



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 3, 2017 – 01:58 PM EDT

PDB ID : 5TX1
EMDB ID: : EMD-8471
Title : Cryo-Electron microscopy structure of species-D human adenovirus 26
Authors : Reddy, V.; Yu, X.; Veesler, D.
Deposited on : unknown
Resolution : 3.70 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

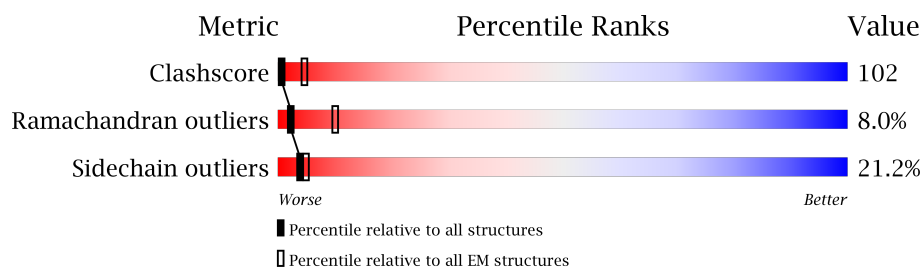
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

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



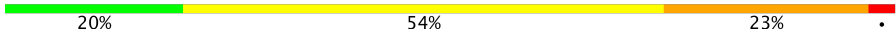

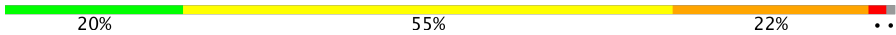
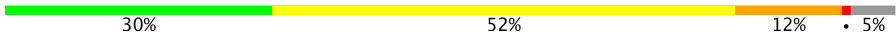
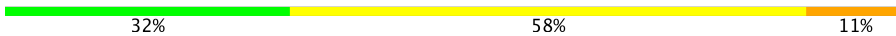
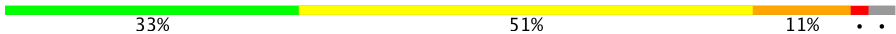
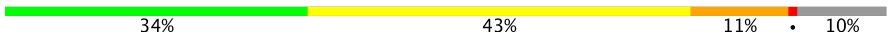
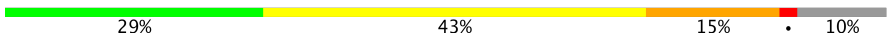
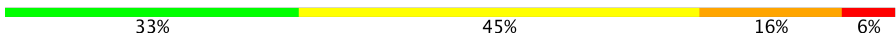

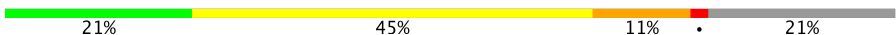
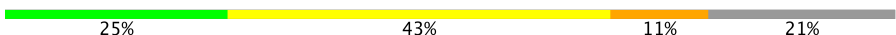












Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	952	23% 58% 16% .
1	B	952	19% 58% 20% .
1	C	952	18% 57% 21% ..
1	D	952	24% 57% 18% ..
1	E	952	20% 56% 21% ..
1	F	952	16% 54% 25% .
1	G	952	21% 54% 23% ..
1	H	952	17% 54% 25% ..
1	I	952	18% 55% 24% .

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Mol	Chain	Length	Quality of chain
1	J	952	
1	K	952	
1	L	952	
2	N	497	
3	O	19	
4	M	388	
5	P	134	
5	Q	134	
5	R	134	
5	S	134	
6	U	227	
6	V	227	
7	1	31	
7	2	31	
7	3	31	
7	4	31	
7	5	31	
7	6	31	
7	7	31	
7	8	31	
7	9	31	
8	X	10	
8	Y	10	
8	Z	10	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 105738 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Hexon protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	951	Total	C	N	O	S	0	0
			7551	4796	1276	1444	35		
1	B	949	Total	C	N	O	S	0	0
			7536	4787	1274	1441	34		
1	C	946	Total	C	N	O	S	0	0
			7519	4777	1271	1437	34		
1	D	947	Total	C	N	O	S	0	0
			7526	4780	1272	1440	34		
1	E	947	Total	C	N	O	S	0	0
			7526	4780	1272	1440	34		
1	F	950	Total	C	N	O	S	0	0
			7544	4792	1275	1442	35		
1	G	947	Total	C	N	O	S	0	0
			7526	4780	1272	1440	34		
1	H	947	Total	C	N	O	S	0	0
			7526	4780	1272	1440	34		
1	I	949	Total	C	N	O	S	0	0
			7536	4787	1274	1441	34		
1	J	951	Total	C	N	O	S	0	0
			7551	4795	1276	1446	34		
1	K	951	Total	C	N	O	S	0	0
			7551	4795	1276	1446	34		
1	L	947	Total	C	N	O	S	0	0
			7524	4780	1272	1438	34		

- Molecule 2 is a protein called Penton.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	473	Total	C	N	O	S	0	0
			3803	2416	643	730	14		

- Molecule 3 is a protein called Fiber.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	O	19	Total	C	N	O	0	0
			162	105	27	30		

- Molecule 4 is a protein called PIIIa.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	376	Total	C	N	O	S	0	0
			2938	1832	530	567	9		

- Molecule 5 is a protein called PIX.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	120	Total	C	N	O	S	0	0
			871	535	155	177	4		
5	Q	120	Total	C	N	O	S	0	0
			875	538	155	178	4		
5	R	134	Total	C	N	O	S	0	0
			965	592	169	199	5		
5	S	121	Total	C	N	O	S	0	0
			881	542	156	180	3		

- Molecule 6 is a protein called PVIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	U	180	Total	C	N	O	S	0	0
			1391	876	239	270	6		
6	V	180	Total	C	N	O	S	0	0
			1391	876	239	270	6		

- Molecule 7 is a protein called PVI.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1	31	Total	C	N	O	S	0	0
			236	146	44	45	1		
7	2	27	Total	C	N	O	S	0	0
			211	132	39	39	1		
7	3	26	Total	C	N	O	S	0	0
			202	127	37	37	1		
7	4	27	Total	C	N	O	S	0	0
			211	132	39	39	1		
7	5	26	Total	C	N	O	S	0	0
			202	127	37	37	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	27	Total	C	N	O	S	0	0
			211	132	39	39	1		
7	7	26	Total	C	N	O	S	0	0
			202	127	37	37	1		
7	8	31	Total	C	N	O	S	0	0
			236	146	44	45	1		
7	9	26	Total	C	N	O	S	0	0
			202	127	37	37	1		

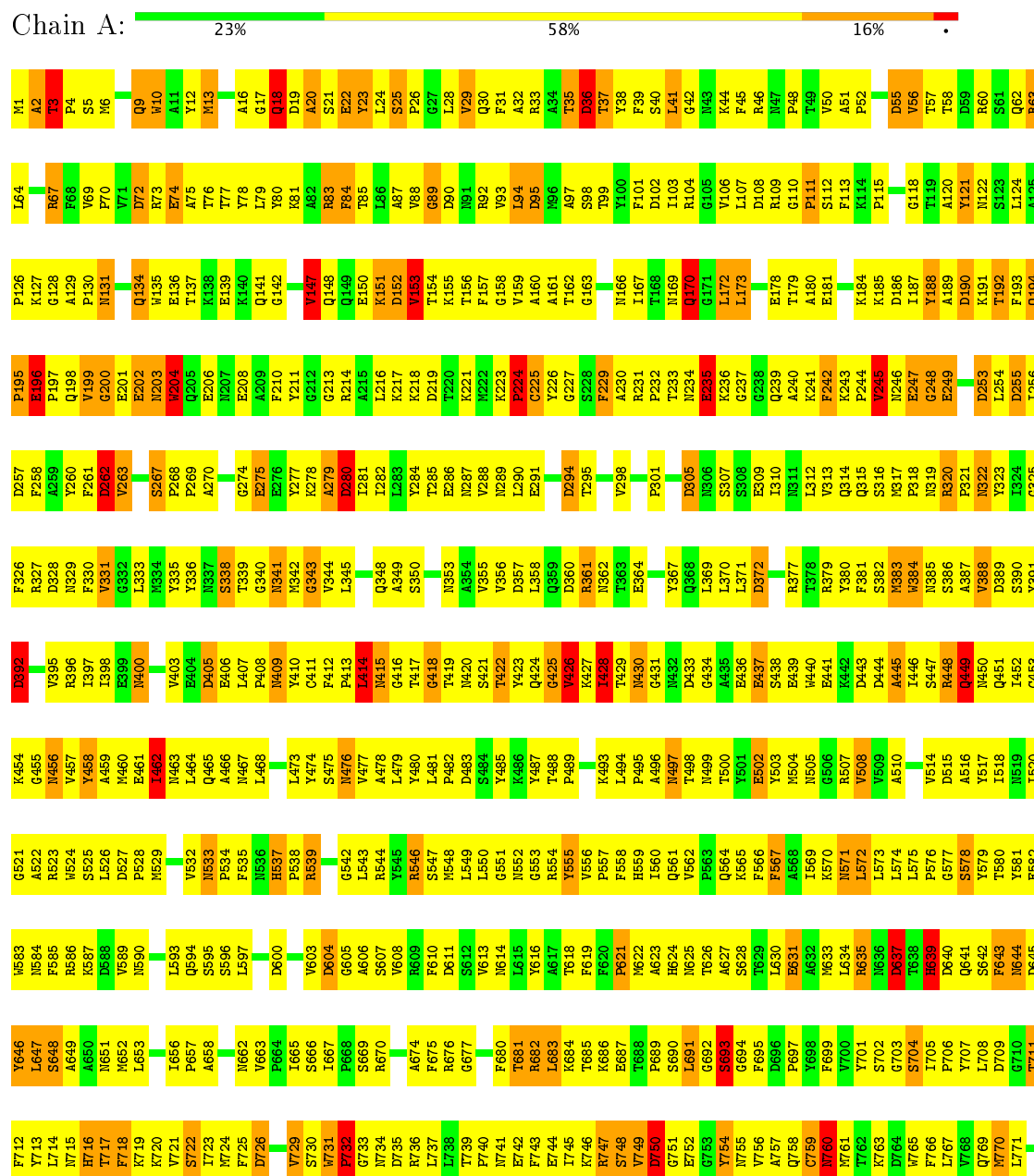
- Molecule 8 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	X	10	Total	C	N	O	0	0
			51	30	10	11		
8	Y	10	Total	C	N	O	0	0
			51	30	10	11		
8	Z	6	Total	C	N	O	0	0
			30	18	6	6		

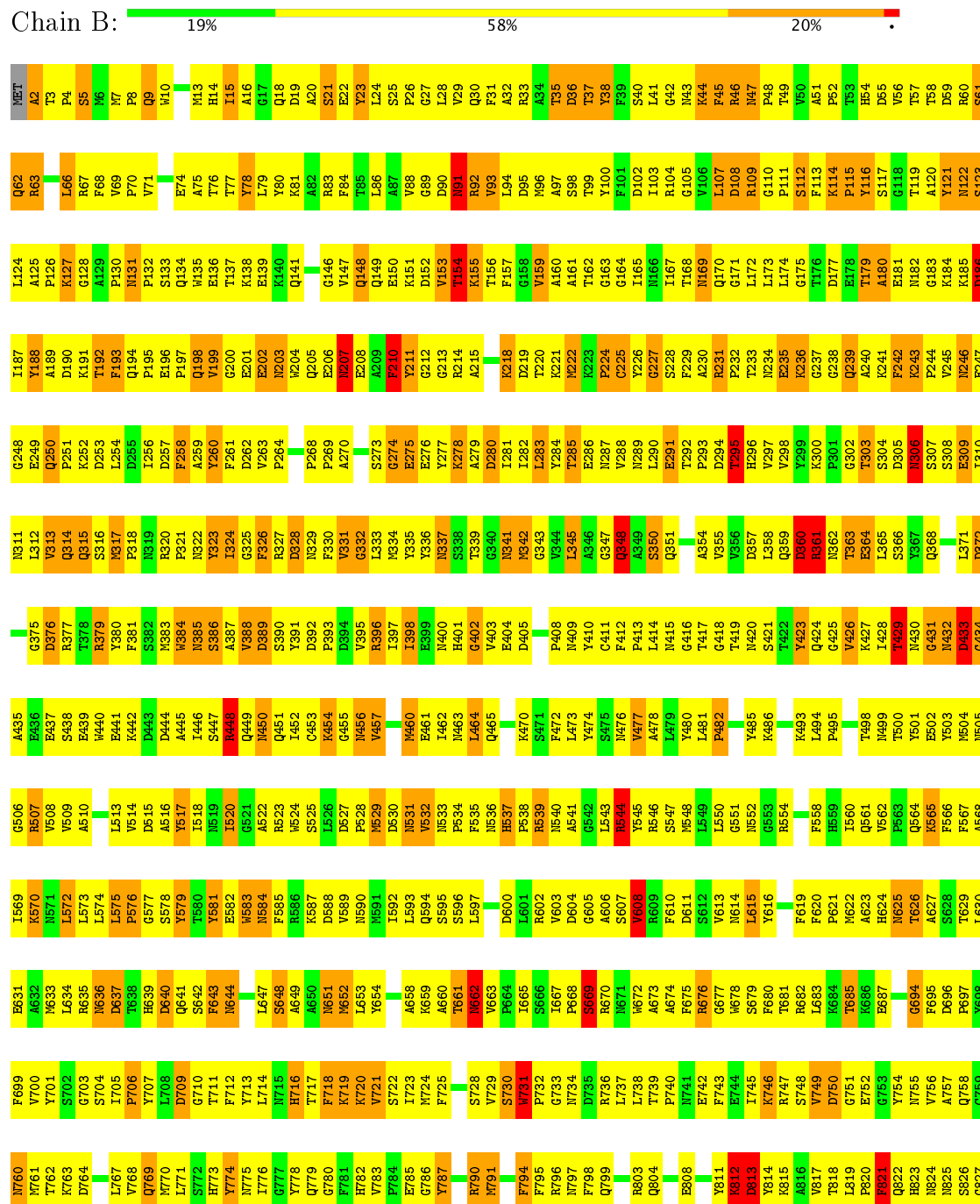
3 Residue-property plots

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. 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. 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: Hexon protein



- Molecule 1: Hexon protein

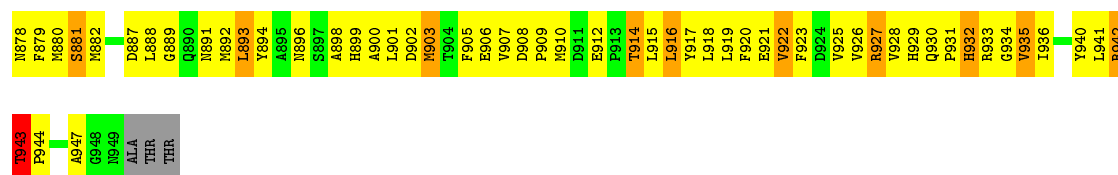


A900	F828
L901	
D902	Y831
M903	L832
T904	A833
F905	P834
E906	T835
V907	M836
D908	R837
P909	G838
N910	G839
D911	D840
E912	P841
P913	L842
T914	P843
L915	A844
L916	N845
L917	F846
L918	P847
L919	L848
F920	
E921	L851
V922	
F923	Y856
D924	P857
V925	M858
V926	Y859
L927	T860
V928	N861
H929	K862
Q930	K863
P931	F864
H932	L865
R933	C866
	D867
I936	K868
E937	Y869
A938	M870
V939	M871
Y940	
L941	F875
R942	S876
N943	S877
K944	M878
F945	F879
P946	M880
	S881
G948	M882
N949	
A950	L885
THR	T886
	D887
	L888
	G889
	D890
	N891
	M892
	L893
	H899

• Molecule 1: Hexon protein

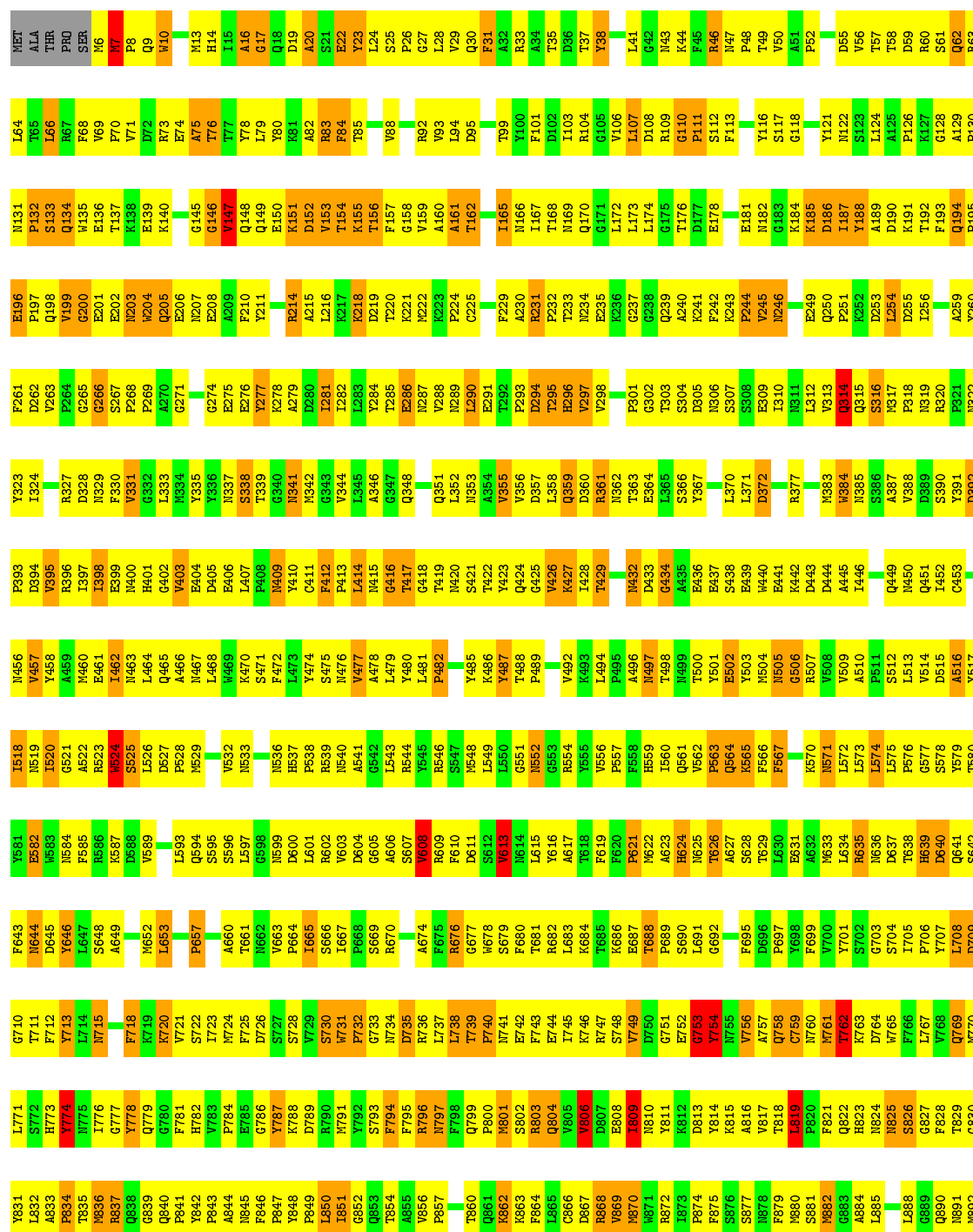
Chain C: 18% 57% 21%

MET	P863	A125	Y188	G248	L310	D872	E441	Y501	P563	H624	K886	D750	A816
ALA	L64	P126	A189	E249	N311	S373	K442	E502	Q564	M625	E887	G751	V817
THR	L65	K127	D190	P251	L312	R377	D443	Y503	F565	T626	T688	T752	T818
P4	T66	G128	K191	P251	V313		D444	M504	F566	A627	P689	G753	L819
S5	R67	A129	T192	K252	Q314		A445	M505	F567	S628	S690	T754	P820
M6	T68	F193	F193	D253	Q315	Y390	A446	G506	A568	T629	L691	N755	F821
N7	V69	M131	Q194	L254	S316	F381	S447	R507	I569	L630	G694	V756	Q822
P8	P70	P132	F195	D255	R317	S382	S448	Y508	K570	E631	F695	A757	H823
Q9	D72	S133	E196	L256	P318	K383	Q449	V509	L572	A632		G758	N824
R8	R73	W10	Q198	F258	N319	M384	Q450	A510	L573	M633		G759	N825
	K73		Q199	F259	R320	M385	Q451		L574	L634		N760	S826
	A75		G200	A259	P321	S386	C452		L575	M635		N761	G827
	T76		E201	F261	Y323	F388	K453	M513	L576	M636		T762	F828
	T77		E202	V262	I324	D389	G455	D515	P576	D637		K763	
	T78		N203	V263	G325	K390	M456	A516	G577	T638		D764	Y831
	L79		Q204	P264	F326	Y391	V457	Y517	S578	M639		T765	L832
	K80		Q205	G265	G327	F392	V458	M518	F579	D640		F766	N833
	K81		E206	G266	D328	F393	V459	M519	T580	Q641		L767	P834
	A82		K207	S267	N329	D394	M460	E520	Y581	S642		V768	T835
	R83		E208	P268	F330	Y395	M461		E582	F643		Q769	M836
	F84		A209	P269		K396	I462	M523	M583	M644		T770	R837
	A87		Y211	A270	L333	I397	M463	M524	M584	D645		T771	Q838
	Y88		G212		N334	I398	M464	S525	F585	Y646		G710	G839
	G89		G213		Y335	E399	L467	L526	R586	L647		T711	Q840
	D90		K214		Y336	M400	Q465	D527	K587	S648		F712	P841
	N91		K215		N337	E401	Q466	P528	D588	A649		Y713	Y842
	R92		K216		R338	G402	L468	M529	V589	A650		L714	P843
	F31		K217		T339	H403	M469	D530	M590	M651		T715	A844
	A32		K218		G340	E404	K470	V532	M591	M652		H716	N845
	R94		K155		K341	D405	S471	M533	L592	L653		T717	G846
	D95		K156			E406	F472	P534	Q594			F718	P847
	F96		F157		V344	L407	L473	F535	L593	L656		T719	Y848
	A97		K221		L345	P408	Y474	M536	S595	K659		K720	P849
	S98		K222		A346	M409	Y475	M537	S596	A660		T721	L851
	T99		K223		G347	Y410	P482	P538		T661		I723	G852
	Y100		K224		Q348	C411	G416	P539		M662		M724	Q853
	F101		C225		A349	F412	A478	M540		V663		F725	T854
	D102		C226		S350	P413	L479	A541		P664		D726	A855
	I103		Y226		L352	L414	L481	G542		T665		W729	V856
	R104		G227		N353	N415	P482	L543		S666		S730	P857
	L107		S228		K354	N416	L483	M544		L667		H731	S858
	D108		E291		A354	T417	D483	Y545		P668		F732	V859
	K109		P232		V355		S484	M546		S669		Q733	T860
	G110		P233		V356	T422	Y485	S547		R670		G734	Q861
	P111		T233		L358	Y423	K486	M548		P671		D735	K862
	S112		N234		Q359	Q424	Y487	L549		M672		F736	P863
	F113		E235		D360	G425	T488	L550		A673		R737	R864
	K114		Q237		R361	K427	P489	G551		A674		L738	L865
	P115		G238		N362	I428	A490	M552		P675		T739	C866
	Y116		Q239		T363	Y429	V492	G553		G677			D867
	S117		A240		E364		K493	M554		M678		E742	R868
	G118		K241		L365	G434	L494	Y555		Y616		F743	V869
	T119		P242		S366	S303	V566	V556		A617		N809	N870
	A120		K243		Y367	S304	A495	P567		T618		N810	M871
	D59		P244		Q368	E437	M496	M568		F619		T745	R872
	N122		V245		L369	E437	M497	M569		F620		K746	
	S123		S308		L370	S438	T498	I560		P621		T747	D813
	L124		E247		L371	W440	T500	V562		M622		S748	Y814



• Molecule 1: Hexon protein

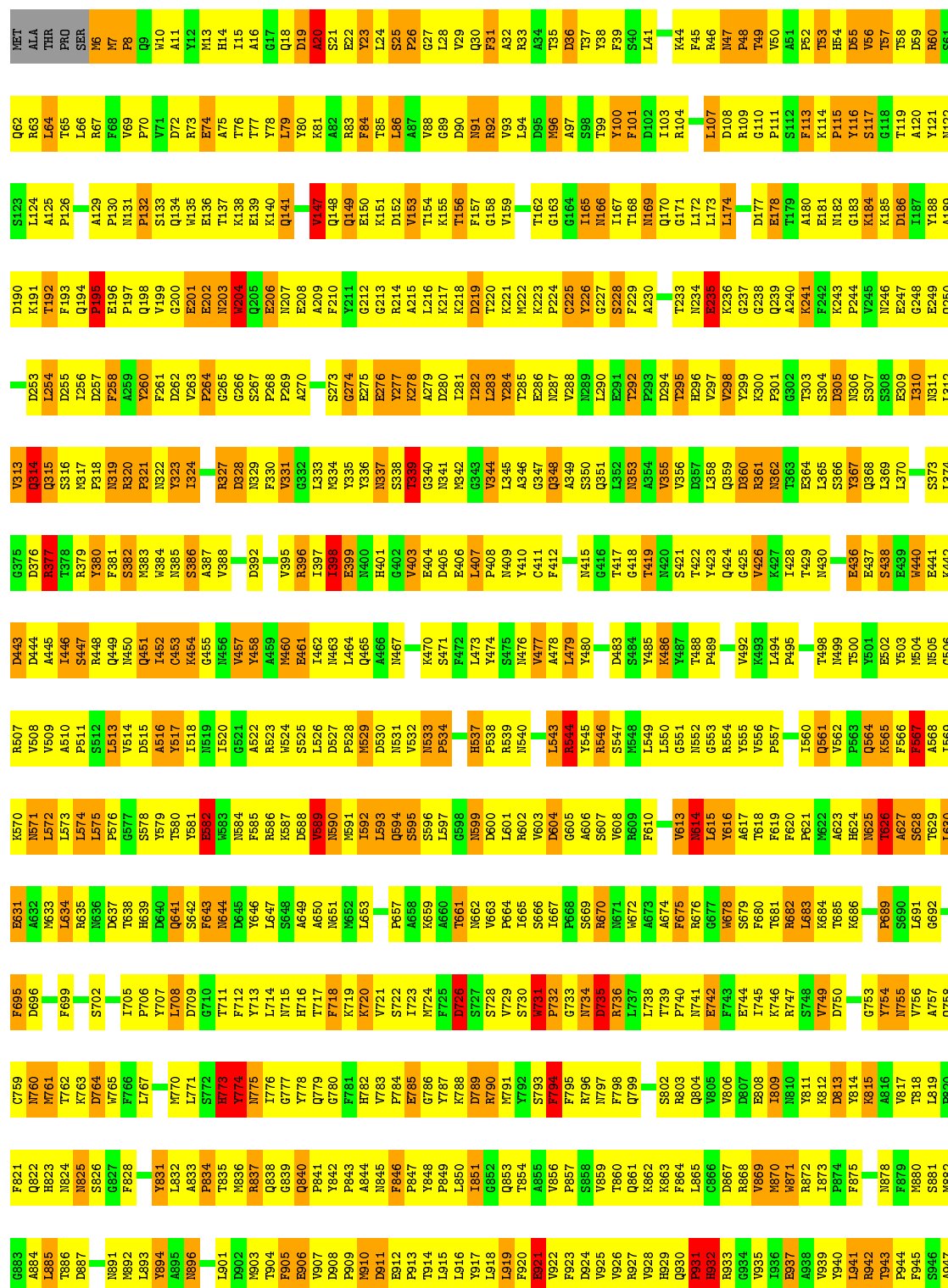
Chain D: 24% 57% 18% ..





● Molecule 1: Hexon protein

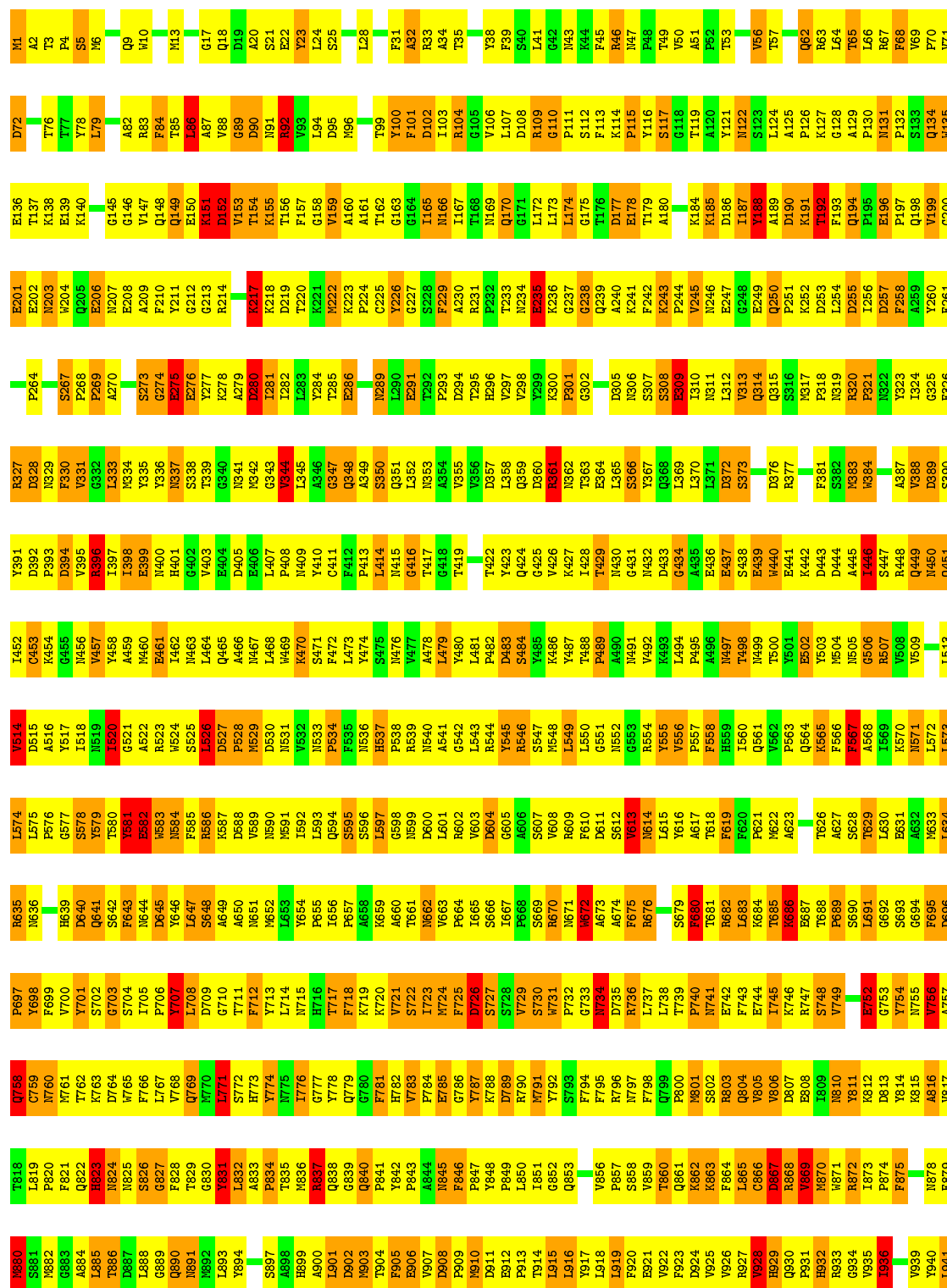
Chain E: 20% 56% 21% . .



6948
T951
T952

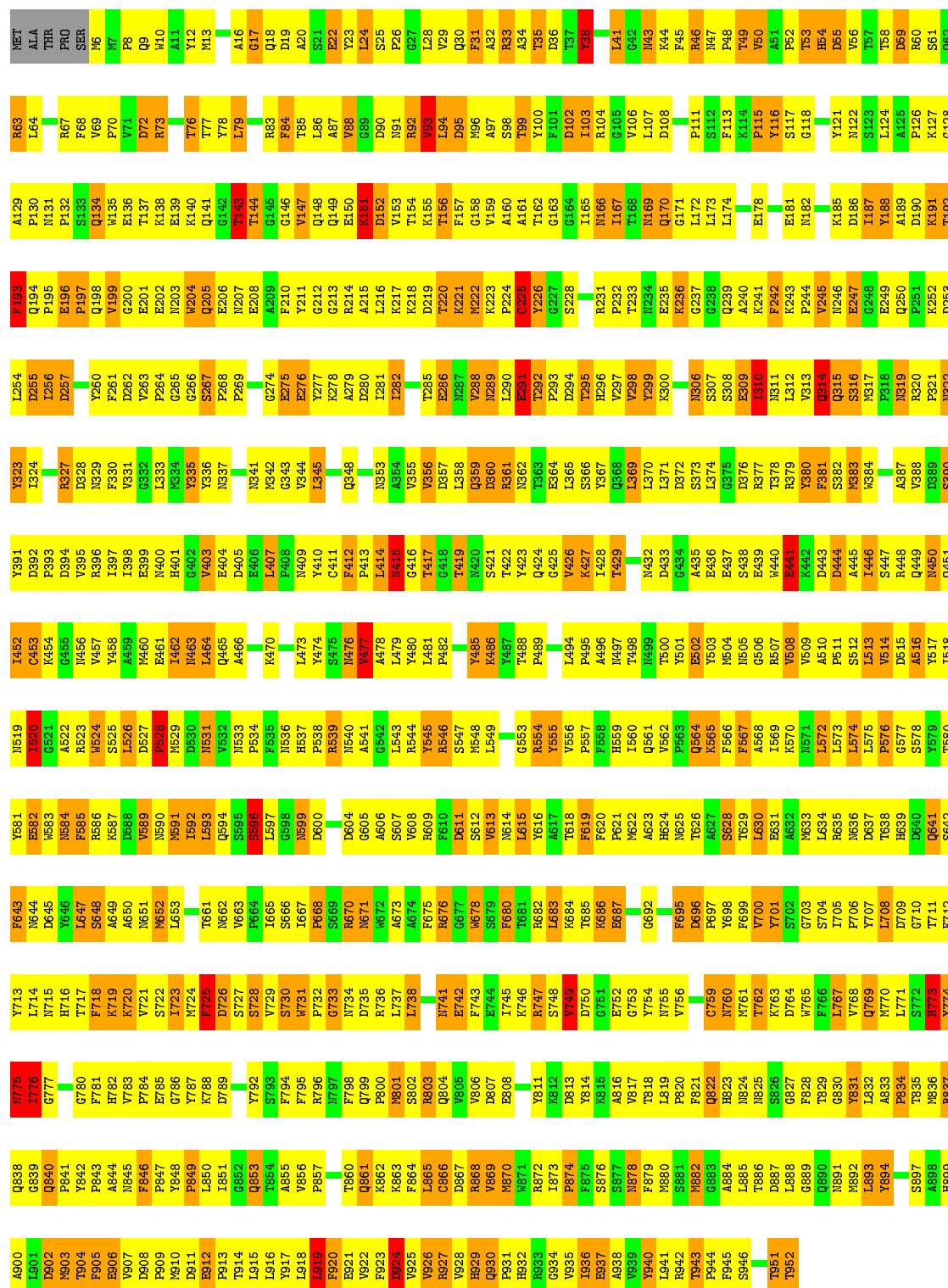
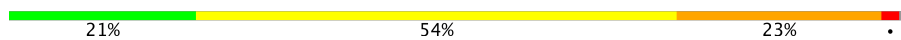
• Molecule 1: Hexon protein

Chain F: 16% 54% 25% .



- Molecule 1: Hexon protein

Chain G:



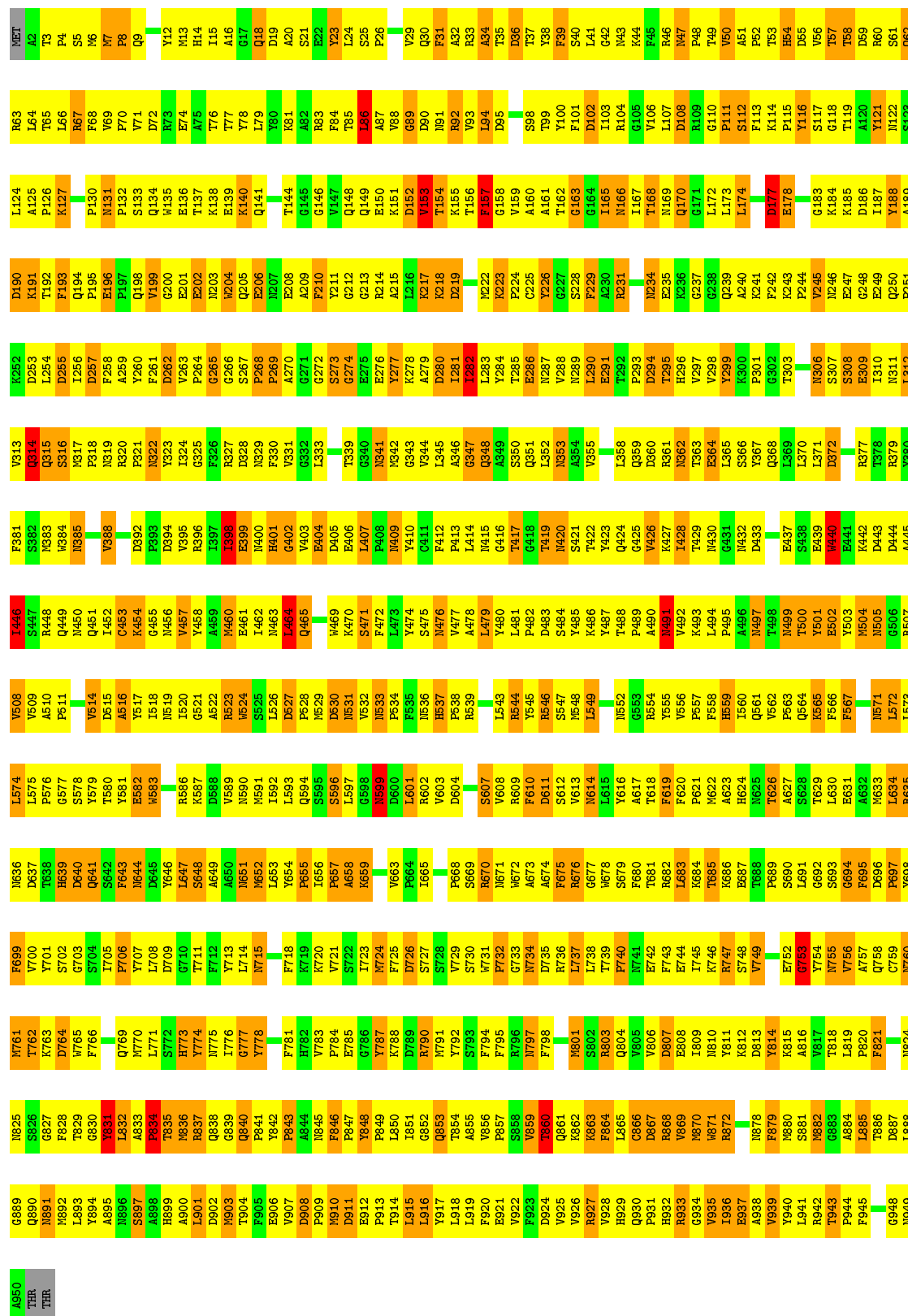
● Molecule 1: Hexon protein

Chain H: 17% 54% 25% 0%

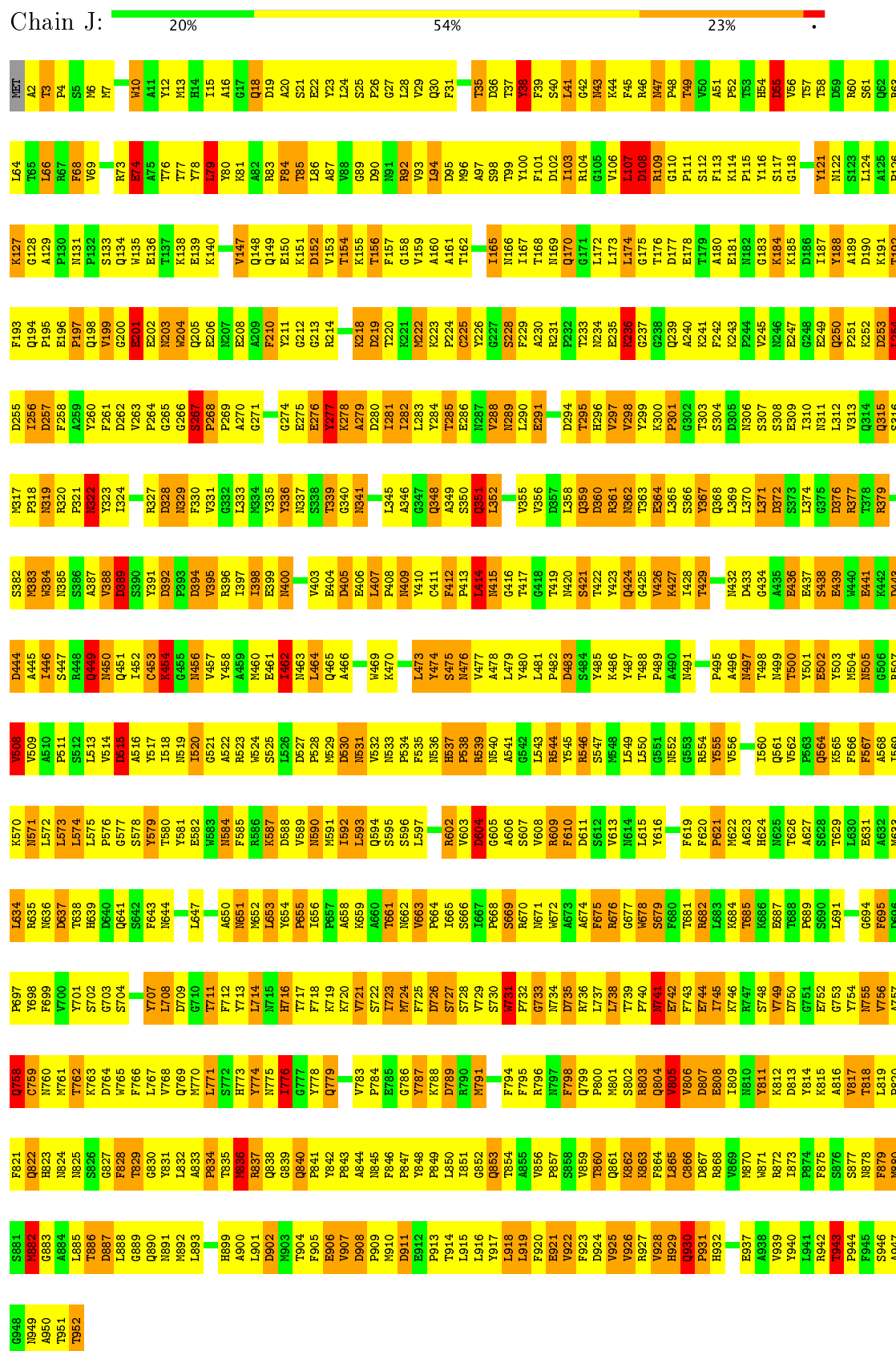
P944	G883	P820	N760	F699	N636	L575	L513	I446	W384	R320	T256	P195	P132	R67
F945	A884	F821	W761	V700	D637	P576	V514	Q449	S385	P321	T256	P195	P132	R67
S946	L885	T762	T762	Y701	T638	S577	D515	Q449	S386	P321	T256	P195	P132	R67
A947	T886	H823	K763	S702	H639	S578	A516	N450	V387	Y323	A259	Q198	W135	V69
G948	D887	N824	D764	T703	D640	Y579	Y517	N451	V388	I324	Y260	V199	E135	W71
N949	L888	N825	W765	S704	Q641	T580	I518	I452	D389	G325	F261	G200	T137	D72
G889	G889	S826	F766	T705	S642	Y581	N519	C453	S390	F326	D262	E201	K138	R73
A950	G889	G827	L767	P706	F643	E582	I520	K454	S391	R327	V263	E202	E139	E74
T952	N891	F828	W768	Y707	N644	W583	G521	G455	D392	D328	G264	N203	K140	A75
	N892	T829	Q769	L708	N644	N584	A522	N456	P593	N329	G265	D265	Q141	W10
L893	L893	G830	N770	D709	L647	K587	R523	V457	D394	F330	G266	D265	Q141	A11
Y894	Y894	R831	L771	G740	S643	D588	N524	Y458	V395	V331	S267	E206	G142	T77
A895	A895	L832	T772	T711	W649	D588	S525	A459	V396	G332	P268	N207	G146	L79
N896	N896	A833	W773	F712	N650	V589	L526	N460	I397	L333	P269	E208	Q147	R80
		P834	Y774	F713	N651	N580	D527	E461	I398	L333	P269	E208	Q147	R80
		T835	W775	L714	N652	M591	P528	I462	E399	Y336	G274	F210	Q149	A82
		N836	L776	W715	L653	L592	N529	N463	W400	Y336	G274	F210	Q149	A82
		R837	G777	H716	W654	L593	L530	L464	H401	S338	E275	Y211	Q150	R83
		Q838	W778	T717	P655	Q594	N531	Q465	G402	T339	E276	R214	D152	F84
		N902	Y779	F718	L656	S595	V532	A466	V403	G340	Y277	A215	V153	T85
		N903	Q779	W719	P657	S596	N533	N467	D405	N341	K278	L216	T154	L86
		Q840	F780	K720	P664	L597	P534	L468	D404	N341	A279	K217	K155	A87
F905	T904	P841	F781	K720	A658	L597	P534	L468	D404	N341	A279	K217	K155	V88
A950	F905	R841	H782	W721	N659	G598	F535	N469	E406	G343	D280	K218	T156	G89
	E906	Y842	H782	W721	N659	G598	F535	N469	E406	G343	D280	K218	T156	G89
	N907	P843	W783	S722	A660	N599	N536	K470	L407	V344	I281	D219	F157	D90
		A844	F784	I723	T661	D600	H537	S471	P408	L345	I282	D219	F157	D90
		N908	E785	W724	N662	L601	P538	F472	N409	A346	L282	T220	G158	N91
		N909	G786	F725	V663	R602	R539	L473	Y410	A346	L282	T220	G158	N91
		D911	Y787	W726	P664	V603	N540	Y474	C411	G347	Y284	K222	V159	R92
		F912	K788	S727	L665	D604	A541	S475	C411	T283	A161	K222	A160	V93
		N913	D789	W728	S666	G605	G542	N476	P412	G349	E286	K224	T162	D95
		L914	W790	Y729	L667	A606	L543	V477	L414	S350	N287	C225	G163	F31
		N915	F791	S730	P668	S607	R544	A478	N415	Q351	L290	G227	G164	A97
		G852	Y792	W731	N670	F608	Y545	N479	G416	N353	E291	N166	T167	S98
		Q853	F793	F732	N670	R609	Y545	N479	G416	N353	E291	N166	T167	S98
			G794	G733	N671	F610	M548	L481	T417	A354	T292	K230	T168	F101
			F795	G733	N671	F610	M548	L481	T417	A354	T292	K230	T168	F101
			W796	W734	A672	D611	L549	P482	T419	V355	D294	R231	N169	D102
			N796	W734	A672	D611	L549	P482	T419	V355	D294	R231	N169	D102
			N797	W736	N673	S612	M552	D483	T422	L358	T295	P232	Q170	I103
			Y797	F736	N676	V613	G553	S484	Y423	Q359	H296	T233	G171	R104
			F798	L737	L677	N614	R553	Y485	T423	D360	G297	T233	G171	R104
			Q799	L738	L677	L615	R554	K486	Y424	N234	V298	K241	L172	G105
			P800	T739	N678	V616	Y555		G425	R361	Y299	K241	L172	G105
			N801	F740	S679	A617	V556	P489	Y426	N362	K300	G237	L174	L107
			S802	W741	T681	F618	P557		K427	T363	K300	G237	G175	D108
			R803	E742	T681	F619	P557	L494	R427	E364	P301	G238	G177	R109
			Q804	F743	T681	F619	P557	P495	K428	L365	D298	Q239	D177	T49
			W805	E744	L683	F620	I560	A496	N430	S366	A240	K241	E178	V50
			N806	I745	N684	P621	O561	N497	G431	Y367	K304	K241	E178	V50
			W806	W746	K684	M622	O561	N497	G431	Y367	K304	K241	E178	V50
			N807	K746	T685	A623	V562	T498	N432	L369	S307	F242	E180	P52
			E808	R747	W686	H624	P563	N499	D433	L370	S308	F242	E180	P52
			R808	R747	W686	H624	P563	N499	D433	L370	S308	F242	E180	P52
			L809	W748	T688	N625	O564	T500	E436	L371	E309	N246	K184	H54
			N810	W749	W688	T626	K565	Y501	E437	D372	I310	K246	K185	V56
			Y811	F750	P689	A627	V566	E502	E437	S373	N311	E247	D186	T57
			K812	W751	S690	S628	P567	Y503	S438	L374	I312	K248	D187	T58
			D813	F752	L691	T629	A568	Y503	E439	L374	I312	K248	D187	T58
			L814	W753	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			K815	F754	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N816	Y754	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			A816	W755	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			W817	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N818	F756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			Y817	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N818	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N819	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N820	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N821	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N822	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N823	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N824	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N825	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N826	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N827	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N828	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N829	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N830	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N831	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N832	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N833	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N834	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N835	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N836	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N837	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N838	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N839	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N840	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N841	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N842	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N843	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N844	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N845	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N846	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N847	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N848	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N849	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N850	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N851	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N852	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N853	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N854	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N855	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N856	W756	G692	L630	I569	R507	W440	R377	V313	E249	E188	Y121
			N857	W756	G692	L630	I569							

- Molecule 1: Hexon protein

Chain I:  18% 55% 24%

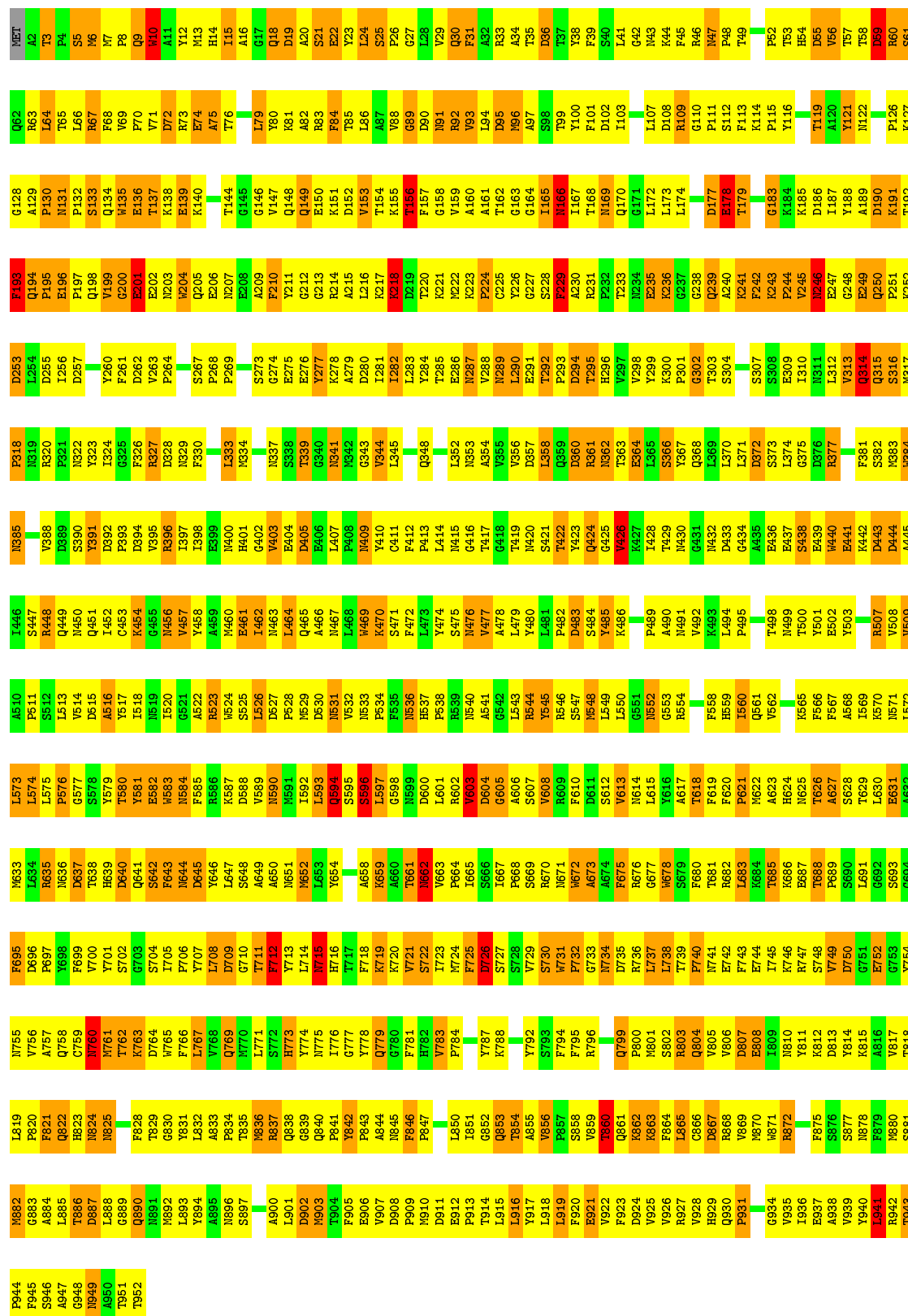


● Molecule 1: Hexon protein



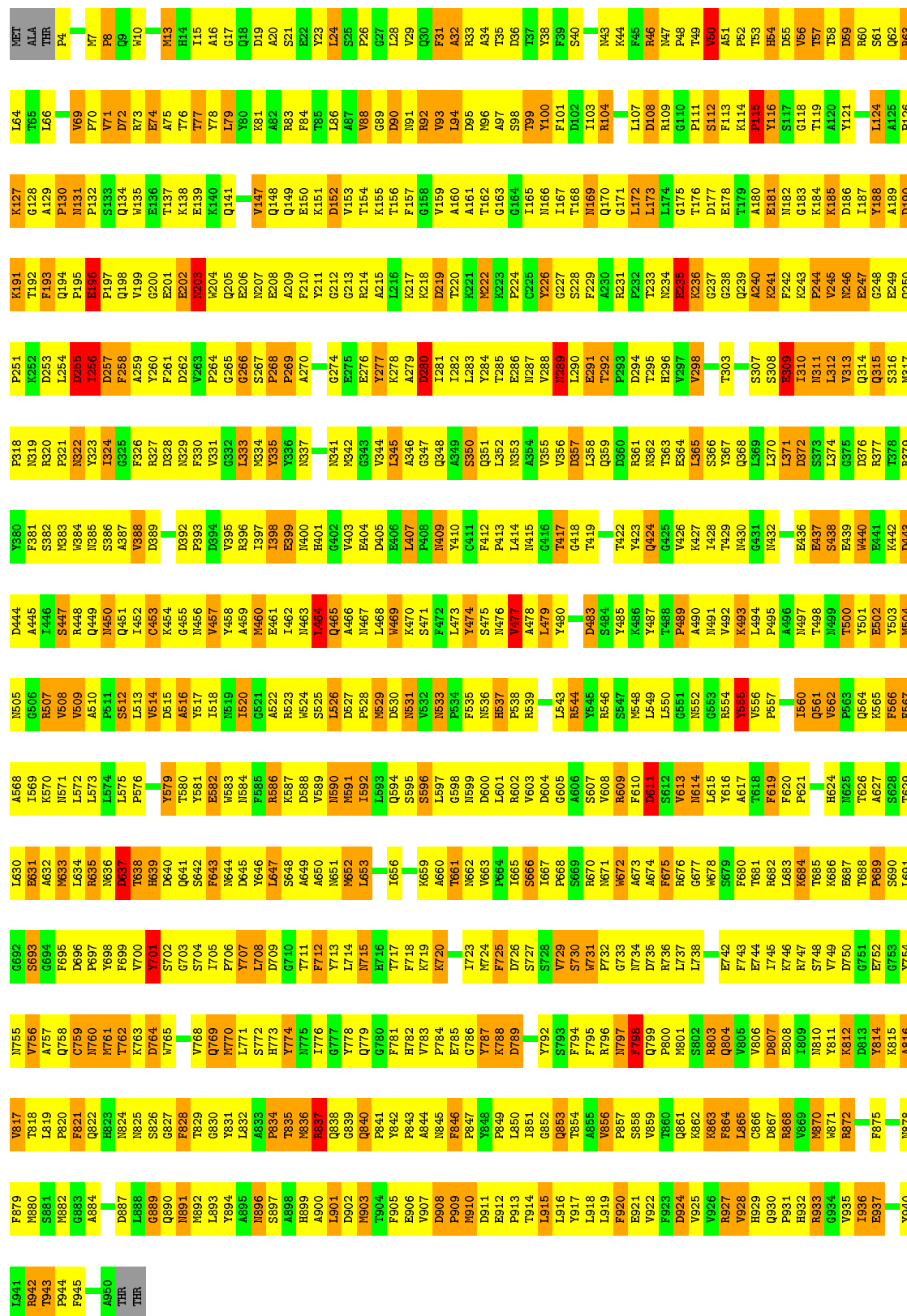
● Molecule 1: Hexon protein

Chain K: 18% 55% 24%

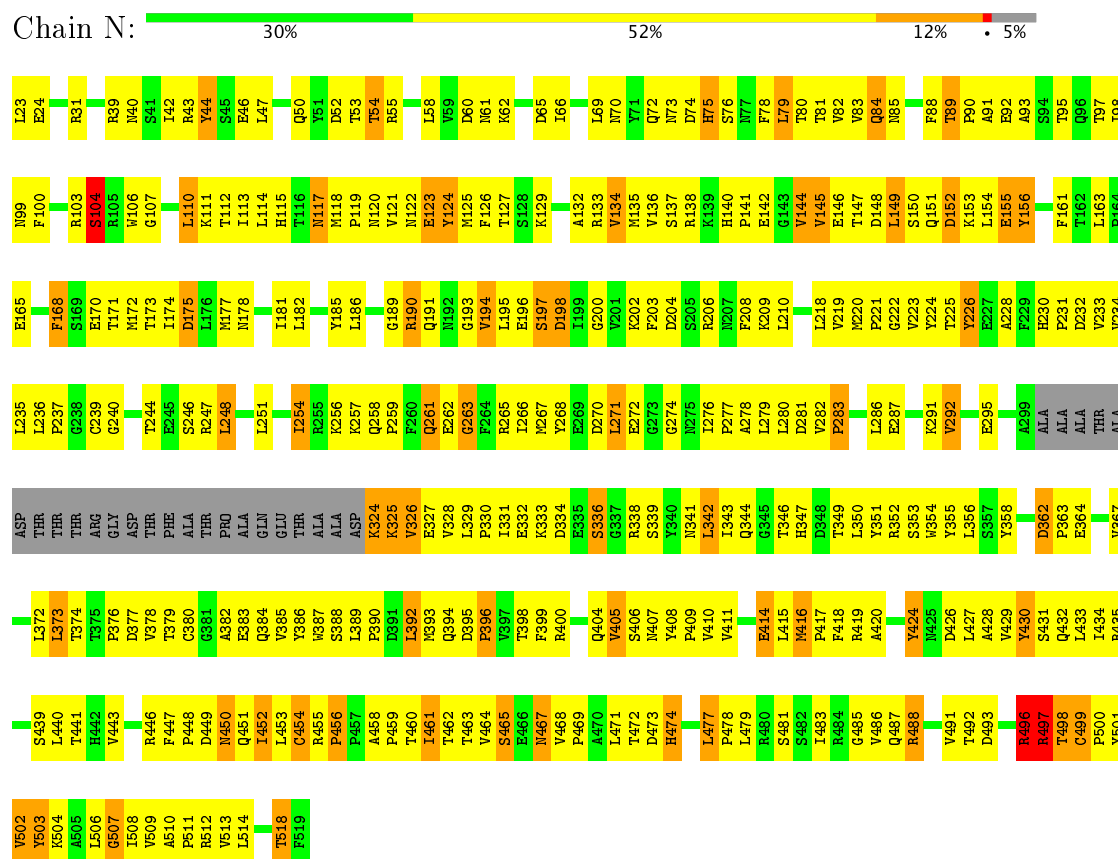


● Molecule 1: Hexon protein

Chain L:  20% 55% 22%



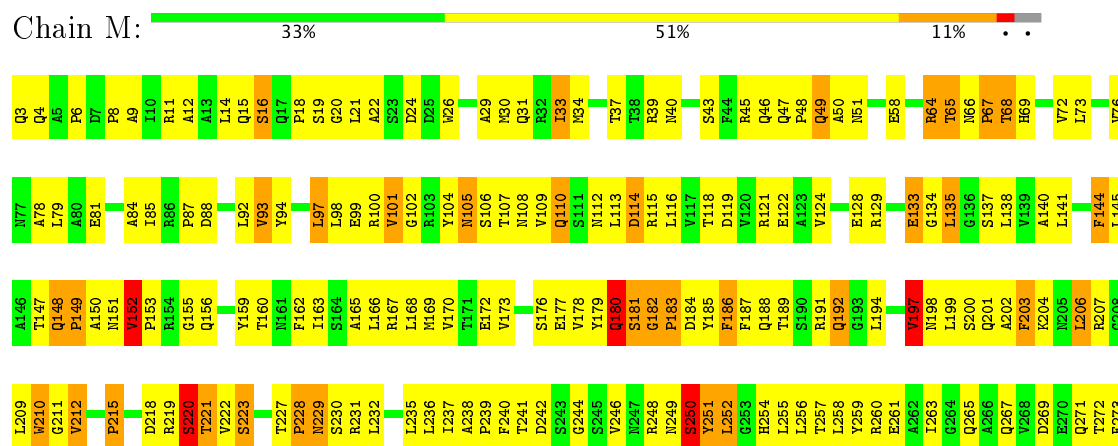
- Molecule 2: Penton

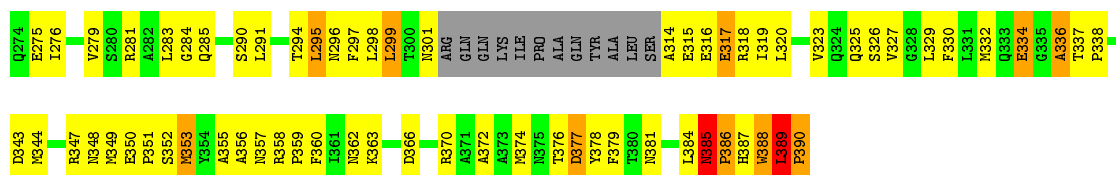


- Molecule 3: Fiber



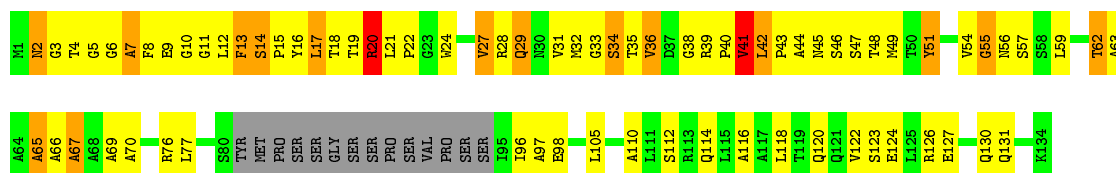
- Molecule 4: PIH1a





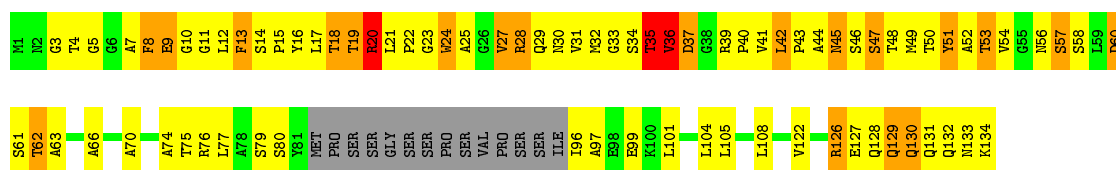
- Molecule 5: PIX

Chain P: 34% 43% 11% • 10%



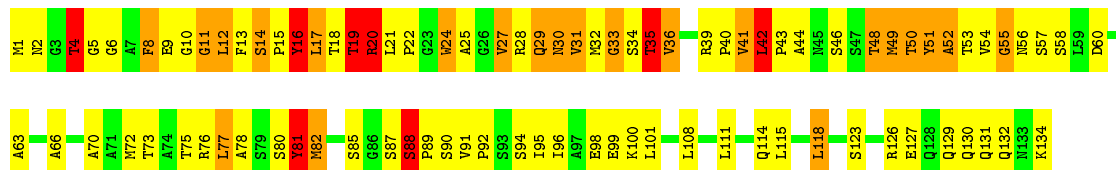
- Molecule 5: PIX

Chain Q: 29% 43% 15% • 10%



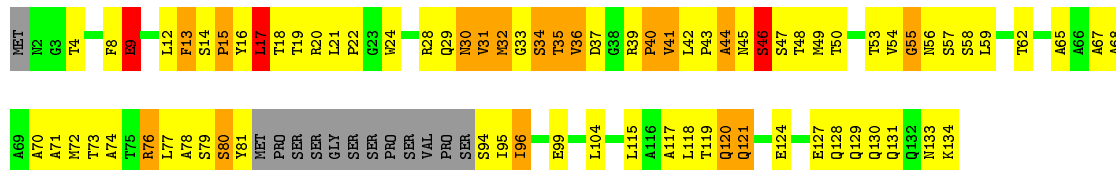
- Molecule 5: PIX

Chain R: 33% 45% 16% 6%



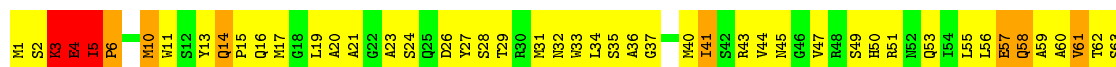
- Molecule 5: PIX

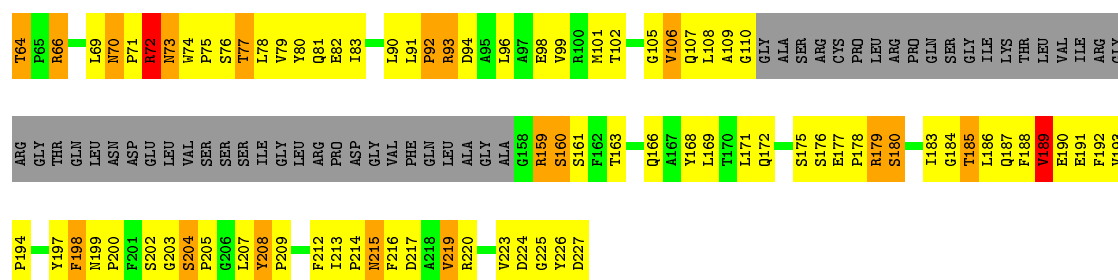
Chain S: 32% 43% 13% • 10%



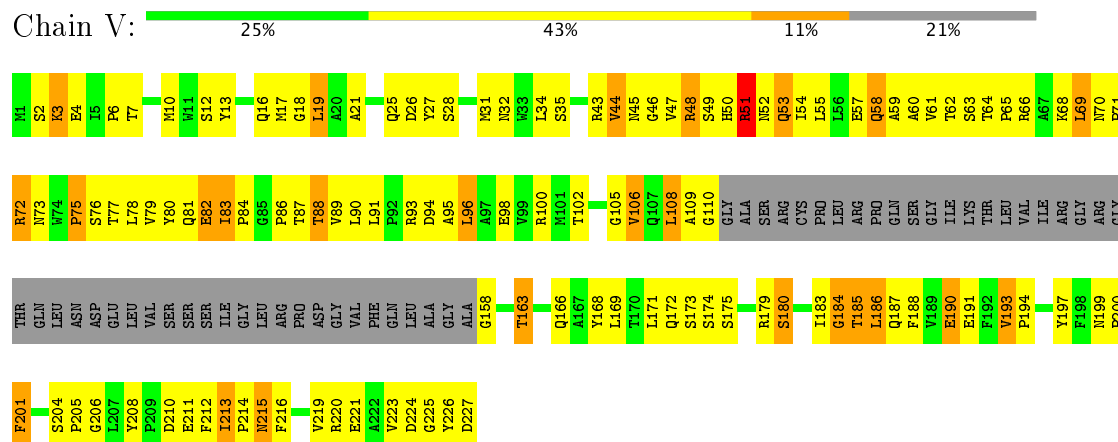
- Molecule 6: PVIII

Chain U: 21% 45% 11% • 21%

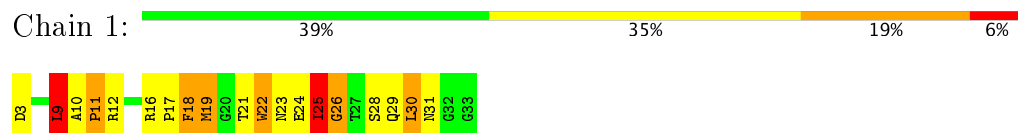




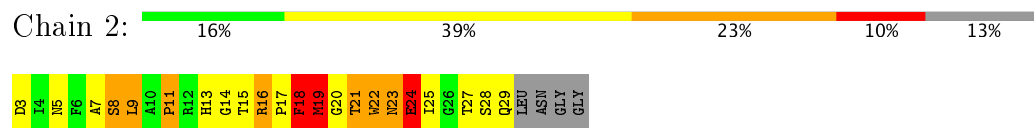
• Molecule 6: PVIII



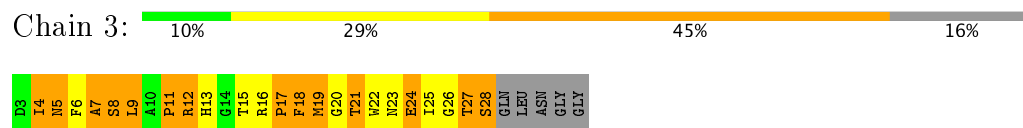
• Molecule 7: PVI



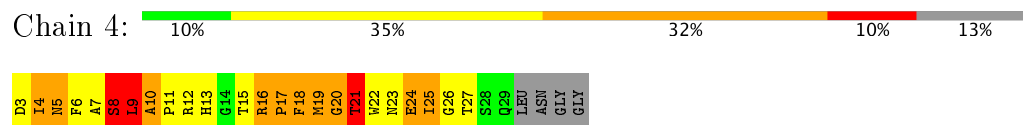
• Molecule 7: PVI



• Molecule 7: PVI



• Molecule 7: PVI

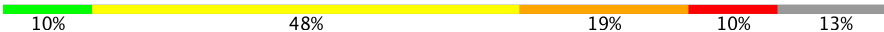


- Molecule 7: PVI

Chain 5: 



- Molecule 7: PVI

Chain 6: 



- Molecule 7: PVI

Chain 7: 



- Molecule 7: PVI

Chain 8: 



- Molecule 7: PVI

Chain 9: 



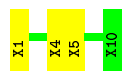
- Molecule 8: Unknown

Chain X: 

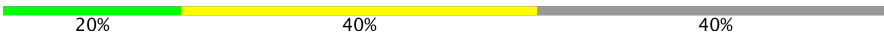


- Molecule 8: Unknown

Chain Y: 



- Molecule 8: Unknown

Chain Z: 

X5	X6	X9	X10	UNK	UNK	UNK
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	19000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.73	5/7757 (0.1%)	1.12	54/10551 (0.5%)
1	B	0.95	15/7743 (0.2%)	1.40	81/10534 (0.8%)
1	C	0.80	5/7726 (0.1%)	1.19	52/10509 (0.5%)
1	D	0.82	10/7732 (0.1%)	1.18	47/10517 (0.4%)
1	E	0.90	12/7732 (0.2%)	1.28	78/10517 (0.7%)
1	F	0.86	6/7751 (0.1%)	1.27	70/10544 (0.7%)
1	G	0.92	9/7732 (0.1%)	1.57	70/10517 (0.7%)
1	H	0.92	11/7732 (0.1%)	1.33	69/10517 (0.7%)
1	I	0.78	1/7743 (0.0%)	1.18	53/10534 (0.5%)
1	J	1.01	11/7758 (0.1%)	1.26	49/10554 (0.5%)
1	K	0.84	3/7758 (0.0%)	1.22	55/10554 (0.5%)
1	L	0.77	2/7731 (0.0%)	1.18	45/10516 (0.4%)
2	N	0.71	4/3896 (0.1%)	0.98	15/5302 (0.3%)
3	O	1.04	0/167	1.66	1/225 (0.4%)
4	M	0.75	5/2990 (0.2%)	1.04	20/4067 (0.5%)
5	P	0.86	1/879 (0.1%)	1.44	15/1190 (1.3%)
5	Q	1.04	1/884 (0.1%)	1.45	13/1197 (1.1%)
5	R	0.82	0/978	1.30	13/1328 (1.0%)
5	S	0.78	0/890	1.22	7/1206 (0.6%)
6	U	0.73	0/1428	1.06	2/1946 (0.1%)
6	V	0.68	0/1428	1.01	5/1946 (0.3%)
7	1	1.45	2/242 (0.8%)	1.89	7/326 (2.1%)
7	2	1.20	0/217	1.73	6/294 (2.0%)
7	3	0.92	0/208	1.73	10/282 (3.5%)
7	4	1.26	2/217 (0.9%)	1.66	10/294 (3.4%)
7	5	1.21	0/208	1.71	7/282 (2.5%)
7	6	1.04	0/217	1.56	9/294 (3.1%)
7	7	1.06	1/208 (0.5%)	1.70	5/282 (1.8%)
7	8	1.28	1/242 (0.4%)	1.67	3/326 (0.9%)
7	9	1.16	0/208	1.46	2/282 (0.7%)
All	All	0.86	107/108402 (0.1%)	1.26	873/147433 (0.6%)

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	0	2
1	B	0	5
1	C	0	1
1	E	0	2
1	F	0	3
1	G	1	3
1	H	0	2
1	I	0	1
1	J	0	2
1	L	0	2
5	P	0	1
All	All	1	24

The worst 5 of 107 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	277	TYR	CB-CG	-49.00	0.78	1.51
1	B	433	ASP	CB-CG	-28.79	0.91	1.51
1	H	328	ASP	CB-CG	-21.23	1.07	1.51
1	G	776	ILE	CB-CG1	-20.98	0.95	1.54
1	D	297	VAL	CB-CG1	19.99	1.94	1.52

The worst 5 of 873 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	774	TYR	CB-CG-CD1	-63.44	82.93	121.00
1	G	774	TYR	CB-CG-CD2	60.92	157.55	121.00
1	B	210	PHE	CB-CG-CD2	-28.19	101.07	120.80
1	J	277	TYR	CA-CB-CG	25.09	161.06	113.40
1	B	210	PHE	CB-CG-CD1	25.02	138.31	120.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	G	776	ILE	CB

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	GLN	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
1	B	429	THR	Mainchain,Peptide
1	B	431	GLY	Mainchain
1	B	432	ASN	Sidechain
1	B	433	ASP	Mainchain

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	7551	0	7220	1552	0
1	B	7536	0	7195	2040	0
1	C	7519	0	7187	1985	0
1	D	7526	0	7193	1420	0
1	E	7526	0	7186	1709	0
1	F	7544	0	7214	2019	0
1	G	7526	0	7193	1614	0
1	H	7526	0	7184	1842	0
1	I	7536	0	7203	1663	0
1	J	7551	0	7211	1876	0
1	K	7551	0	7216	1769	0
1	L	7524	0	7194	1819	0
2	N	3803	0	3723	530	0
3	O	162	0	148	25	0
4	M	2938	0	2905	414	0
5	P	871	0	873	278	0
5	Q	875	0	873	338	0
5	R	965	0	962	318	0
5	S	881	0	877	157	0
6	U	1391	0	1342	374	0
6	V	1391	0	1344	199	0
7	1	236	0	219	95	0
7	2	211	0	196	66	0
7	3	202	0	188	68	0
7	4	211	0	196	95	0
7	5	202	0	188	65	0
7	6	211	0	196	74	0
7	7	202	0	188	29	0
7	8	236	0	219	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	9	202	0	188	86	0
8	X	51	0	14	6	0
8	Y	51	0	13	3	0
8	Z	30	0	8	9	0
All	All	105738	0	101256	21102	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 102.

The worst 5 of 21102 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:162:THR:HG21	1:J:193:PHE:CD2	1.16	1.65
1:A:407:LEU:HD21	1:C:474:TYR:CD2	1.30	1.64
1:F:950:ALA:CB	1:H:893:LEU:HD12	1.19	1.63
1:H:94:LEU:CD1	1:H:619:PHE:CD1	1.80	1.62
1:L:199:VAL:CG1	1:L:206:GLU:CG	1.75	1.61

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 PDB entries followed by that with respect to all EM entries.

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	947/952 (100%)	670 (71%)	190 (20%)	87 (9%)	1	13
1	B	947/952 (100%)	714 (75%)	173 (18%)	60 (6%)	1	23
1	C	944/952 (99%)	646 (68%)	207 (22%)	91 (10%)	1	12
1	D	945/952 (99%)	683 (72%)	195 (21%)	67 (7%)	1	20
1	E	945/952 (99%)	705 (75%)	170 (18%)	70 (7%)	1	18
1	F	948/952 (100%)	681 (72%)	178 (19%)	89 (9%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	945/952 (99%)	684 (72%)	194 (20%)	67 (7%)	1	20
1	H	945/952 (99%)	654 (69%)	216 (23%)	75 (8%)	1	16
1	I	947/952 (100%)	669 (71%)	192 (20%)	86 (9%)	1	13
1	J	949/952 (100%)	672 (71%)	206 (22%)	71 (8%)	1	18
1	K	949/952 (100%)	718 (76%)	160 (17%)	71 (8%)	1	18
1	L	945/952 (99%)	638 (68%)	235 (25%)	72 (8%)	1	17
2	N	469/497 (94%)	366 (78%)	76 (16%)	27 (6%)	2	24
3	O	17/19 (90%)	13 (76%)	3 (18%)	1 (6%)	2	24
4	M	372/388 (96%)	281 (76%)	63 (17%)	28 (8%)	1	18
5	P	116/134 (87%)	84 (72%)	25 (22%)	7 (6%)	2	24
5	Q	116/134 (87%)	89 (77%)	22 (19%)	5 (4%)	3	32
5	R	132/134 (98%)	97 (74%)	26 (20%)	9 (7%)	1	21
5	S	117/134 (87%)	83 (71%)	26 (22%)	8 (7%)	1	21
6	U	176/227 (78%)	131 (74%)	32 (18%)	13 (7%)	1	18
6	V	176/227 (78%)	126 (72%)	36 (20%)	14 (8%)	1	16
7	1	29/31 (94%)	20 (69%)	6 (21%)	3 (10%)	0	10
7	2	25/31 (81%)	15 (60%)	7 (28%)	3 (12%)	0	7
7	3	24/31 (77%)	12 (50%)	7 (29%)	5 (21%)	0	2
7	4	25/31 (81%)	13 (52%)	6 (24%)	6 (24%)	0	1
7	5	24/31 (77%)	14 (58%)	9 (38%)	1 (4%)	3	32
7	6	25/31 (81%)	15 (60%)	3 (12%)	7 (28%)	0	0
7	7	24/31 (77%)	13 (54%)	5 (21%)	6 (25%)	0	0
7	8	29/31 (94%)	20 (69%)	6 (21%)	3 (10%)	0	10
7	9	24/31 (77%)	15 (62%)	4 (17%)	5 (21%)	0	2
All	All	13276/13597 (98%)	9541 (72%)	2678 (20%)	1057 (8%)	2	16

5 of 1057 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	ALA
1	A	89	GLY
1	A	151	LYS
1	A	199	VAL
1	A	248	GLY

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 PDB entries followed by that with respect to all EM entries.

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	817/818 (100%)	696 (85%)	121 (15%)	3	24
1	B	815/818 (100%)	662 (81%)	153 (19%)	2	12
1	C	814/818 (100%)	651 (80%)	163 (20%)	1	10
1	D	814/818 (100%)	675 (83%)	139 (17%)	2	17
1	E	814/818 (100%)	645 (79%)	169 (21%)	1	9
1	F	816/818 (100%)	603 (74%)	213 (26%)	0	4
1	G	814/818 (100%)	616 (76%)	198 (24%)	1	6
1	H	814/818 (100%)	604 (74%)	210 (26%)	0	5
1	I	815/818 (100%)	627 (77%)	188 (23%)	1	7
1	J	817/818 (100%)	609 (74%)	208 (26%)	0	5
1	K	817/818 (100%)	605 (74%)	212 (26%)	0	5
1	L	814/818 (100%)	635 (78%)	179 (22%)	1	7
2	N	428/443 (97%)	370 (86%)	58 (14%)	4	28
3	O	16/16 (100%)	14 (88%)	2 (12%)	5	31
4	M	317/327 (97%)	279 (88%)	38 (12%)	6	32
5	P	89/102 (87%)	77 (86%)	12 (14%)	4	28
5	Q	89/102 (87%)	73 (82%)	16 (18%)	2	14
5	R	102/102 (100%)	81 (79%)	21 (21%)	1	9
5	S	90/102 (88%)	72 (80%)	18 (20%)	1	10
6	U	153/190 (80%)	120 (78%)	33 (22%)	1	8
6	V	153/190 (80%)	124 (81%)	29 (19%)	2	11
7	1	24/24 (100%)	18 (75%)	6 (25%)	1	5
7	2	22/24 (92%)	13 (59%)	9 (41%)	0	0
7	3	21/24 (88%)	15 (71%)	6 (29%)	0	3
7	4	22/24 (92%)	18 (82%)	4 (18%)	2	13
7	5	21/24 (88%)	15 (71%)	6 (29%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	6	22/24 (92%)	21 (96%)	1 (4%)	32 69
7	7	21/24 (88%)	20 (95%)	1 (5%)	30 67
7	8	24/24 (100%)	20 (83%)	4 (17%)	2 18
7	9	21/24 (88%)	14 (67%)	7 (33%)	0 2
All	All	11416/11606 (98%)	8992 (79%)	2424 (21%)	4 8

5 of 2424 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	683	LEU
1	H	924	ASP
4	M	248	ARG
1	G	840	GLN
1	H	369	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 513 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	415	ASN
1	H	769	GLN
2	N	404	GLN
1	G	540	ASN
1	H	311	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	4
1	J	2
1	H	2
1	A	2
1	G	1
1	D	1
1	E	1

The worst 5 of 13 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	179:THR	C	180:ALA	N	2.03
1	B	432:ASN	C	433:ASP	N	1.65
1	B	429:THR	C	430:ASN	N	1.19
1	J	276:GLU	C	277:TYR	N	1.19
1	G	776:ILE	C	777:GLY	N	1.18