (82%)	156 (18%)	2	3
1	O	873/875 (100%)	715 (82%)	158 (18%)	1	3
1	P	873/875 (100%)	665 (76%)	208 (24%)	0	1
All	All	13968/14000 (100%)	11417 (82%)	2551 (18%)	1	3

5 of 2551 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	523	TRP
1	J	277	GLU
1	P	71	GLU
1	H	724	GLU
1	I	293	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 370 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	262	GLN
1	I	950	GLN
1	O	1008	GLN
1	H	460	ASN
1	I	38	ASN

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 carbohydrates 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%)	-1.08	0 100 100	2, 24, 54, 79	0
1	B	1021/1023 (99%)	-1.10	0 100 100	2, 23, 54, 81	0
1	C	1021/1023 (99%)	-1.06	0 100 100	4, 21, 52, 80	0
1	D	1021/1023 (99%)	-1.10	0 100 100	4, 25, 56, 81	0
1	E	1021/1023 (99%)	-0.94	1 (0%) 95 96	8, 34, 61, 86	0
1	F	1021/1023 (99%)	-1.03	0 100 100	2, 23, 55, 78	0
1	G	1021/1023 (99%)	-1.07	0 100 100	3, 27, 58, 82	0
1	H	1021/1023 (99%)	-0.92	1 (0%) 95 96	6, 33, 61, 89	0
1	I	1021/1023 (99%)	-1.02	0 100 100	4, 30, 59, 80	0
1	J	1021/1023 (99%)	-1.02	0 100 100	8, 28, 56, 85	0
1	K	1021/1023 (99%)	-0.89	1 (0%) 95 96	10, 35, 64, 92	0
1	L	1021/1023 (99%)	-0.86	1 (0%) 95 96	6, 35, 63, 84	0
1	M	1021/1023 (99%)	-0.80	2 (0%) 95 95	12, 39, 65, 80	0
1	N	1021/1023 (99%)	-0.97	0 100 100	9, 30, 59, 89	0
1	O	1021/1023 (99%)	-1.00	0 100 100	11, 31, 60, 81	0
1	P	1021/1023 (99%)	-0.47	15 (1%) 73 75	14, 43, 69, 89	0
All	All	16336/16368 (99%)	-0.96	21 (0%) 95 96	2, 30, 60, 92	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	81	ALA	4.1
1	P	313	VAL	3.4
1	P	143	PHE	3.3
1	P	70	PRO	3.1
1	P	141	ILE	3.0

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 carbohydrates 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(\AA^2)	Q<0.9
2	MG	F	1101	1/1	0.78	0.19	35,35,35,35	0
2	MG	K	1101	1/1	0.89	0.08	34,34,34,34	0
2	MG	G	1101	1/1	0.91	0.17	32,32,32,32	0
2	MG	O	1101	1/1	0.92	0.12	40,40,40,40	0
2	MG	P	1101	1/1	0.93	0.12	49,49,49,49	0
2	MG	C	1102	1/1	0.93	0.08	28,28,28,28	0
2	MG	M	1101	1/1	0.94	0.14	56,56,56,56	0
2	MG	J	1101	1/1	0.94	0.14	34,34,34,34	0
2	MG	E	1102	1/1	0.95	0.08	32,32,32,32	0
2	MG	D	1102	1/1	0.95	0.13	42,42,42,42	0
2	MG	L	1102	1/1	0.95	0.04	28,28,28,28	0
2	MG	A	1102	1/1	0.95	0.08	37,37,37,37	0
2	MG	B	1101	1/1	0.96	0.15	25,25,25,25	0
2	MG	H	1101	1/1	0.96	0.15	27,27,27,27	0
2	MG	J	1102	1/1	0.96	0.05	29,29,29,29	0
2	MG	E	1101	1/1	0.96	0.15	39,39,39,39	0
2	MG	D	1101	1/1	0.97	0.12	28,28,28,28	0
2	MG	N	1101	1/1	0.97	0.14	32,32,32,32	0
2	MG	C	1101	1/1	0.97	0.18	23,23,23,23	0
2	MG	L	1101	1/1	0.98	0.14	31,31,31,31	0
2	MG	K	1102	1/1	0.98	0.05	25,25,25,25	0
2	MG	N	1102	1/1	0.98	0.11	26,26,26,26	0
2	MG	A	1101	1/1	0.98	0.15	37,37,37,37	0
2	MG	I	1102	1/1	0.98	0.08	33,33,33,33	0
2	MG	P	1102	1/1	0.99	0.05	26,26,26,26	0
2	MG	I	1101	1/1	0.99	0.13	33,33,33,33	0
2	MG	O	1102	1/1	0.99	0.09	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	H	1102	1/1	0.99	0.06	22,22,22,22	0
2	MG	B	1102	1/1	0.99	0.05	23,23,23,23	0
2	MG	G	1102	1/1	0.99	0.03	18,18,18,18	0
2	MG	F	1102	1/1	0.99	0.07	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.