



## wwPDB EM Validation Summary Report ⓘ

May 14, 2024 – 06:35 am BST

PDB ID : 6Z7N  
EMDB ID : EMD-11108  
Title : The atomic structure of HAdV-F41 at pH 7.4  
Authors : Carlson, L.-A.; Rafie, K.  
Deposited on : 2020-05-31  
Resolution : 3.77 Å (reported)  
Based on initial model : 5TX1

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
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>.

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

EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

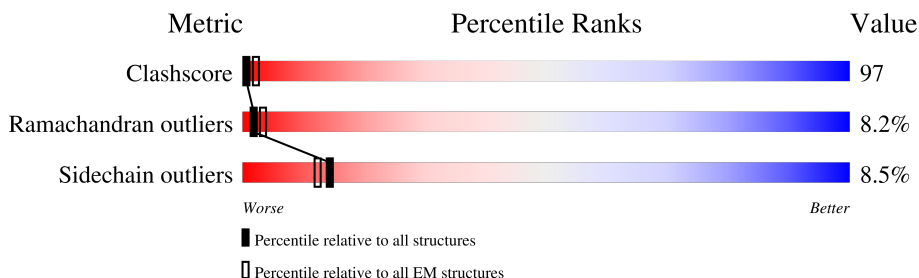
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.77 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.



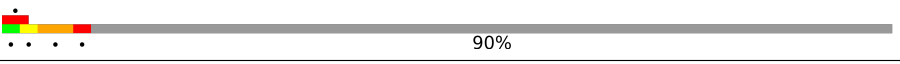
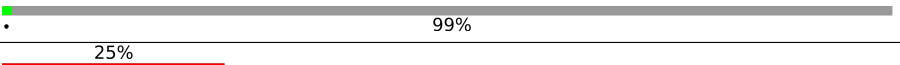
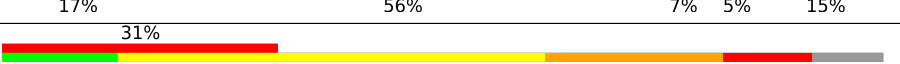
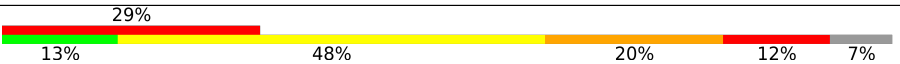
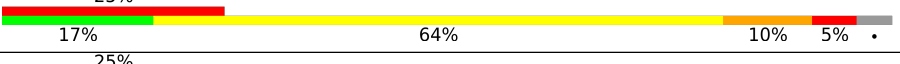
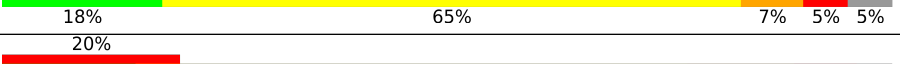
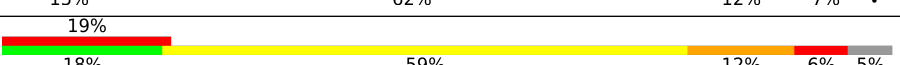
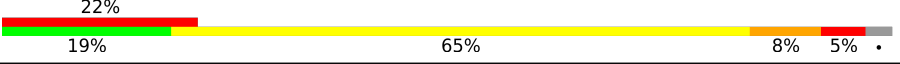
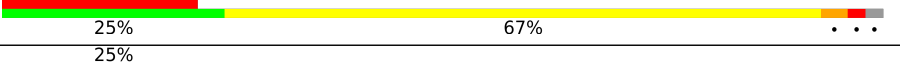
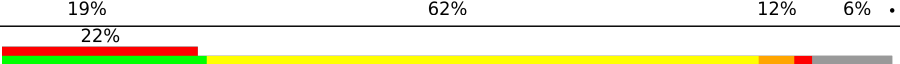
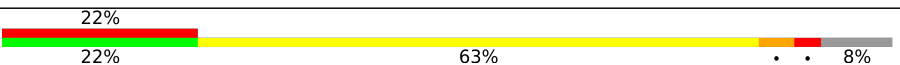
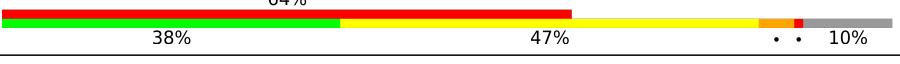
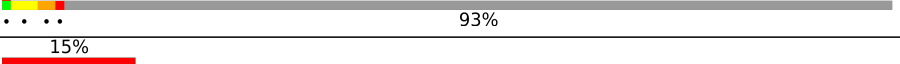
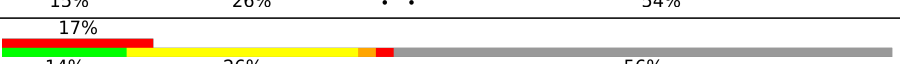


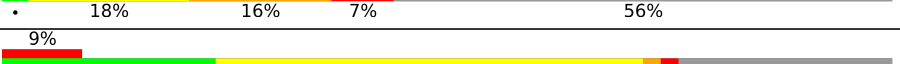
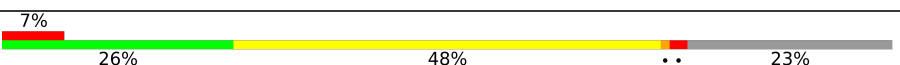

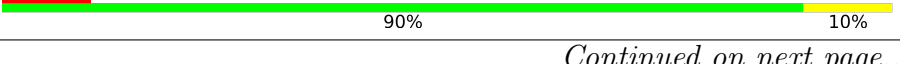



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	266	 95%
1	1	266	 94%
1	2	266	 98%
1	3	266	 95%
1	4	266	 93%
1	5	266	 94%
1	6	266	 99%
1	7	266	 99%




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Mol	Chain	Length	Quality of chain
1	8	266	
1	9	266	
2	A	925	
2	B	925	
2	C	925	
2	D	925	
2	E	925	
2	F	925	
2	G	925	
2	H	925	
2	I	925	
2	J	925	
2	K	925	
2	L	925	
3	M	508	
4	N	348	
5	O	579	
6	P	133	
6	Q	133	
6	R	133	
6	S	133	
7	T	233	
7	U	233	
8	X	7	
9	V	10	

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Mol	Chain	Length	Quality of chain
9	W	10	 50% 40% 10%
9	Z	10	 20% 80% 10% 10%
10	Y	6	 17% 50% 50%

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 94362 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 Pre-protein VI.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	12	Total	C	N	O	S	0	0
			94	59	20	14	1		
1	1	16	Total	C	N	O	S	0	0
			124	79	25	19	1		
1	2	6	Total	C	N	O	S	0	0
			48	31	9	7	1		
1	3	12	Total	C	N	O	S	0	0
			98	63	17	17	1		
1	4	19	Total	C	N	O	S	0	0
			147	91	29	26	1		
1	5	16	Total	C	N	O	S	0	0
			123	76	22	24	1		
1	6	3	Total	C	N	O		0	0
			28	17	8	3			
1	7	3	Total	C	N	O		0	0
			28	17	8	3			
1	8	26	Total	C	N	O	S	0	0
			197	122	38	36	1		
1	9	3	Total	C	N	O		0	0
			28	17	8	3			

- Molecule 2 is a protein called Hexon protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	788	Total	C	N	O	S	0	0
			6307	4029	1063	1180	35		
2	B	847	Total	C	N	O	S	0	0
			6761	4305	1146	1277	33		
2	C	860	Total	C	N	O	S	0	0
			6862	4368	1163	1296	35		
2	D	887	Total	C	N	O	S	0	0
			7057	4493	1194	1335	35		
2	E	878	Total	C	N	O	S	0	0
			6988	4451	1180	1321	36		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	889	Total	C	N	O	S	0	0
			7070	4499	1196	1339	36		
2	G	880	Total	C	N	O	S	0	0
			7008	4462	1183	1328	35		
2	H	894	Total	C	N	O	S	0	0
			7095	4513	1202	1344	36		
2	I	908	Total	C	N	O	S	0	0
			7212	4584	1222	1370	36		
2	J	907	Total	C	N	O	S	0	0
			7203	4577	1219	1371	36		
2	K	840	Total	C	N	O	S	0	0
			6702	4271	1130	1265	36		
2	L	855	Total	C	N	O	S	0	0
			6831	4358	1155	1283	35		

- Molecule 3 is a protein called Penton protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	458	Total	C	N	O	S	0	0
			3659	2322	630	696	11		

- Molecule 4 is a protein called Core-capsid bridging protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	24	Total	C	N	O	S	0	0
			198	124	34	37	3		

- Molecule 5 is a protein called Pre-hexon-linking protein IIIa.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	O	267	Total	C	N	O	S	0	0
			2088	1309	371	404	4		

- Molecule 6 is a protein called Hexon-interlacing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	58	Total	C	N	O	S	0	0
			419	262	74	80	3		
6	Q	50	Total	C	N	O	S	0	0
			366	233	65	67	1		
6	R	30	Total	C	N	O	S	0	0
			228	147	41	39	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	58	Total	C	N	O	S	0	0
			419	262	74	80	3		

- Molecule 7 is a protein called Pre-hexon-linking protein VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	178	Total	C	N	O	S	0	0
			1368	859	234	270	5		
7	U	179	Total	C	N	O	S	0	0
			1372	861	235	271	5		

- Molecule 8 is a protein called Fiber protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	X	7	Total	C	N	O	0	0
			64	46	8	10		

- Molecule 9 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	W	9	Total	C	N	O	0	0
			45	27	9	9		
9	V	10	Total	C	N	O	0	0
			50	30	10	10		
9	Z	9	Total	C	N	O	0	0
			45	27	9	9		

- Molecule 10 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	Y	6	Total	C	N	O	0	0
			30	18	6	6		





- Molecule 1: Pre-protein VI

Chain 3:  95%

[illegible]

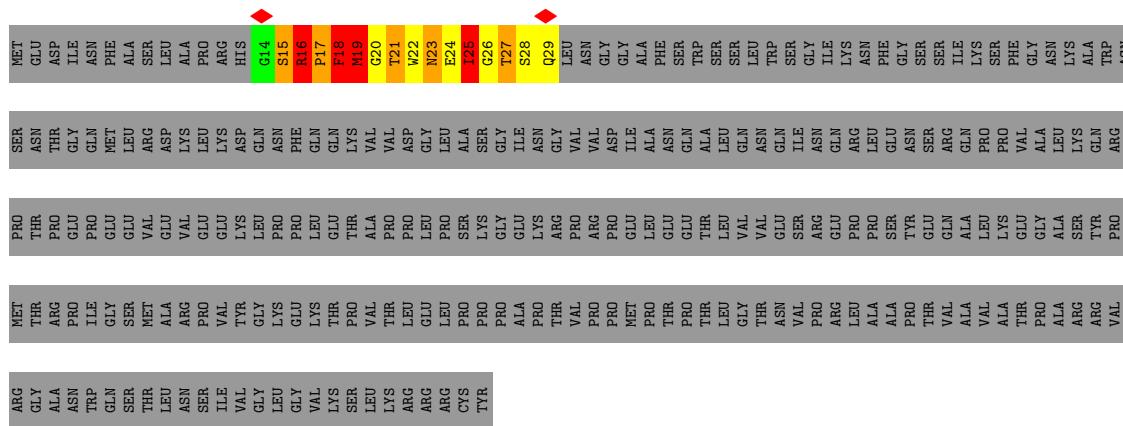
- Molecule 1: Pre-protein VI

Chain 4:  5% .. 93%

[illegible]

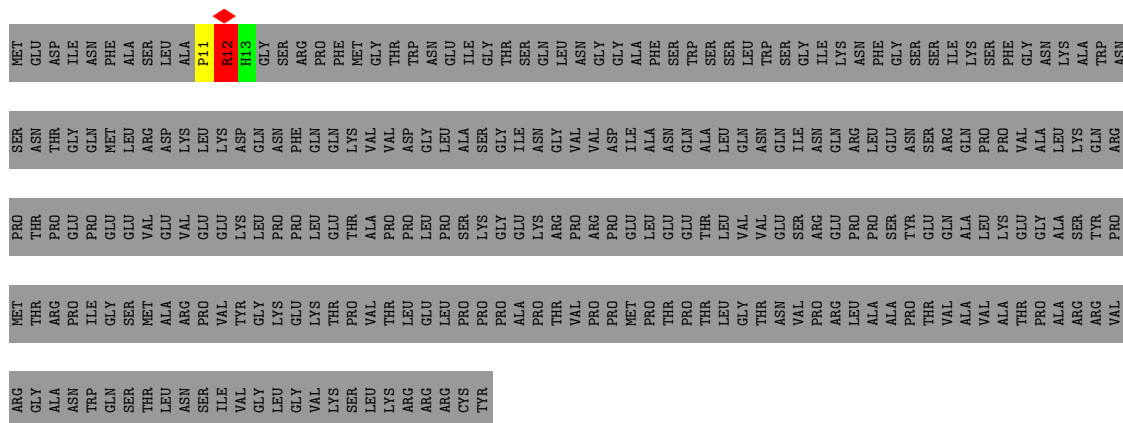
- Molecule 1: Pre-protein VI

Chain 5:  94%



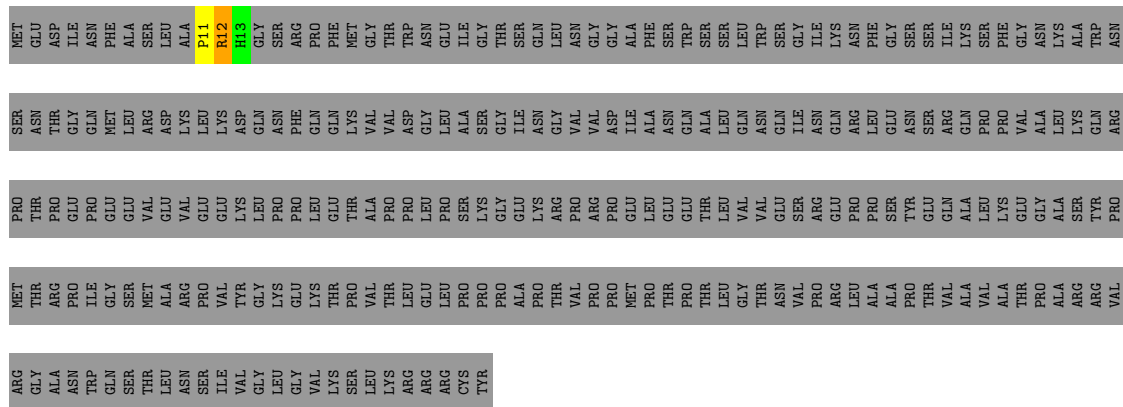
- Molecule 1: Pre-protein VI

Chain 6:  99%



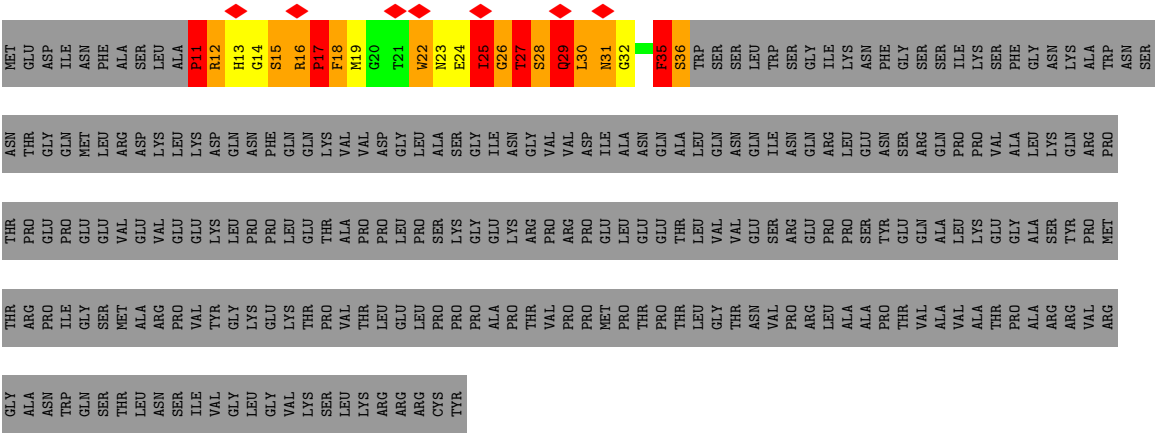
- Molecule 1: Pre-protein VI

Chain 7:  99%



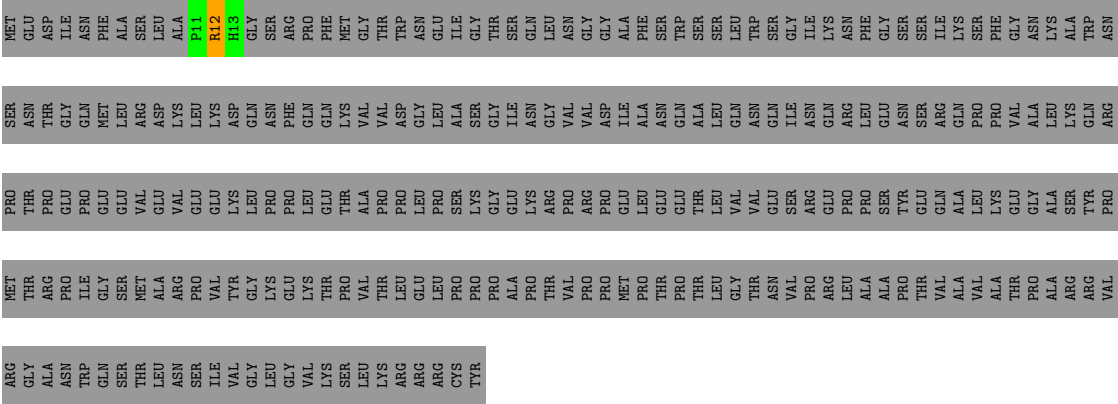
- Molecule 1: Pre-protein VI

Chain 8:  90%



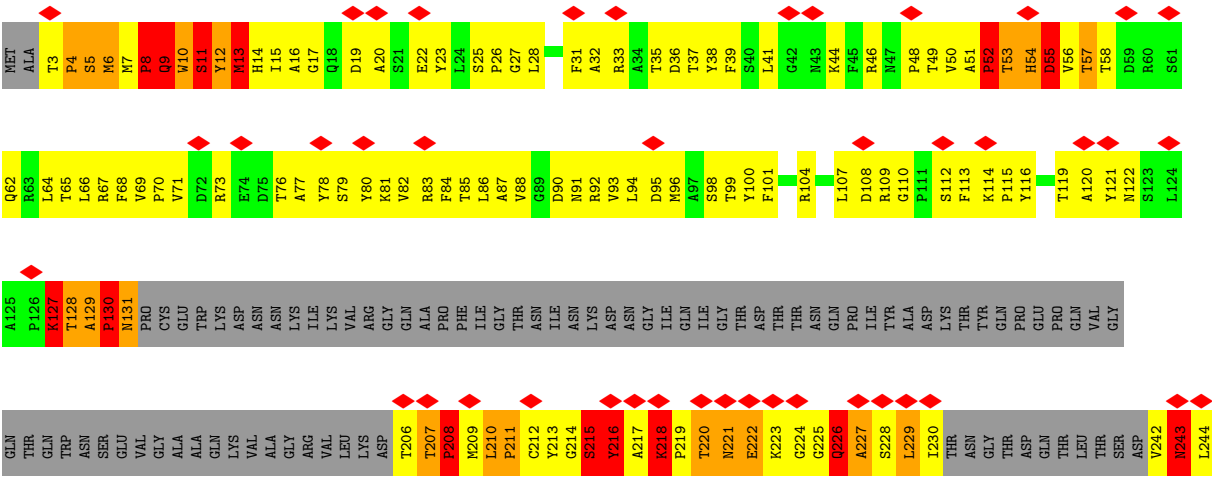
● Molecule 1: Pre-protein VI

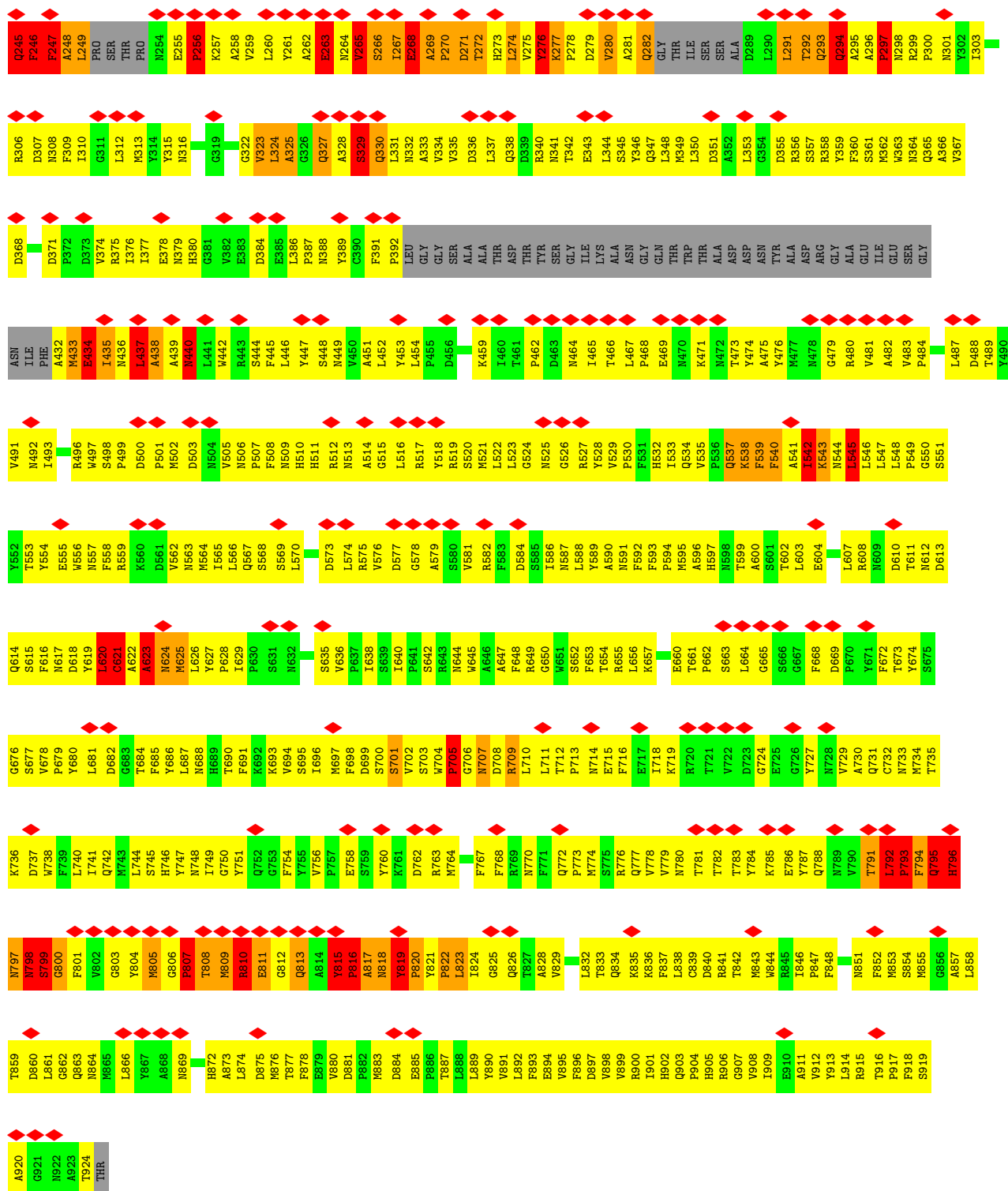
Chain 9: . 99%



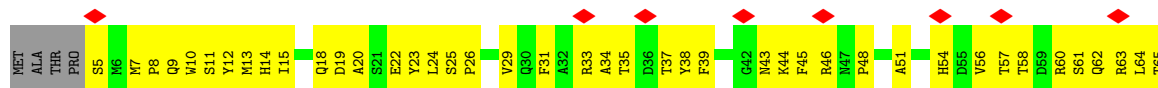
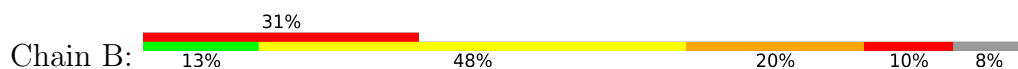
● Molecule 2: Hexon protein

Chain A: 17% 25% 56% 7% 5% 15%

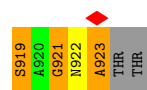




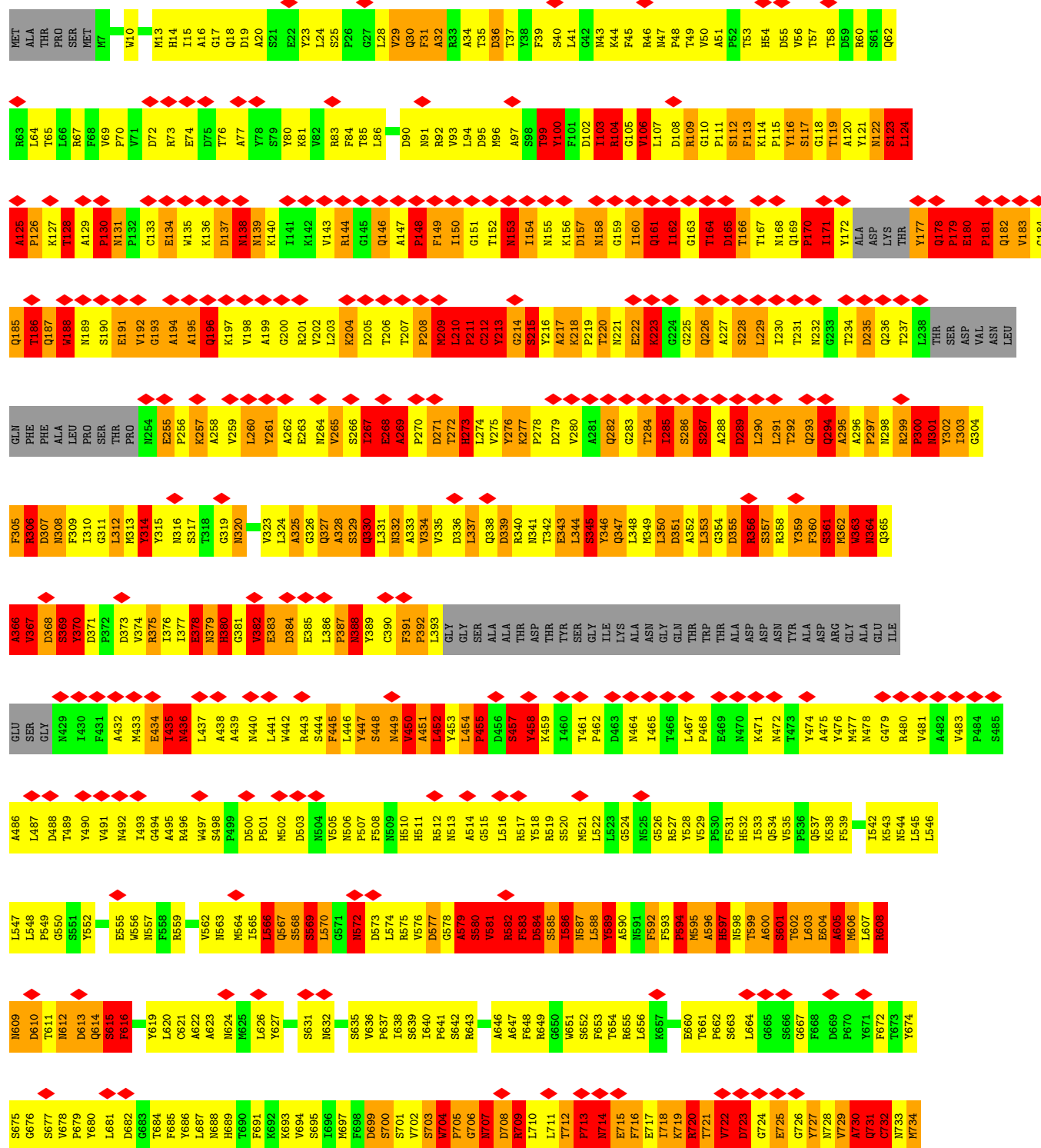
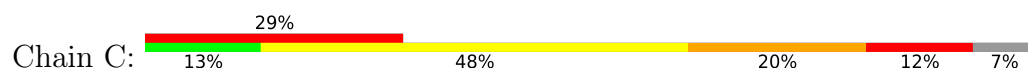
• Molecule 2: Hexon protein

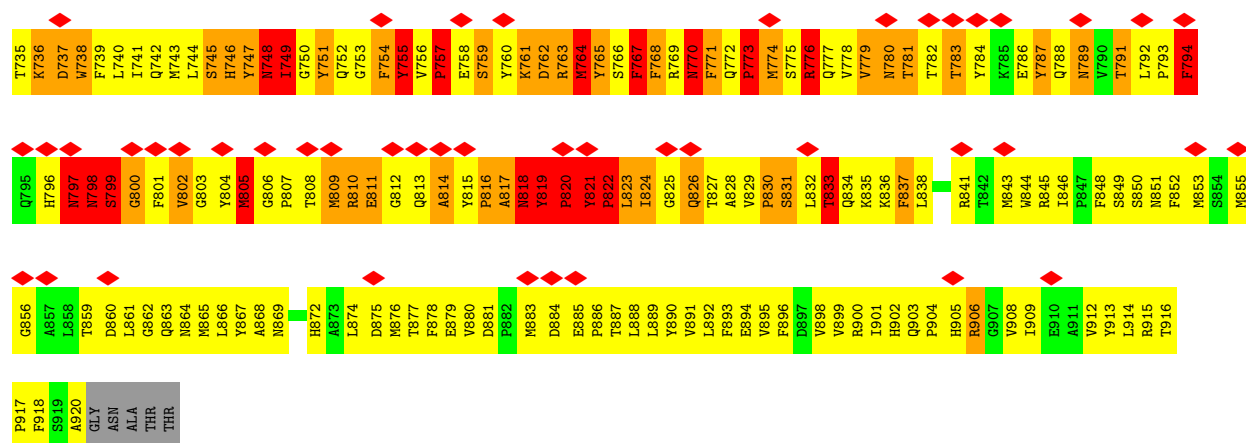


L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1074	L1075	L1076	L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088	L1089	L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100	L1101	L1102	L1103	L1104	L1105	L1106	L1107	L1108	L1109	L1110	L1111	L1112	L1113	L1114	L1115	L1116	L1117	L1118	L1119	L1120	L1121	L1122	L1123	L1124	L1125	L1126	L1127	L1128																																																																																																																																																																																																																																																																																																																																																																															
SER	GLY	PHE	VAL	GLY	TYR	MET	GLY	THR	PRO	MET	ARG	GLU	GLY	GLN	ALA	TYR	P816	P817	P818	P819	P820	P821	P822	P823	P824	P825	P826	P827	P828	P829	P830	P831	P832	P833	P834	P835	P836	P837	P838	P839	P840	P841	P842	P843	P844	P845	P846	P847	P848	P849	P850	P851	P852	P853	P854	P855	P856	P857	P858	P859	P860	P861	P862	P863	P864	P865	P866	P867	P868	P869	P870	P871	P872	P873	P874	P875	P876	P877	P878	P879	P880	P881	P882	P883	P884	P885	P886	P887	P888	P889	P890	P891	P892	P893	P894	P895	P896	P897	P898	P899	P900	P901	P902	P903	P904	P905	P906	P907	P908	P909	P910	P911	P912	P913	P914	P915	P916	P917	P918	P919	P920	P921	P922	P923	P924	P925	P926	P927	P928	P929	P930	P931	P932	P933	P934	P935	P936	P937	P938	P939	P940	P941	P942	P943	P944	P945	P946	P947	P948	P949	P950	P951	P952	P953	P954	P955	P956	P957	P958	P959	P960	P961	P962	P963	P964	P965	P966	P967	P968	P969	P970	P971	P972	P973	P974	P975	P976	P977	P978	P979	P980	P981	P982	P983	P984	P985	P986	P987	P988	P989	P990	P991	P992	P993	P994	P995	P996	P997	P998	P999	L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1074	L1075	L1076	L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088	L1089	L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100	L1101	L1102	L1103	L1104	L1105	L1106	L1107	L1108	L1109	L1110	L1111	L1112	L1113	L1114	L1115	L1116	L1117	L1118	L1119	L1120	L1121	L1122	L1123	L1124	L1125	L1126	L1127	L1128																																																																																																																																																																																																																																																																																																																				
L489	L490	L491	L492	L493	L494	L495	L496	L497	D500	P501	P502	D503	P504	P505	P506	P507	P508	P509	P510	P511	P512	P513	P514	P515	P516	P517	P518	P519	P520	P521	P522	P523	P524	P525	P526	P527	P528	P529	P530	P531	P532	P533	P534	P535	P536	P537	P538	P539	P540	P541	P542	P543	P544	P545	P546	P547	P548	P549	P550	P551	P552	P553	P554	P555	P556	P557	P558	P559	P560	P561	P562	P563	P564	P565	P566	P567	P568	P569	P570	P571	P572	P573	P574	P575	P576	P577	P578	P579	P580	P581	P582	P583	P584	P585	P586	P587	P588	P589	P590	P591	P592	P593	P594	P595	P596	P597	P598	P599	P600	P601	P602	P603	P604	P605	P606	P607	P608	P609	P610	P611	P612	P613	P614	P615	P616	P617	P618	P619	P620	P621	P622	P623	P624	P625	P626	P627	P628	P629	P630	P631	P632	P633	P634	P635	P636	P637	P638	P639	P640	P641	P642	P643	P644	P645	P646	P647	P648	P649	P650	P651	P652	P653	P654	P655	P656	P657	P658	P659	P660	P661	P662	P663	P664	P665	P666	P667	P668	P669	P670	P671	P672	P673	P674	P675	P676	P677	P678	P679	P680	P681	P682	P683	P684	P685	P686	P687	P688	P689	P690	P691	P692	P693	P694	P695	P696	P697	P698	P699	P700	P701	P702	P703	P704	P705	P706	P707	P708	P709	P710	P711	P712	P713	P714	P715	P716	P717	P718	P719	P720	P721	P722	P723	P724	P725	P726	P727	P728	P729	P730	P731	P732	P733	P734	P735	P736	P737	P738	P739	P740	P741	P742	P743	P744	P745	P746	P747	P748	P749	P750	P751	P752	P753	P754	P755	P756	P757	P758	P759	P760	P761	P762	P763	P764	P765	P766	P767	P768	P769	P770	P771	P772	P773	P774	P775	P776	P777	P778	P779	P780	P781	P782	P783	P784	P785	P786	P787	P788	P789	P790	P791	P792	P793	P794	P795	P796	P797	P798	P799	P800	P801	P802	P803	P804	P805	P806	P807	P808	P809	P810	P811	P812	P813	P814	P815	P816	P817	P818	P819	P820	P821	P822	P823	P824	P825	P826	P827	P828	P829	P830	P831	P832	P833	P834	P835	P836	P837	P838	P839	P840	P841	P842	P843	P844	P845	P846	P847	P848	P849	P850	P851	P852	P853	P854	P855	P856	P857	P858	P859	P860	P861	P862	P863	P864	P865	P866	P867	P868	P869	P870	P871	P872	P873	P874	P875	P876	P877	P878	P879	P880	P881	P882	P883	P884	P885	P886	P887	P888	P889	P890	P891	P892	P893	P894	P895	P896	P897	P898	P899	P900	P901	P902	P903	P904	P905	P906	P907	P908	P909	P910	P911	P912	P913	P914	P915	P916	P917	P918	P919	P920	P921	P922	P923	P924	P925	P926	P927	P928	P929	P930	P931	P932	P933	P934	P935	P936	P937	P938	P939	P940	P941	P942	P943	P944	P945	P946	P947	P948	P949	P950	P951	P952	P953	P954	P955	P956	P957	P958	P959	P960	P961	P962	P963	P964	P965	P966	P967	P968	P969	P970	P971	P972	P973	P974	P975	P976	P977	P978	P979	P980	P981	P982	P983	P984	P985	P986	P987	P988	P989	P990	P991	P992	P993	P994	P995	P996	P997	P998	P999	L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1074	L1075	L1076	L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088	L1089	L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100	L1101	L1102	L1103	L1104	L1105	L1106	L1107	L1108	L1109	L1110	L1111	L1112	L1113	L1114	L1115	L1116	L1117	L1118	L1119	L1120	L1121	L1122	L1123	L1124	L1125	L1126	L1127	L1128
F309	L310	G311	L312	M313	M314	Y315	N316	T317	G318	M319	M320	M321	V323	L324	A325	G326	Q327	N328	A329	S329	Q330	L331	N332	A333	V334	V335	D336	L337	Q338	L339	V340	N341	T342	S343	L344	S345	Y346	Q347	L348	M349	L350	D351	A352	L353	G354	D355	R356	S357	R358	Y359	F360	S361	M362	S363	N364	I365	Q366	S367	D368	S369	Y370	D371	P372	D373	V374	E375	L376	L377	E378	N379	H380	M381	G382	E383	D384	E385	L386	P387	T388	C389	P390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	F404	A405	A406	A407	A408	A409	A410	A411	A412	A413	A414	A415	A416	A417	A418	A419	A420	A421	A422	A423	A424	A425	A426	A427	A428	A429	A430	A431	A432	A433	A434	A435	A436	A437	A438	A439	A440	A441	A442	A443	A444	A445	A446	A447	A448	A449	A450	A451	A452	A453	A454	A455	A456	A457	A458	A459	A460	A461	A462	A463	A464	A465	A466	A467	A468	A469	A470	A471	A472	A473	A474	A475	A476	A477	A478	A479	A480	A481	A482	A483	A484	A485	A486	A487	A488	A489	A490	A491	A492	A493	A494	A495	A496	A497	A498	A499	A500	A501	A502	A503	A504	A505	A506	A507	A508	A509	A510	A511	A512	A513	A514	A515	A516	A517	A518	A519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552																																																																																																																																																																																																																																																																																																																																																																																																										

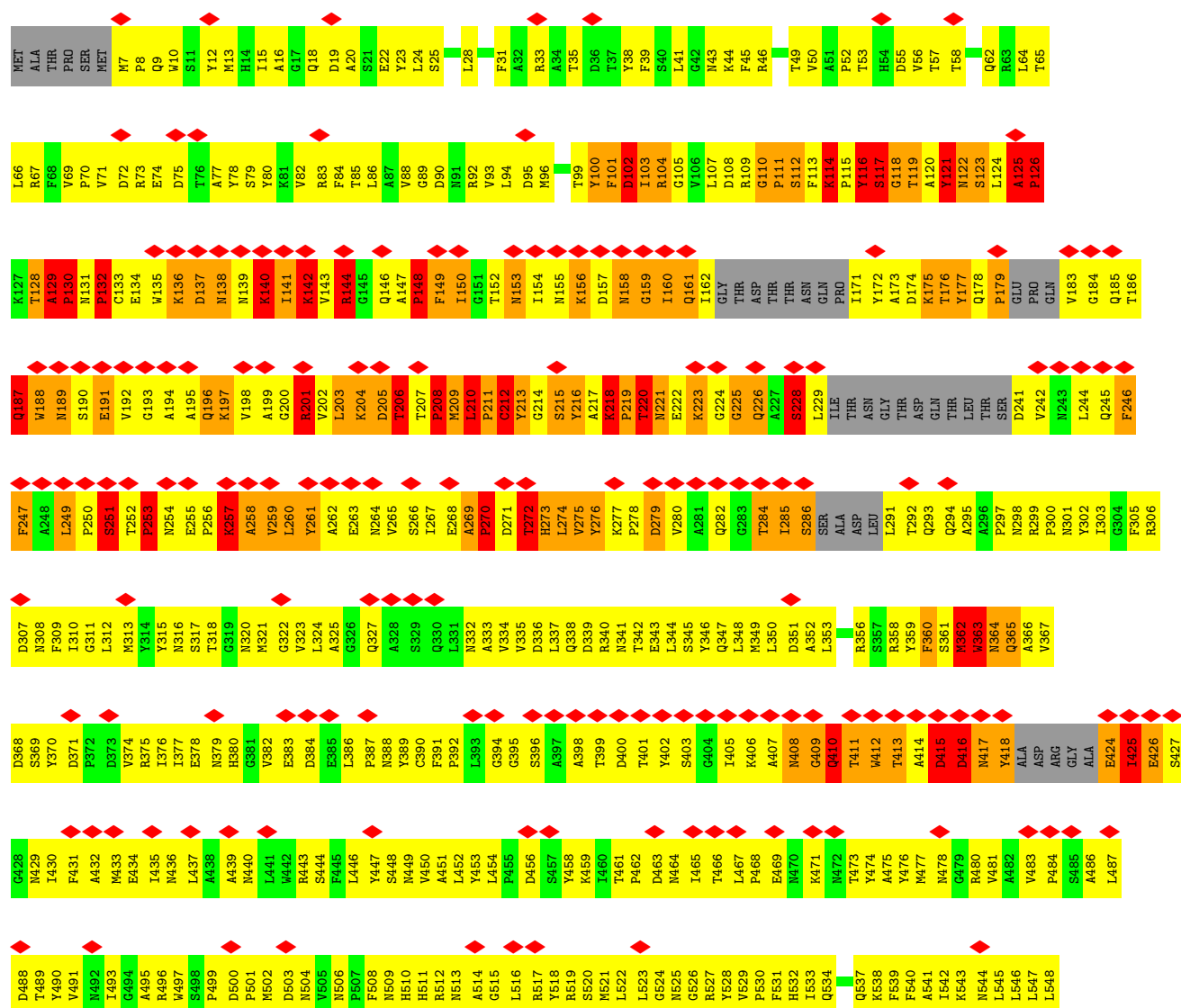


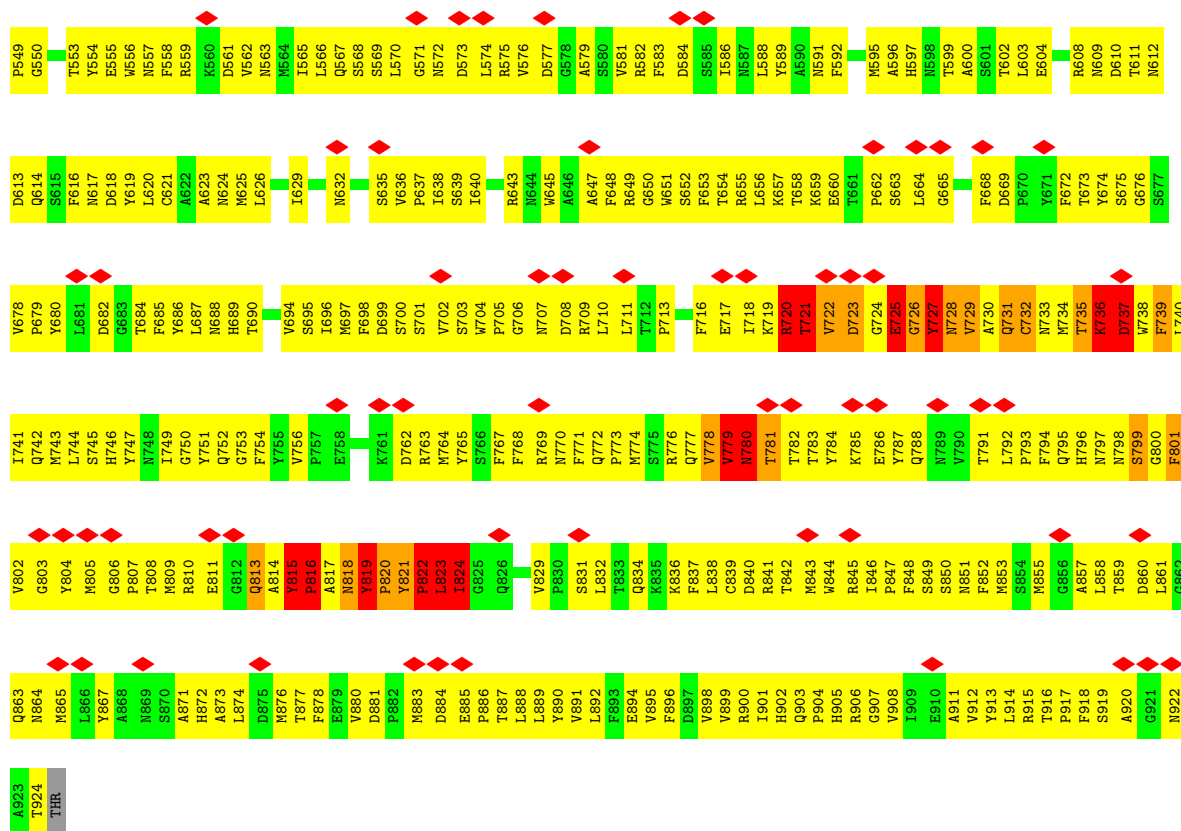
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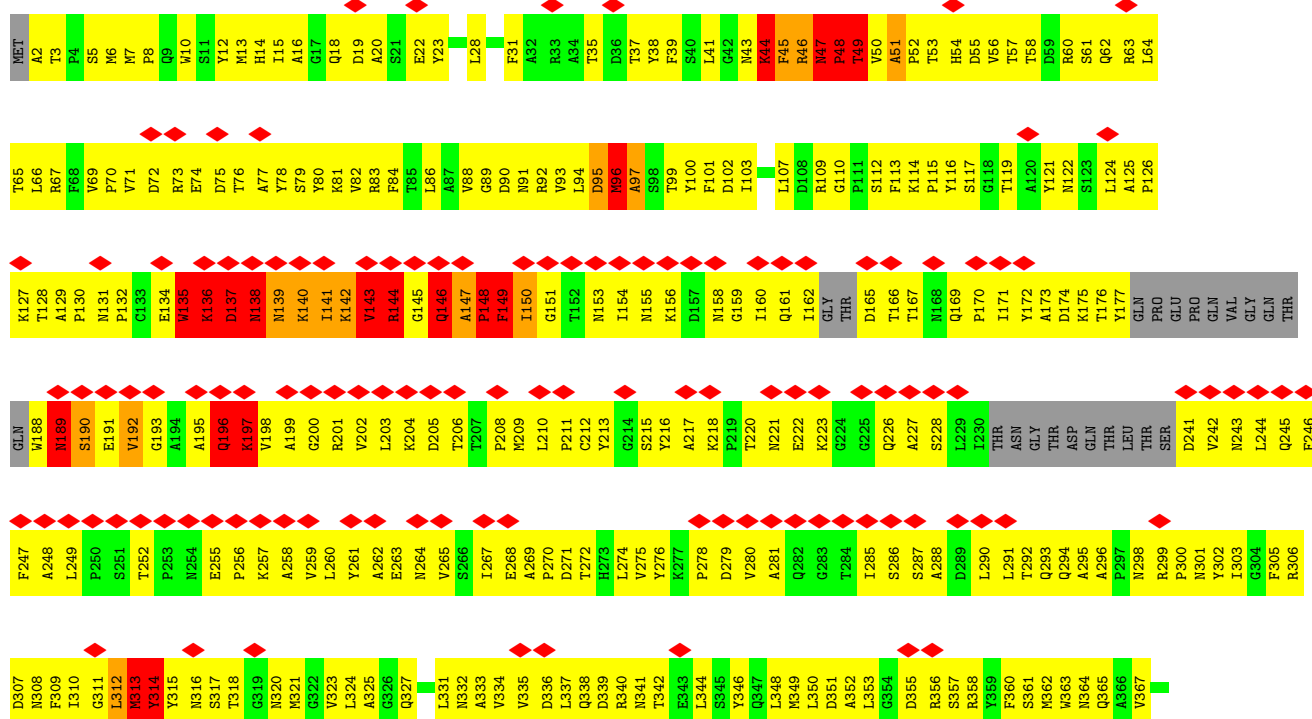


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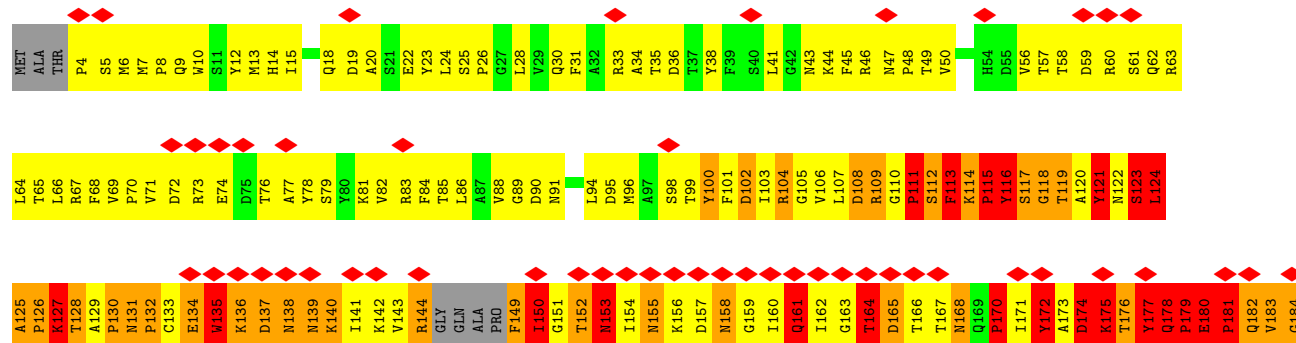
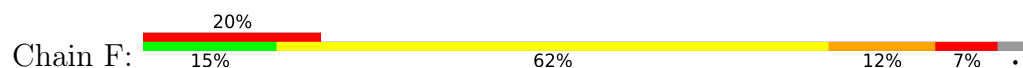


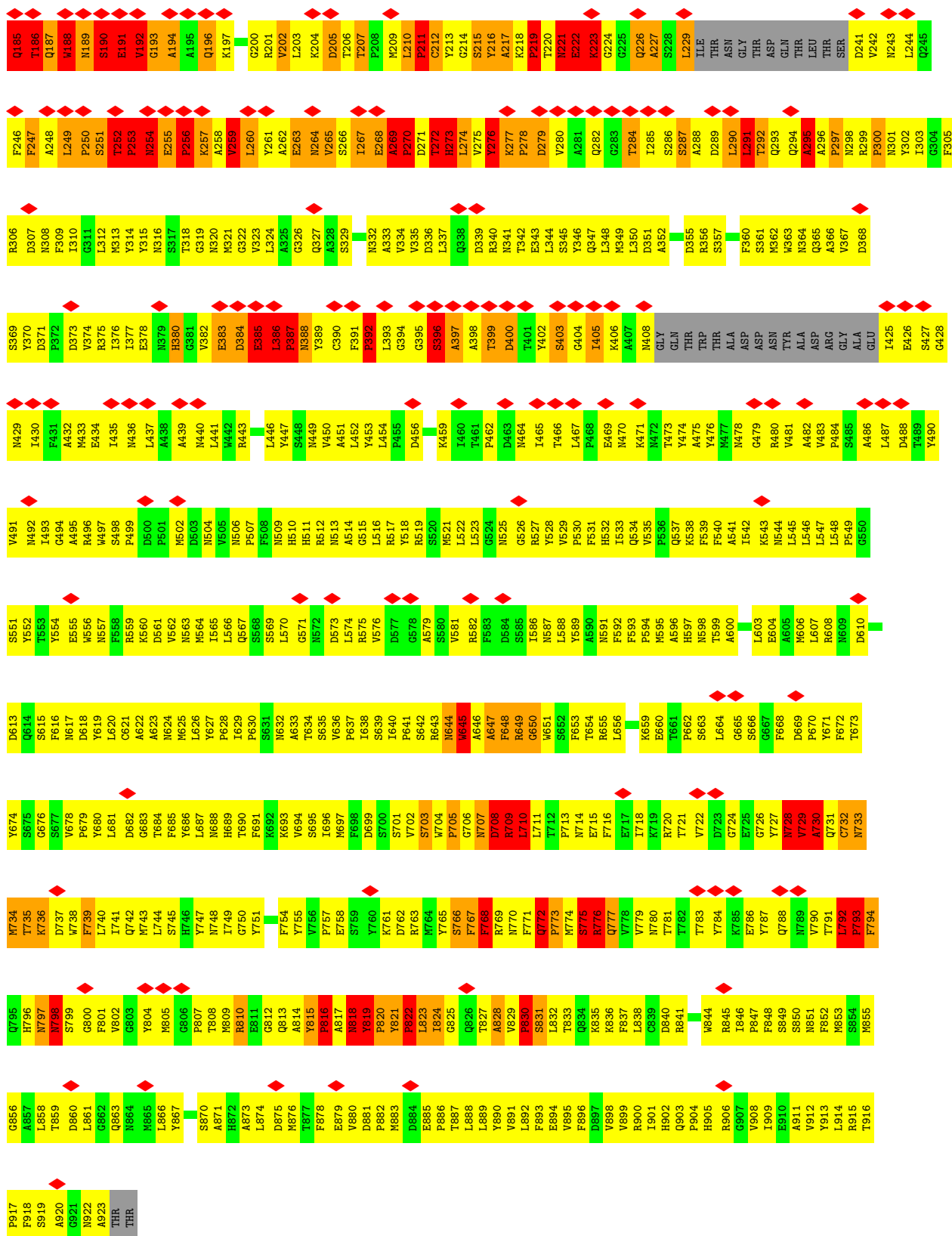
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- Molecule 2: Hexon protein

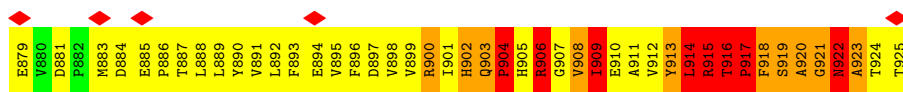




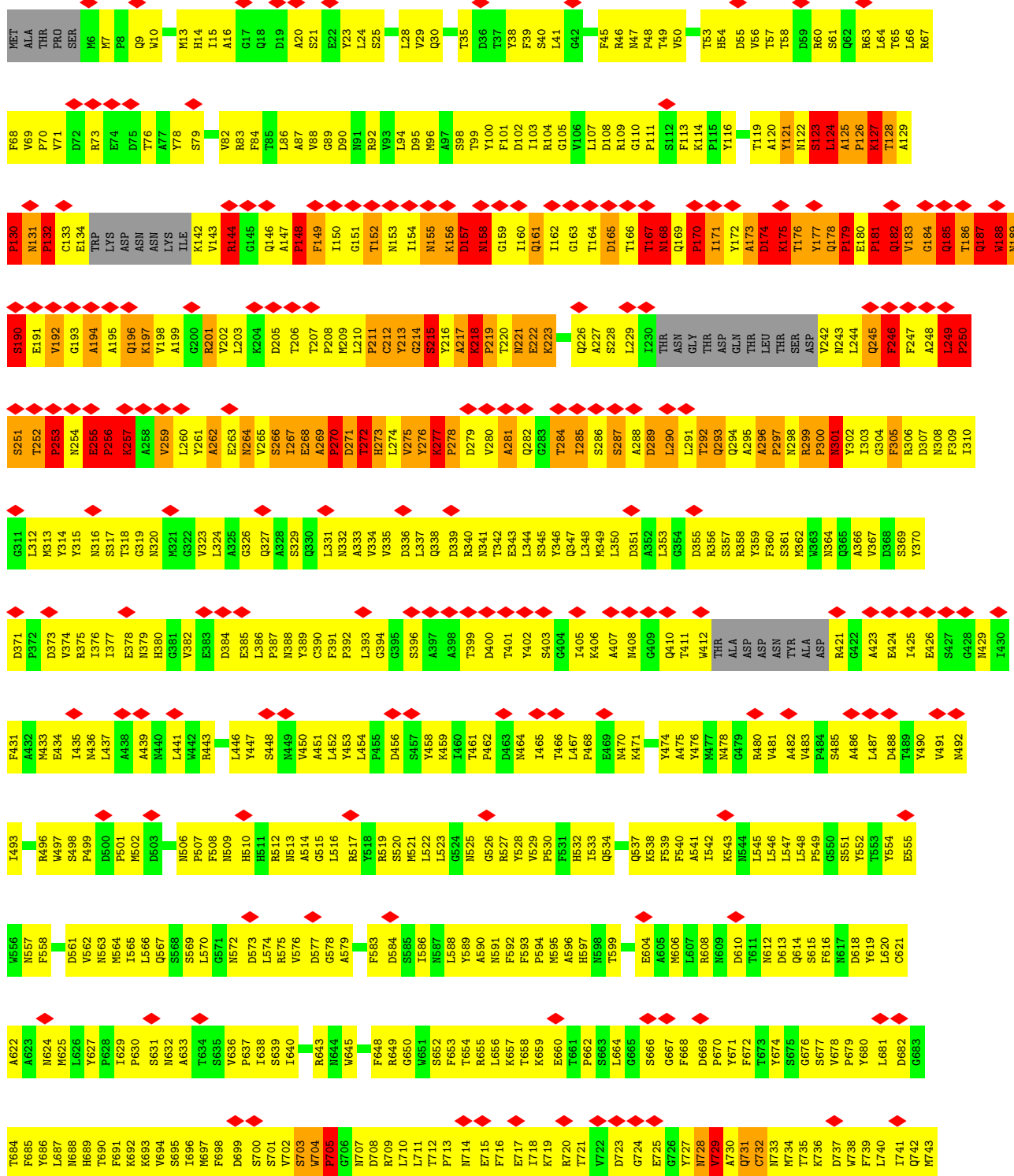
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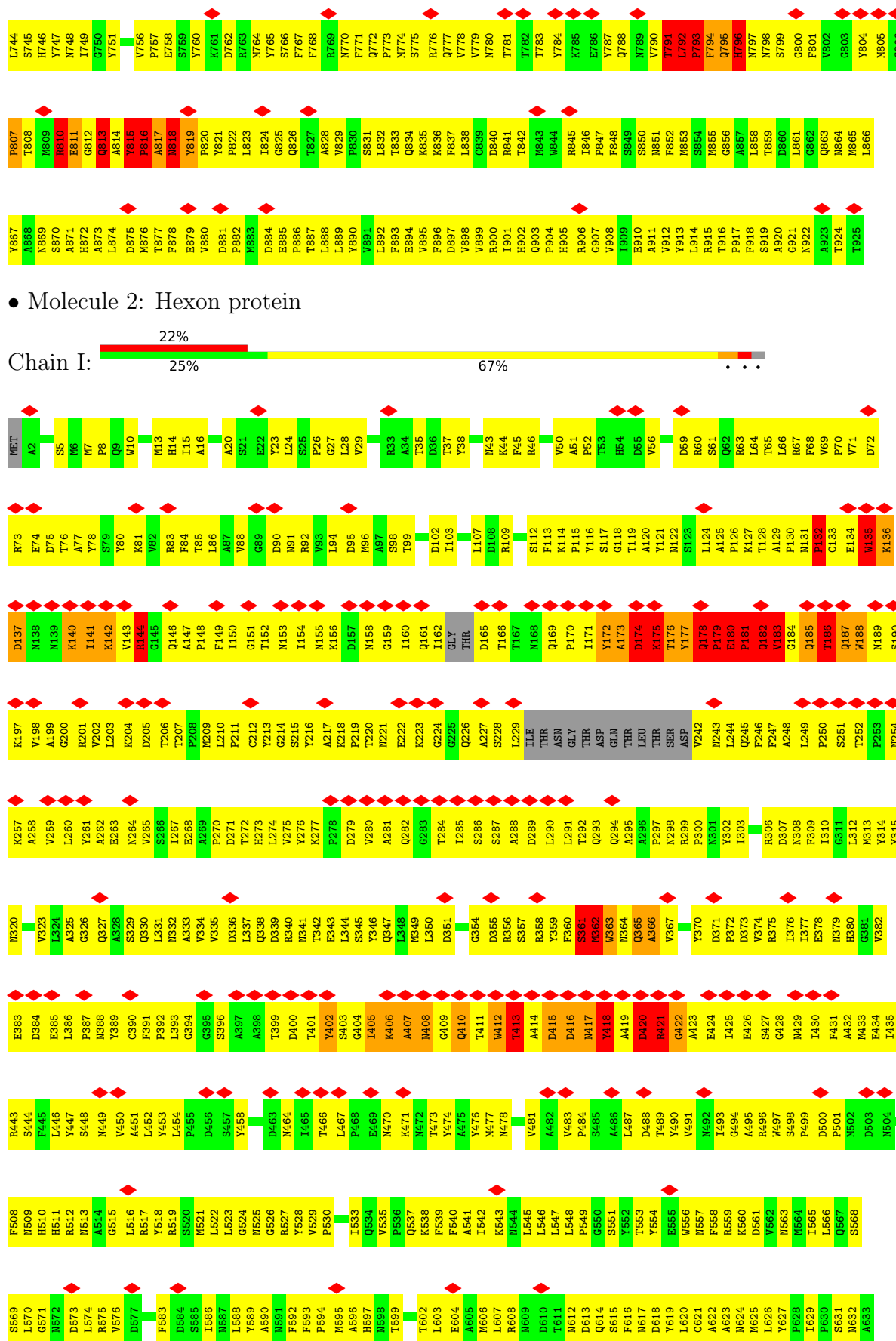


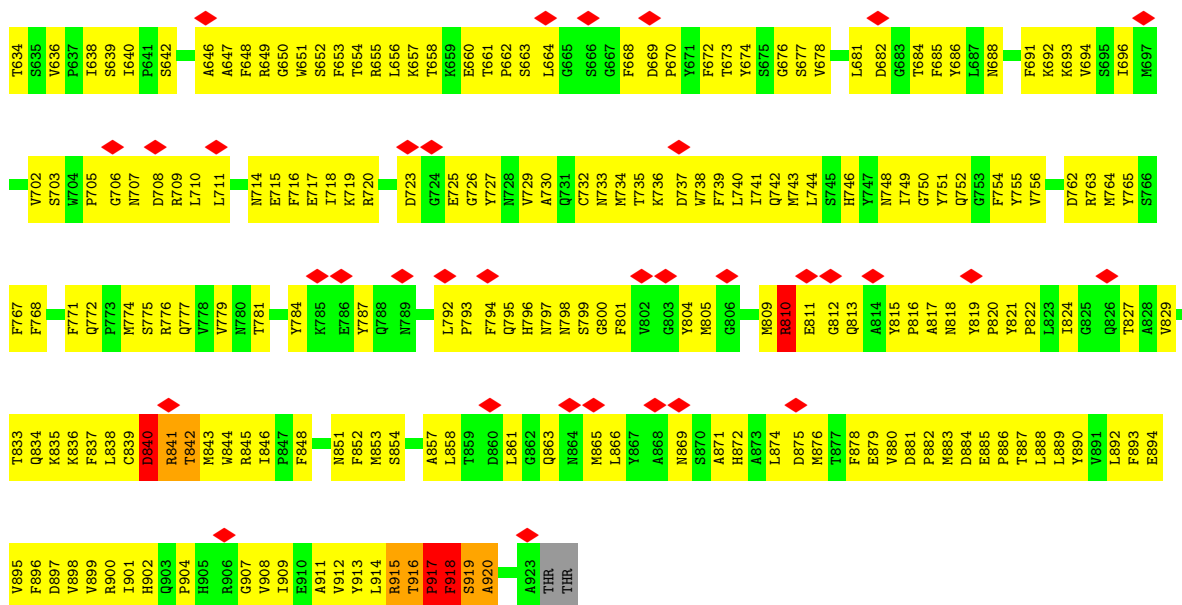




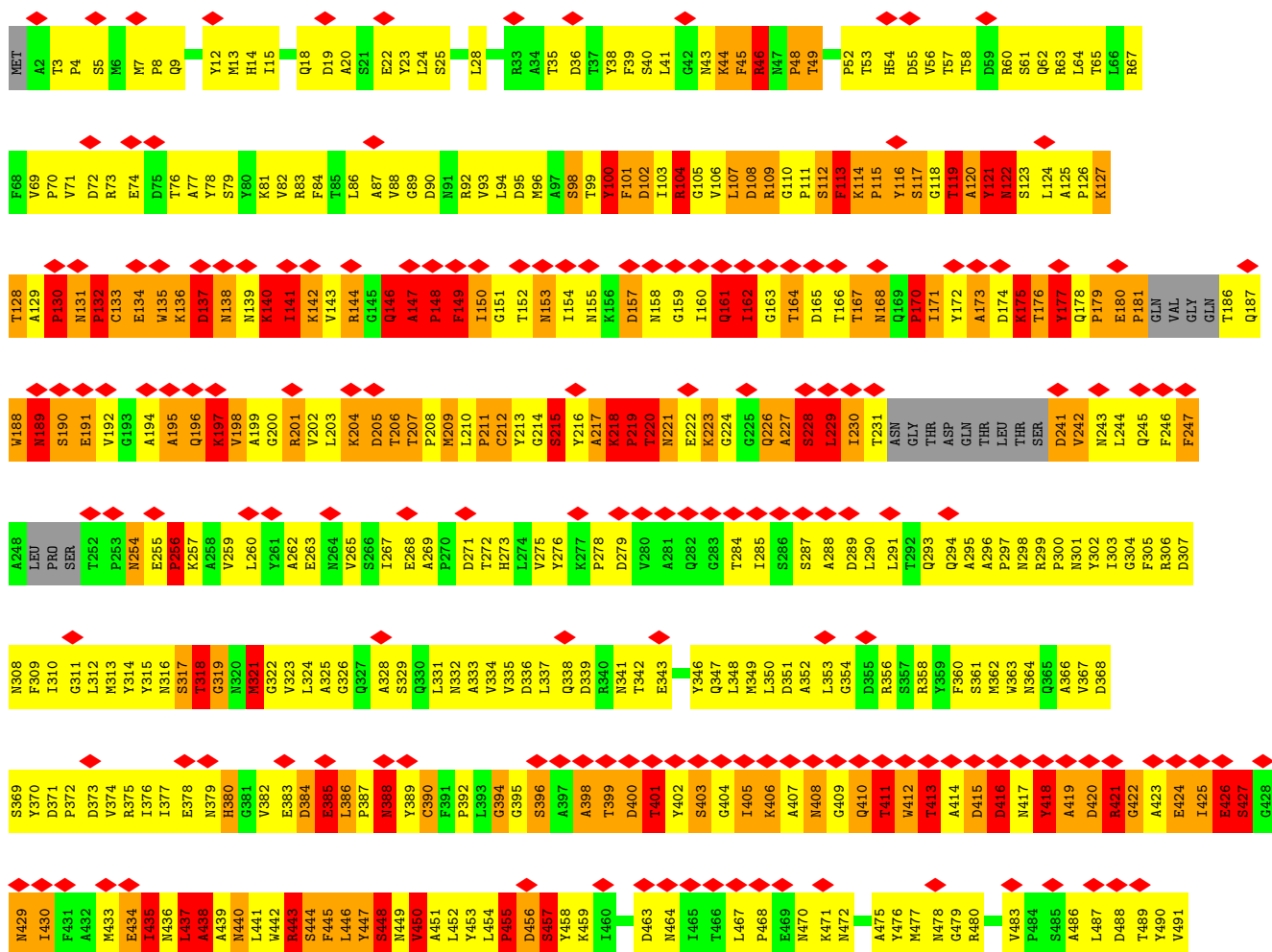
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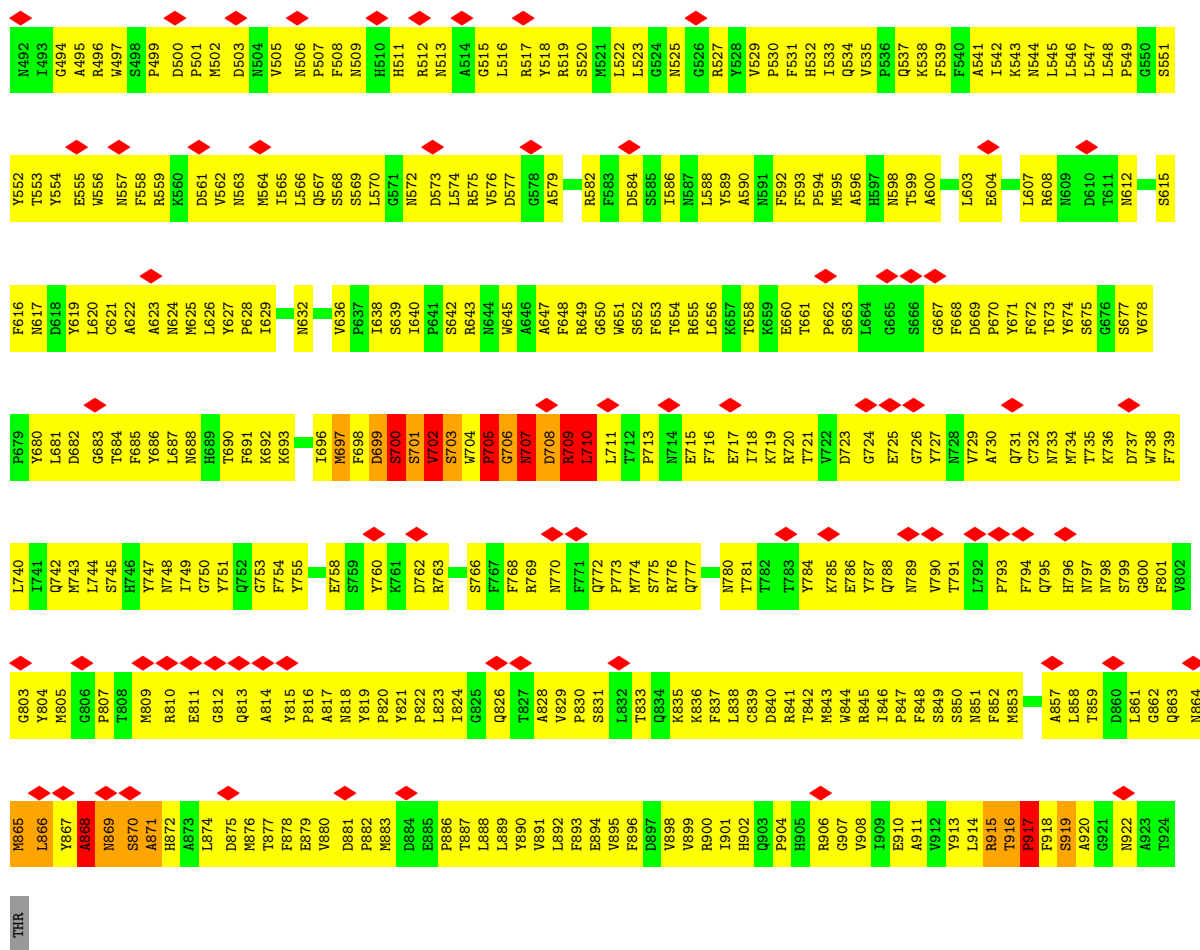




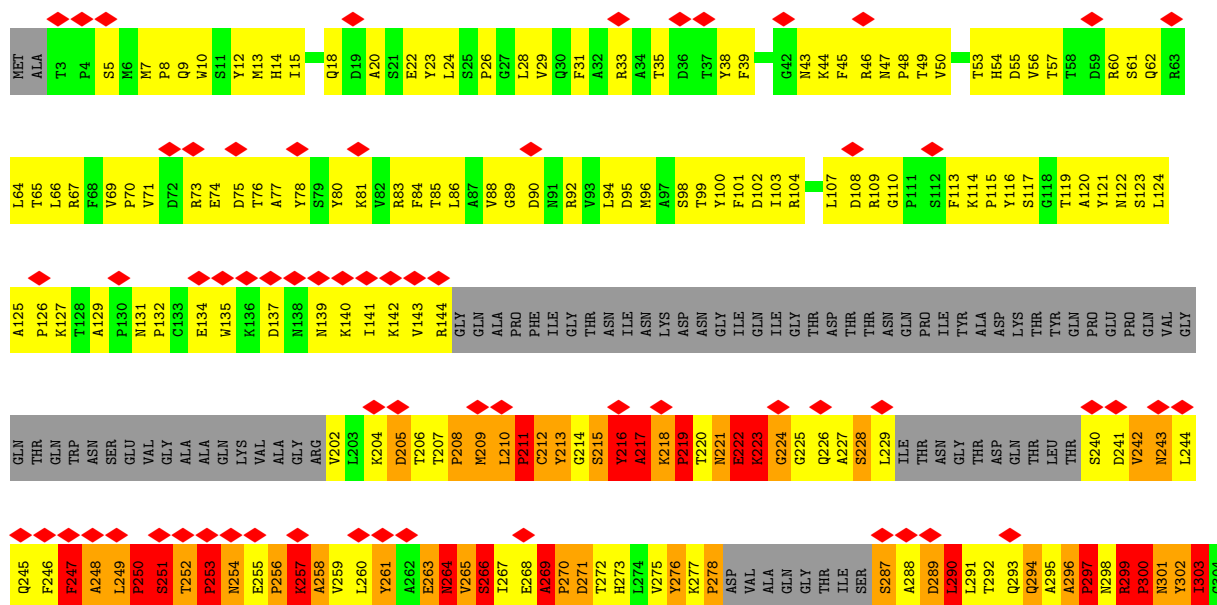


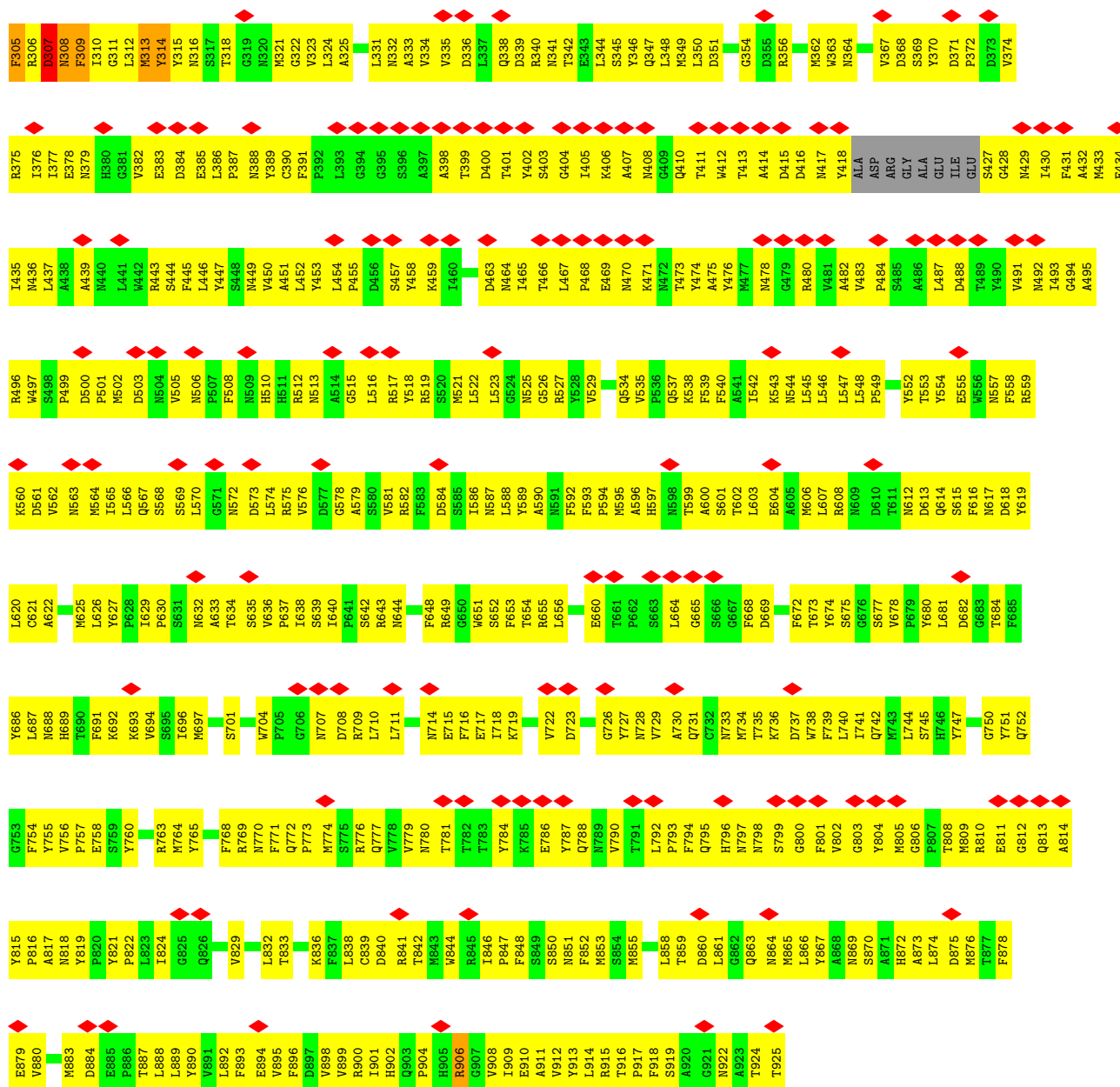
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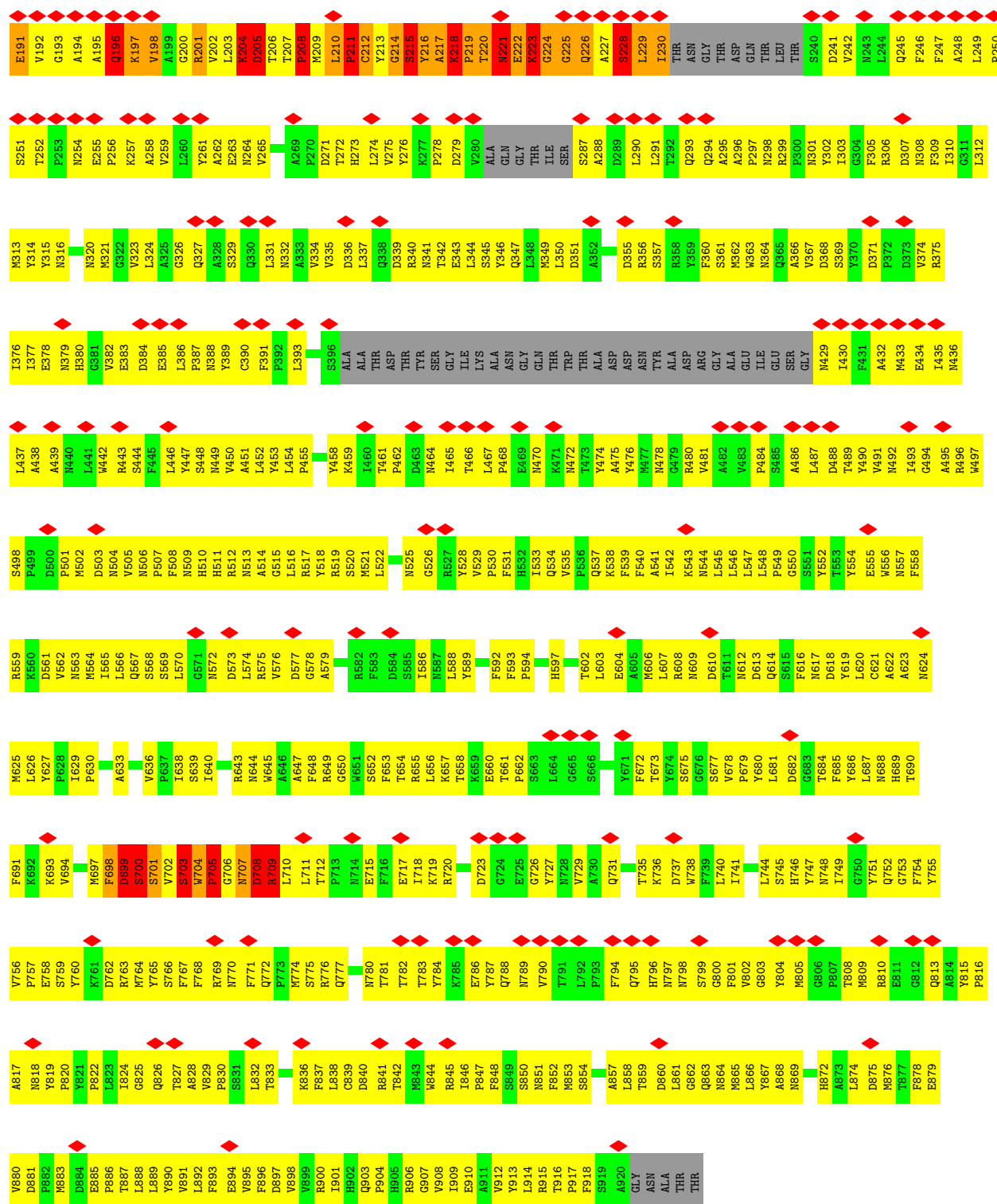


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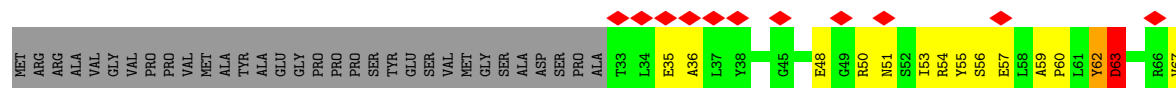








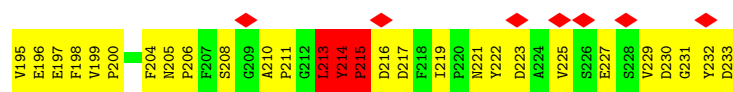
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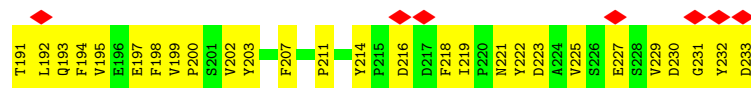
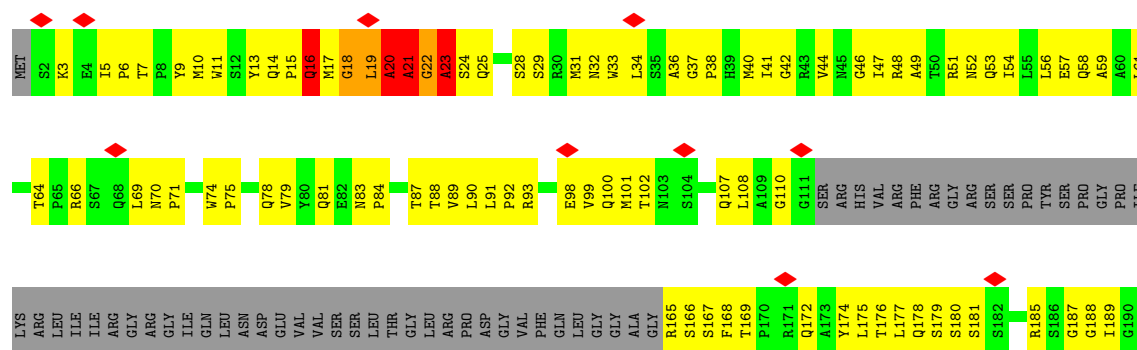




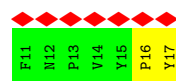




• Molecule 7: Pre-hexon-linking protein VIII



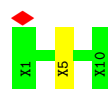
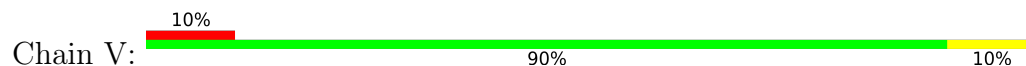
• Molecule 8: Fiber protein



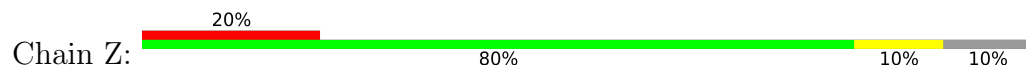
• Molecule 9: Unknown



• Molecule 9: Unknown

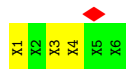


• Molecule 9: Unknown



## ● Molecule 10: Unknown

Chain Y: 



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	19472	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.03	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.067	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size ( $\text{\AA}$ )	936.9, 936.9, 936.9	wwPDB
Map dimensions	900, 900, 900	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.041, 1.041, 1.041	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  >5	RMSZ	# Z  >5
1	0	1.51	2/97 (2.1%)	2.07	4/129 (3.1%)
1	1	1.83	4/129 (3.1%)	2.04	7/174 (4.0%)
1	2	1.09	0/49	1.94	1/64 (1.6%)
1	3	0.89	0/101	1.13	1/136 (0.7%)
1	4	1.46	2/152 (1.3%)	1.75	4/205 (2.0%)
1	5	1.72	2/126 (1.6%)	2.55	5/169 (3.0%)
1	6	0.55	0/29	1.45	1/37 (2.7%)
1	7	0.94	0/29	1.26	0/37
1	8	1.59	3/203 (1.5%)	2.22	8/272 (2.9%)
1	9	0.82	0/29	0.86	0/37
2	A	0.75	12/6485 (0.2%)	1.10	64/8832 (0.7%)
2	B	1.19	36/6946 (0.5%)	1.56	165/9461 (1.7%)
2	C	1.22	57/7052 (0.8%)	1.59	168/9608 (1.7%)
2	D	0.81	18/7250 (0.2%)	1.11	64/9872 (0.6%)
2	E	0.78	19/7181 (0.3%)	1.12	76/9781 (0.8%)
2	F	0.97	30/7265 (0.4%)	1.32	125/9895 (1.3%)
2	G	1.10	50/7201 (0.7%)	1.28	104/9809 (1.1%)
2	H	0.85	26/7290 (0.4%)	1.15	90/9931 (0.9%)
2	I	0.55	5/7412 (0.1%)	0.80	25/10100 (0.2%)
2	J	0.93	27/7401 (0.4%)	1.20	103/10084 (1.0%)
2	K	0.63	10/6891 (0.1%)	0.86	36/9387 (0.4%)
2	L	0.68	9/7023 (0.1%)	0.90	48/9565 (0.5%)
3	M	0.49	3/3744 (0.1%)	0.87	27/5099 (0.5%)
4	N	1.52	1/199 (0.5%)	2.12	10/265 (3.8%)
5	O	0.76	7/2120 (0.3%)	1.01	21/2882 (0.7%)
6	P	0.84	4/428 (0.9%)	1.01	4/583 (0.7%)
6	Q	0.83	2/375 (0.5%)	1.02	3/514 (0.6%)
6	R	1.37	2/234 (0.9%)	1.37	1/317 (0.3%)
6	S	1.31	4/428 (0.9%)	1.80	11/583 (1.9%)
7	T	0.54	0/1406	0.75	9/1922 (0.5%)
7	U	0.63	4/1410 (0.3%)	0.70	4/1927 (0.2%)
8	X	0.41	0/68	0.30	0/94
All	All	0.88	339/96753 (0.4%)	1.18	1189/131771 (0.9%)



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	2	2	0
1	3	1	0
1	5	1	0
1	8	3	0
2	A	4	1
2	B	5	3
2	C	12	2
2	D	4	3
2	E	2	6
2	F	3	1
2	G	0	4
2	H	1	1
2	I	4	0
2	J	6	1
2	K	1	0
2	L	1	2
3	M	2	1
5	O	2	2
6	P	1	0
6	R	1	0
6	S	1	0
7	T	0	1
7	U	0	1
All	All	57	29

The worst 5 of 339 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	886	PRO	N-CD	-37.96	0.94	1.47
2	L	179	PRO	N-CD	-21.89	1.17	1.47
2	G	392	PRO	N-CD	-20.39	1.19	1.47
2	H	208	PRO	N-CD	-19.71	1.20	1.47
2	J	181	PRO	N-CD	-18.41	1.22	1.47

The worst 5 of 1189 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	886	PRO	CA-N-CD	24.15	145.51	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	816	PRO	N-CA-CB	-22.76	75.99	103.30
2	E	917	PRO	N-CA-CB	-22.19	76.67	103.30
2	E	48	PRO	N-CA-CB	-20.20	79.06	103.30
2	I	132	PRO	N-CA-CB	-20.17	79.10	103.30

5 of 57 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	2	17	PRO	CA
1	2	21	THR	CA
1	3	23	ASN	CA
1	5	27	THR	CA
1	8	16	ARG	CA

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	323	VAL	Mainchain
2	B	180	GLU	Mainchain
2	B	431	PHE	Mainchain
2	B	822	PRO	Mainchain
2	C	125	ALA	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	0	94	0	93	19	0
1	1	124	0	118	30	0
1	2	48	0	47	10	0
1	3	98	0	90	14	0
1	4	147	0	135	40	0
1	5	123	0	111	52	0
1	6	28	0	27	6	0
1	7	28	0	27	10	0
1	8	197	0	181	65	0
1	9	28	0	27	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	6307	0	6043	1301	0
2	B	6761	0	6493	1663	0
2	C	6862	0	6574	1727	0
2	D	7057	0	6749	1560	0
2	E	6988	0	6702	1670	0
2	F	7070	0	6781	1694	0
2	G	7008	0	6715	1527	0
2	H	7095	0	6803	1564	0
2	I	7212	0	6900	1365	0
2	J	7203	0	6888	1583	0
2	K	6702	0	6413	1357	0
2	L	6831	0	6550	1300	0
3	M	3659	0	3605	485	0
4	N	198	0	209	90	0
5	O	2088	0	2087	326	0
6	P	419	0	414	84	0
6	Q	366	0	365	93	0
6	R	228	0	227	62	0
6	S	419	0	413	88	0
7	T	1368	0	1297	228	0
7	U	1372	0	1300	181	0
8	X	64	0	55	2	0
9	V	50	0	14	1	0
9	W	45	0	12	8	0
9	Z	45	0	13	1	0
10	Y	30	0	10	3	0
All	All	94362	0	90488	17849	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 97.

The worst 5 of 17849 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)
2:E:885:GLU:HG2	2:E:886:PRO:CD	1.24	1.68
2:A:704:TRP:CG	2:A:705:PRO:HD2	1.14	1.65
2:L:136:LYS:CG	2:L:140:LYS:HG2	1.25	1.63
3:M:221:LEU:HD11	3:M:336:ASN:CB	1.14	1.62
3:M:221:LEU:CD1	3:M:336:ASN:HB3	1.30	1.61

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	0	10/266 (4%)	3 (30%)	3 (30%)	4 (40%)	0	0
1	1	14/266 (5%)	6 (43%)	2 (14%)	6 (43%)	0	0
1	2	4/266 (2%)	2 (50%)	0	2 (50%)	0	0
1	3	10/266 (4%)	3 (30%)	5 (50%)	2 (20%)	0	2
1	4	17/266 (6%)	7 (41%)	8 (47%)	2 (12%)	0	6
1	5	14/266 (5%)	7 (50%)	4 (29%)	3 (21%)	0	1
1	6	1/266 (0%)	1 (100%)	0	0	100	100
1	7	1/266 (0%)	1 (100%)	0	0	100	100
1	8	24/266 (9%)	10 (42%)	9 (38%)	5 (21%)	0	1
1	9	1/266 (0%)	1 (100%)	0	0	100	100
2	A	776/925 (84%)	555 (72%)	163 (21%)	58 (8%)	1	15
2	B	837/925 (90%)	534 (64%)	178 (21%)	125 (15%)	0	4
2	C	852/925 (92%)	513 (60%)	186 (22%)	153 (18%)	0	2
2	D	875/925 (95%)	604 (69%)	202 (23%)	69 (8%)	1	13
2	E	868/925 (94%)	576 (66%)	230 (26%)	62 (7%)	1	16
2	F	881/925 (95%)	599 (68%)	185 (21%)	97 (11%)	0	7
2	G	870/925 (94%)	611 (70%)	184 (21%)	75 (9%)	1	11
2	H	886/925 (96%)	682 (77%)	146 (16%)	58 (6%)	1	19
2	I	902/925 (98%)	737 (82%)	137 (15%)	28 (3%)	4	33
2	J	899/925 (97%)	639 (71%)	183 (20%)	77 (9%)	1	11
2	K	830/925 (90%)	662 (80%)	138 (17%)	30 (4%)	3	30
2	L	845/925 (91%)	683 (81%)	127 (15%)	35 (4%)	3	27
3	M	452/508 (89%)	365 (81%)	81 (18%)	6 (1%)	12	48
4	N	22/348 (6%)	9 (41%)	6 (27%)	7 (32%)	0	0
5	O	259/579 (45%)	190 (73%)	53 (20%)	16 (6%)	1	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	P	56/133 (42%)	41 (73%)	12 (21%)	3 (5%)	2	22
6	Q	48/133 (36%)	34 (71%)	12 (25%)	2 (4%)	3	26
6	R	28/133 (21%)	13 (46%)	11 (39%)	4 (14%)	0	4
6	S	56/133 (42%)	17 (30%)	16 (29%)	23 (41%)	0	0
7	T	174/233 (75%)	139 (80%)	33 (19%)	2 (1%)	14	51
7	U	175/233 (75%)	139 (79%)	31 (18%)	5 (3%)	4	34
8	X	5/7 (71%)	1 (20%)	4 (80%)	0	100	100
All	All	11692/16200 (72%)	8384 (72%)	2349 (20%)	959 (8%)	2	12

5 of 959 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	20	ALA
1	0	23	HIS
1	0	25	SER
1	1	10	ALA
1	1	12	ARG

### 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	0	10/227 (4%)	7 (70%)	3 (30%)	0	2
1	1	12/227 (5%)	7 (58%)	5 (42%)	0	0
1	2	5/227 (2%)	3 (60%)	2 (40%)	0	0
1	3	10/227 (4%)	6 (60%)	4 (40%)	0	0
1	4	15/227 (7%)	13 (87%)	2 (13%)	4	22
1	5	13/227 (6%)	9 (69%)	4 (31%)	0	2
1	6	3/227 (1%)	2 (67%)	1 (33%)	0	1
1	7	3/227 (1%)	2 (67%)	1 (33%)	0	1
1	8	20/227 (9%)	12 (60%)	8 (40%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	9	3/227 (1%)	2 (67%)	1 (33%)	0	1
2	A	687/797 (86%)	629 (92%)	58 (8%)	11	40
2	B	739/797 (93%)	605 (82%)	134 (18%)	1	11
2	C	748/797 (94%)	621 (83%)	127 (17%)	2	14
2	D	764/797 (96%)	692 (91%)	72 (9%)	8	35
2	E	761/797 (96%)	710 (93%)	51 (7%)	16	48
2	F	770/797 (97%)	693 (90%)	77 (10%)	7	32
2	G	763/797 (96%)	696 (91%)	67 (9%)	10	38
2	H	770/797 (97%)	713 (93%)	57 (7%)	13	44
2	I	782/797 (98%)	754 (96%)	28 (4%)	35	63
2	J	781/797 (98%)	712 (91%)	69 (9%)	10	38
2	K	731/797 (92%)	708 (97%)	23 (3%)	40	65
2	L	744/797 (93%)	712 (96%)	32 (4%)	29	58
3	M	408/447 (91%)	400 (98%)	8 (2%)	55	75
4	N	24/307 (8%)	22 (92%)	2 (8%)	11	40
5	O	228/501 (46%)	219 (96%)	9 (4%)	32	60
6	P	44/97 (45%)	42 (96%)	2 (4%)	27	57
6	Q	38/97 (39%)	35 (92%)	3 (8%)	12	42
6	R	24/97 (25%)	23 (96%)	1 (4%)	30	59
6	S	44/97 (45%)	28 (64%)	16 (36%)	0	0
7	T	148/192 (77%)	143 (97%)	5 (3%)	37	64
7	U	148/192 (77%)	147 (99%)	1 (1%)	84	91
8	X	7/7 (100%)	7 (100%)	0	100	100
All	All	10247/13868 (74%)	9374 (92%)	873 (8%)	14	40

5 of 873 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	820	PRO
2	G	299	ARG
2	L	149	PHE
2	F	116	TYR
2	E	815	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 264 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	316	ASN
2	L	752	GLN
7	T	45	ASN
2	E	509	ASN
2	E	316	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 monosaccharides 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](#)

There are no chain breaks in this entry.

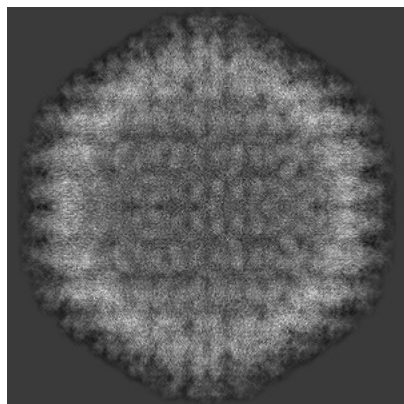
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11108. These allow visual inspection of the internal detail of the map and identification of artifacts.

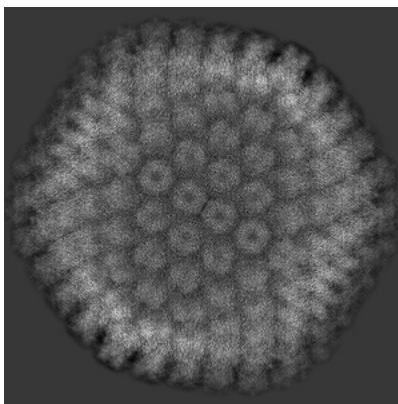
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

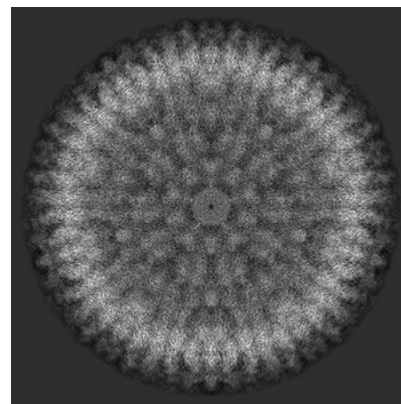
#### 6.1.1 Primary map



X

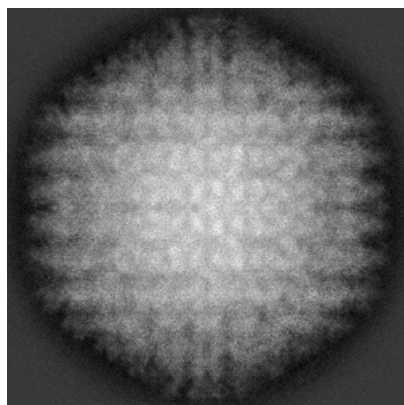


Y

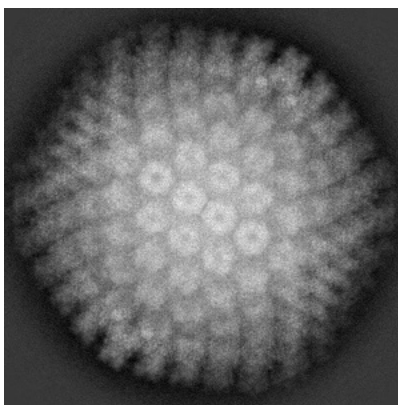


Z

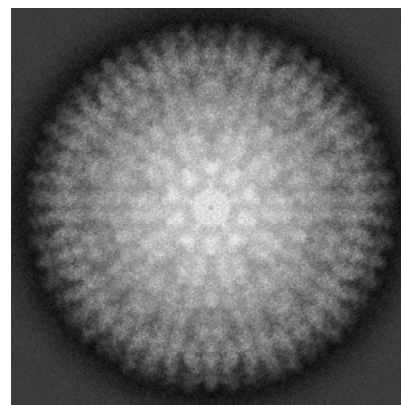
#### 6.1.2 Raw map



X



Y



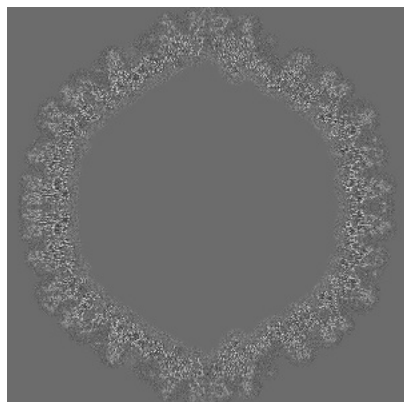
Z

The images above show the map projected in three orthogonal directions.

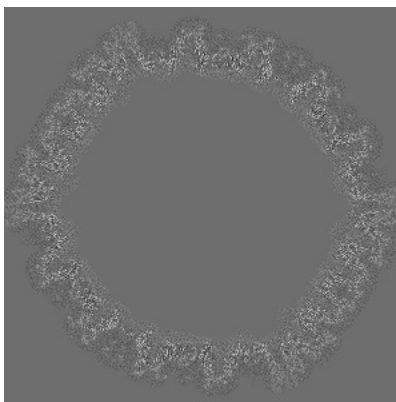


## 6.2 Central slices [i](#)

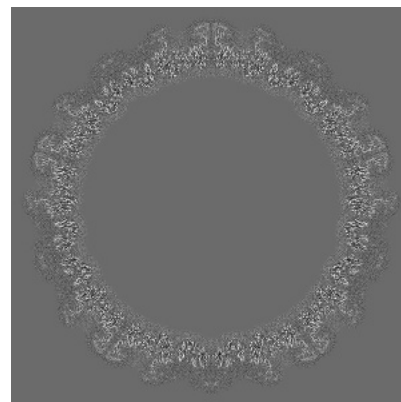
### 6.2.1 Primary map



X Index: 450

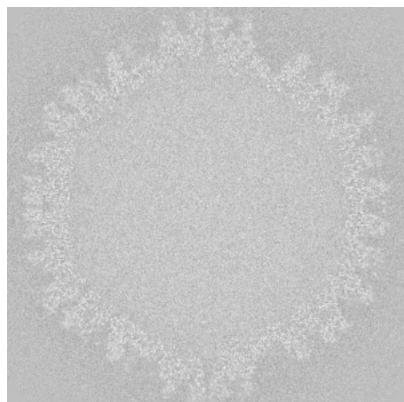


Y Index: 450

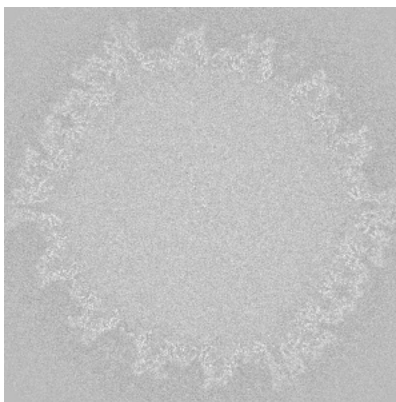


Z Index: 450

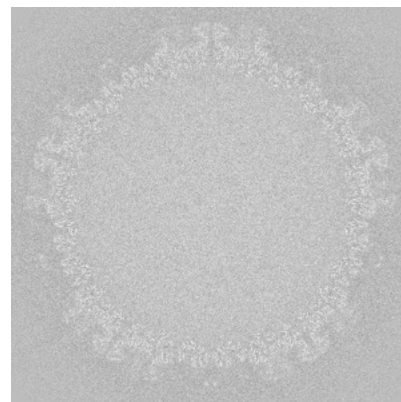
### 6.2.2 Raw map



X Index: 450



Y Index: 450

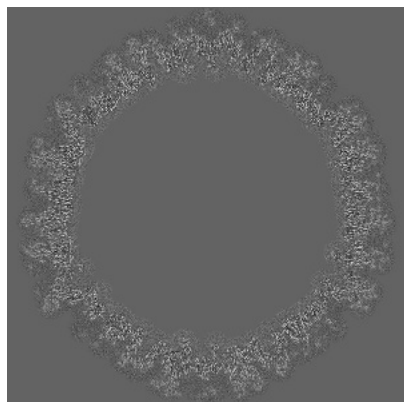


Z Index: 450

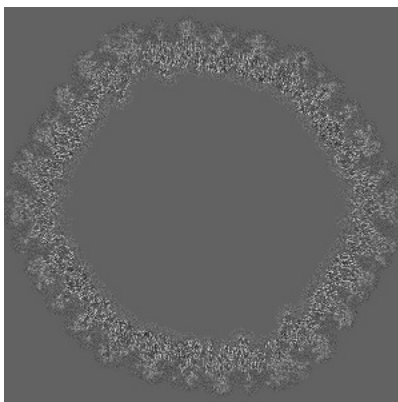
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

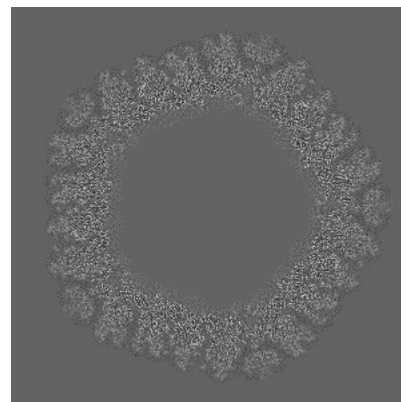
### 6.3.1 Primary map



X Index: 492

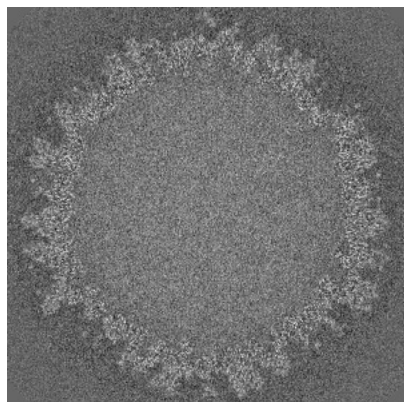


Y Index: 431

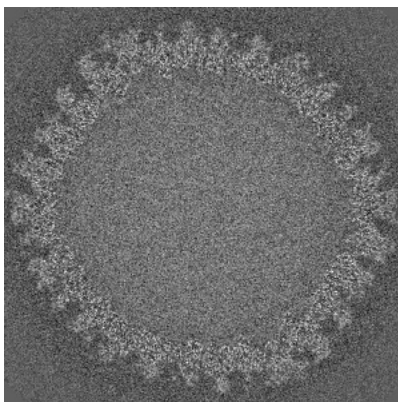


Z Index: 249

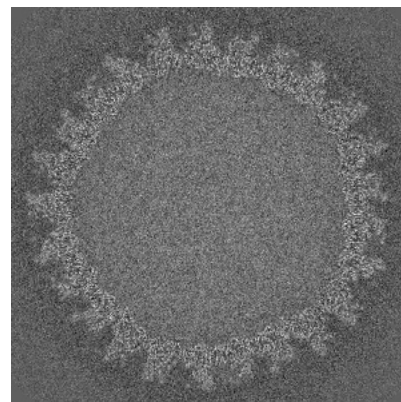
### 6.3.2 Raw map



X Index: 490



Y Index: 431

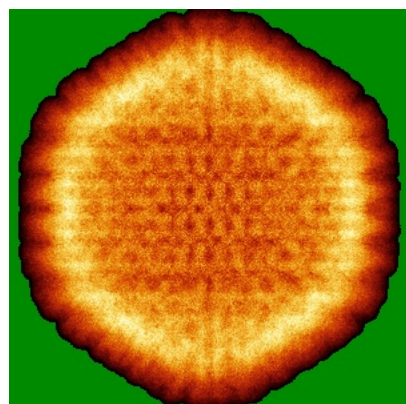


Z Index: 504

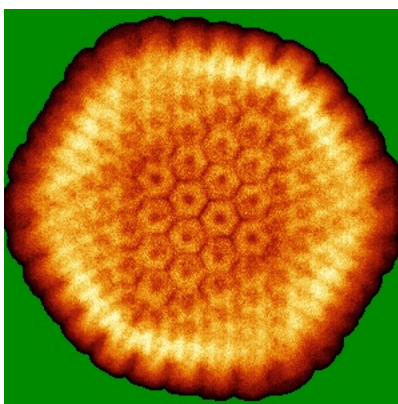
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

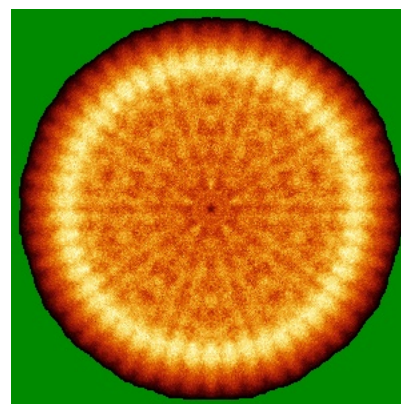
### 6.4.1 Primary map



X

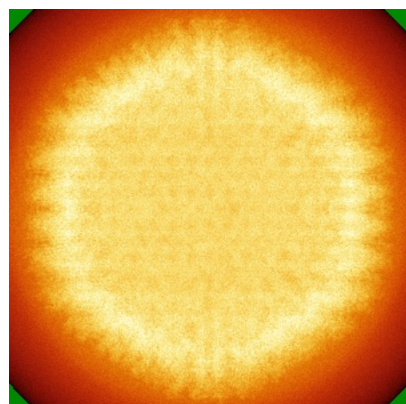


Y

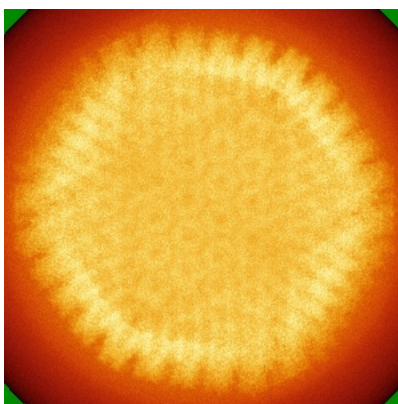


Z

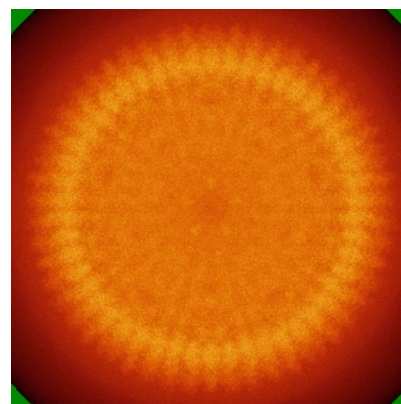
### 6.4.2 Raw map



X



Y



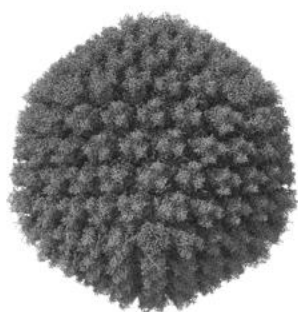
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

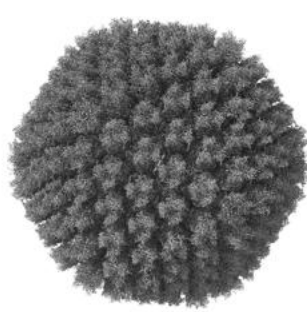


## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



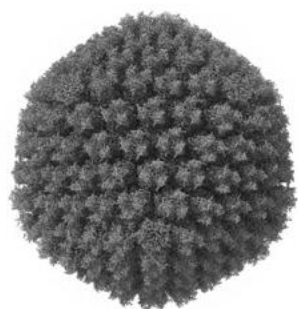
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

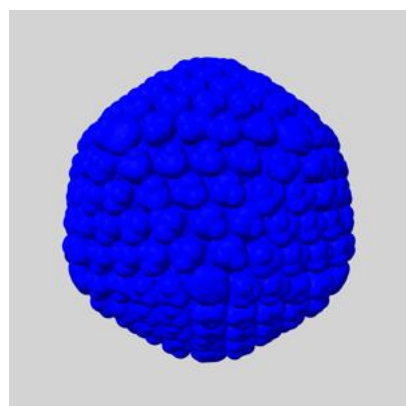
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

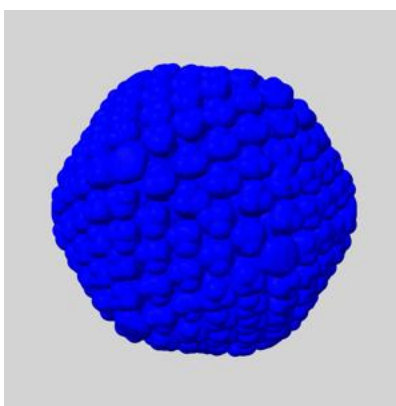
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

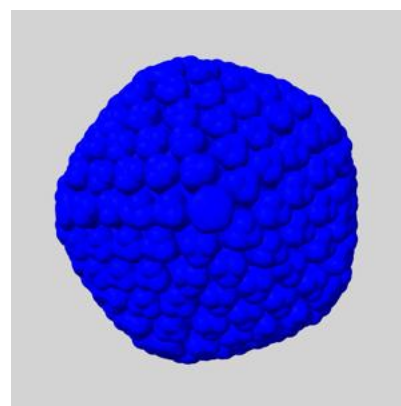
### 6.6.1 emd\_11108\_msk\_1.map [i](#)



X



Y

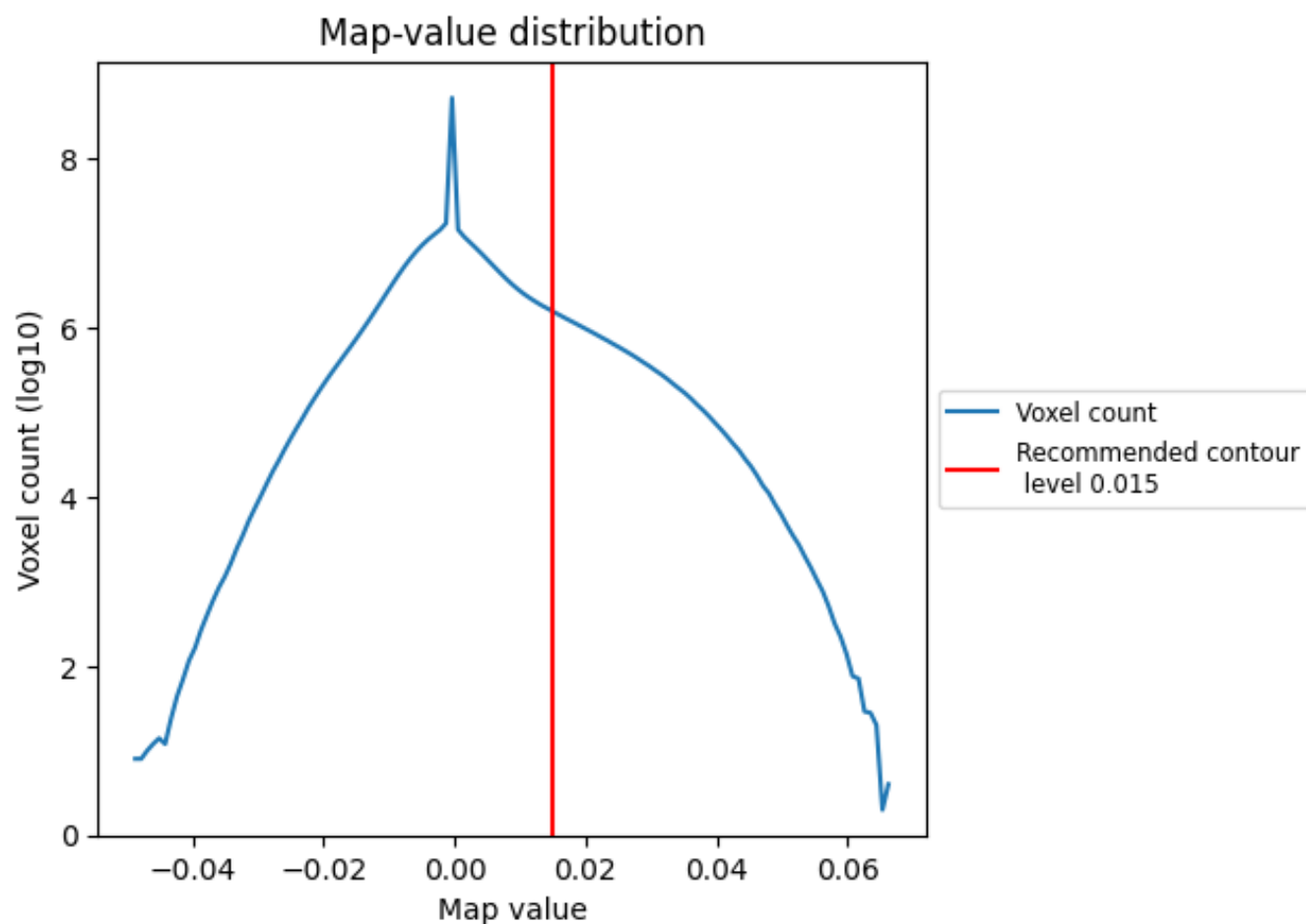


Z

## 7 Map analysis [i](#)

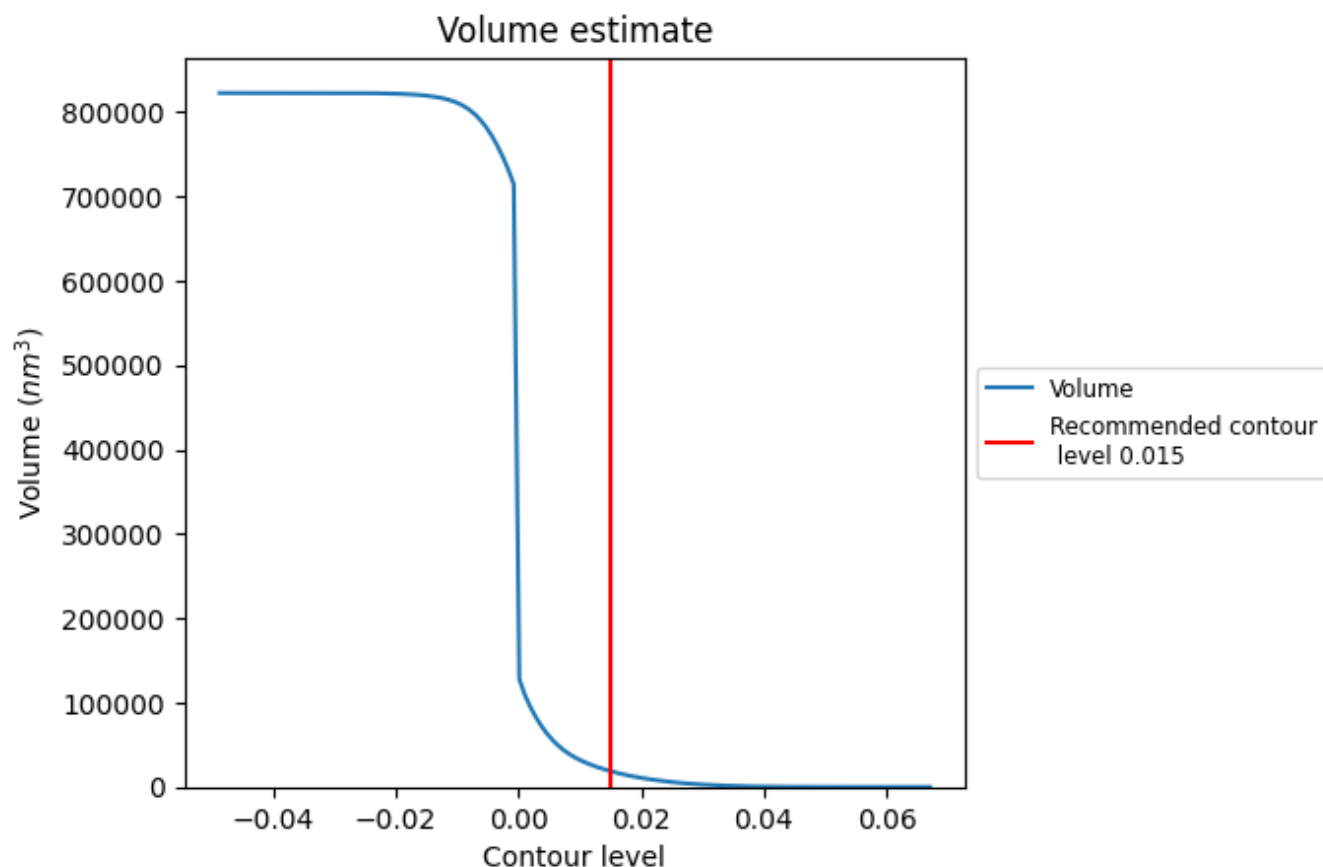
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

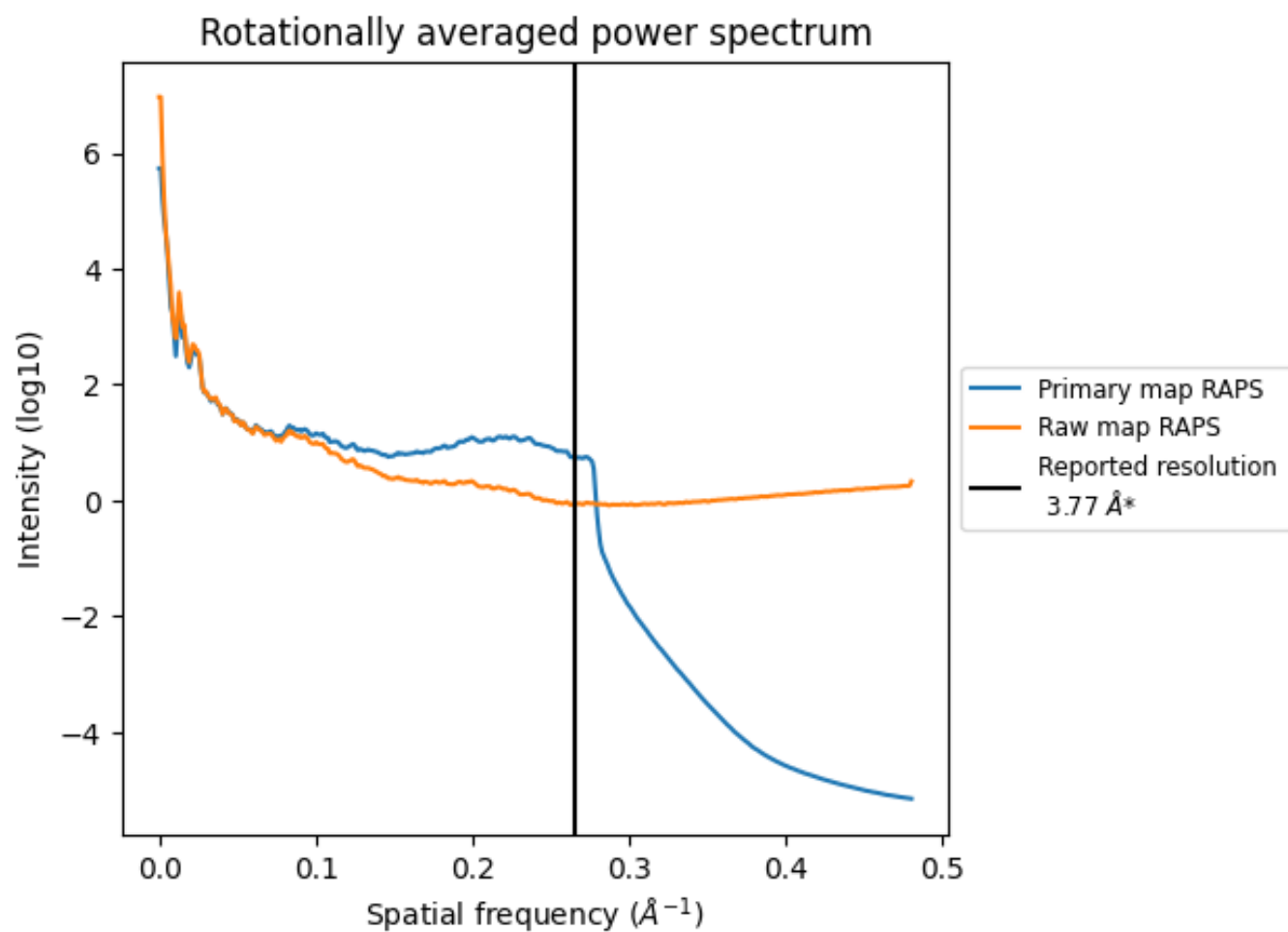
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 18776  $\text{nm}^3$ ; this corresponds to an approximate mass of 16961 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



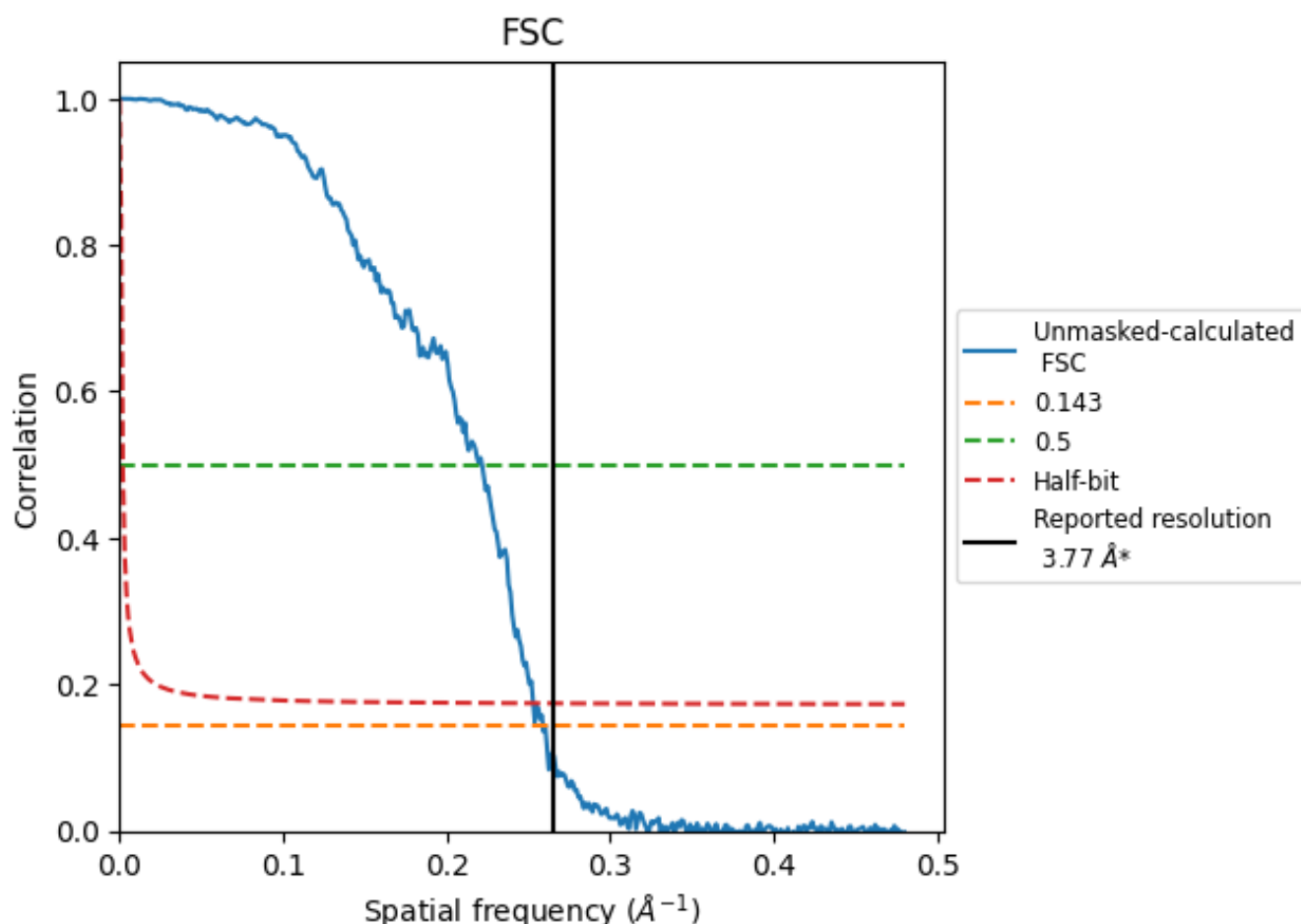
\*Reported resolution corresponds to spatial frequency of 0.265 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.265  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.77	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.86	4.51	3.95

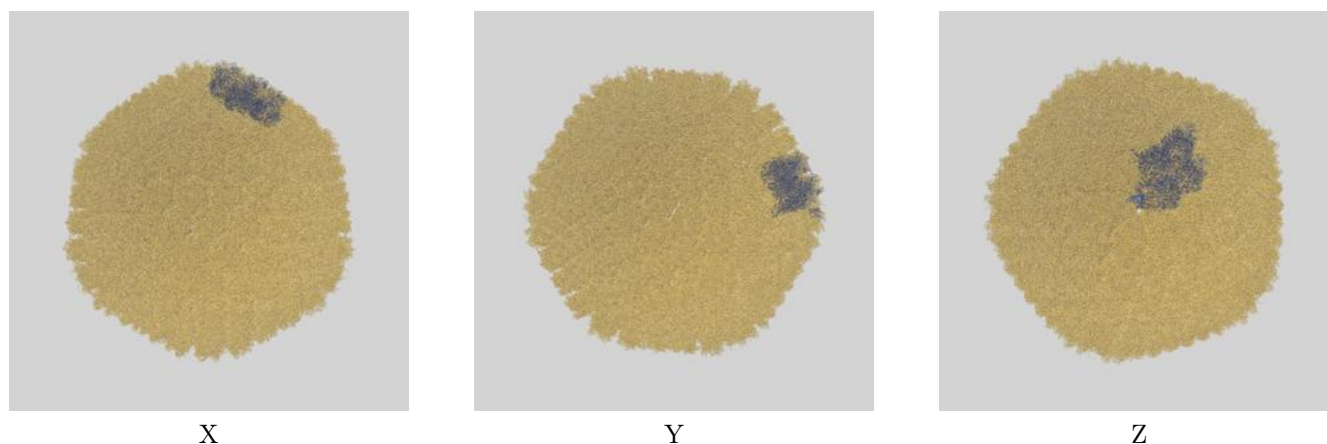
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

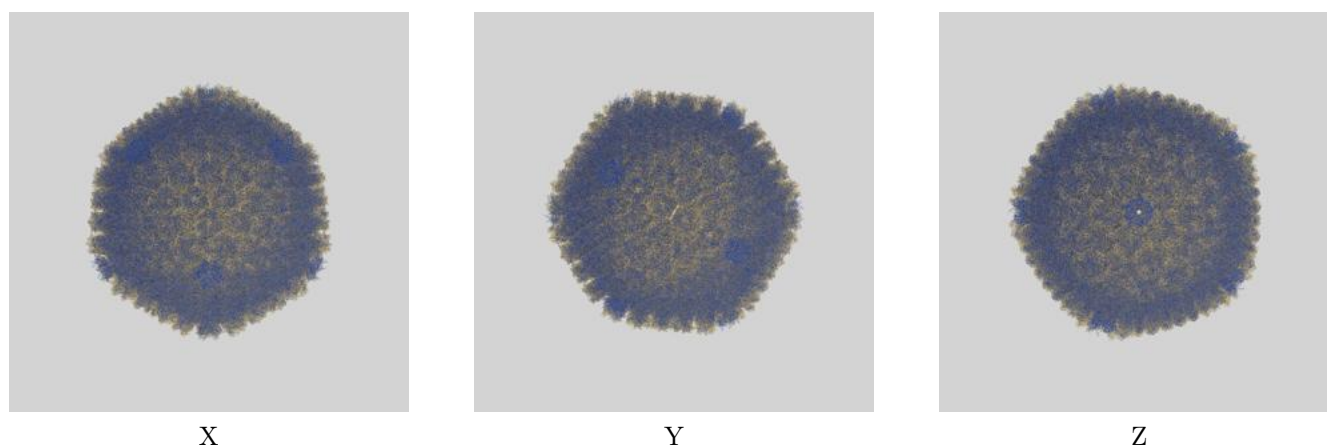
This section contains information regarding the fit between EMDB map EMD-11108 and PDB model 6Z7N. Per-residue inclusion information can be found in section [3](#) on page [8](#).

### 9.1 Map-model overlays

#### 9.1.1 Map-model overlay [i](#)

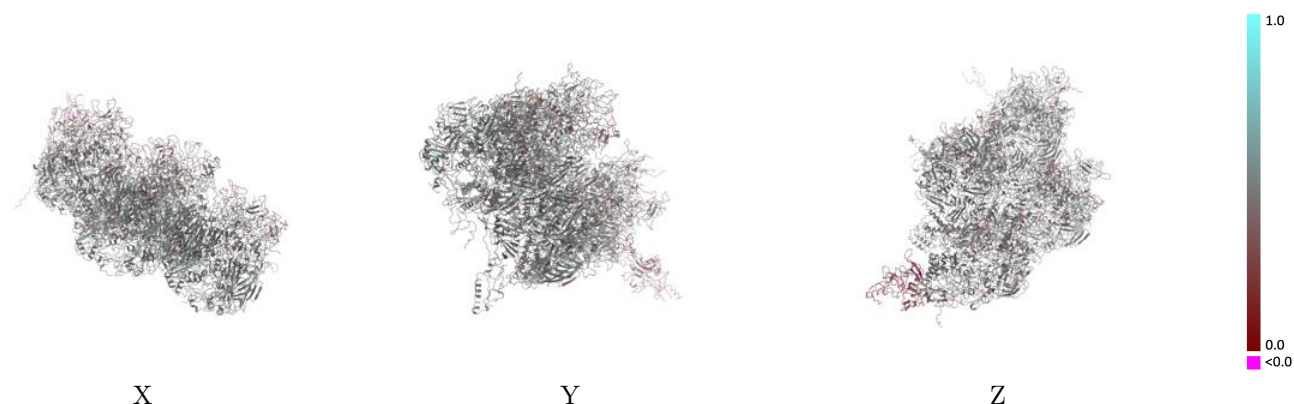


#### 9.1.2 Map-model assembly overlay [i](#)



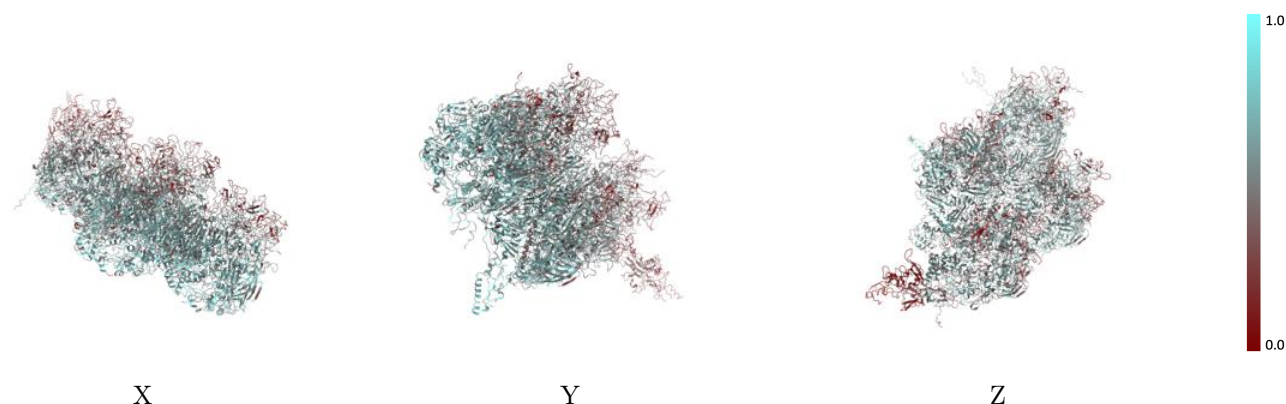
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



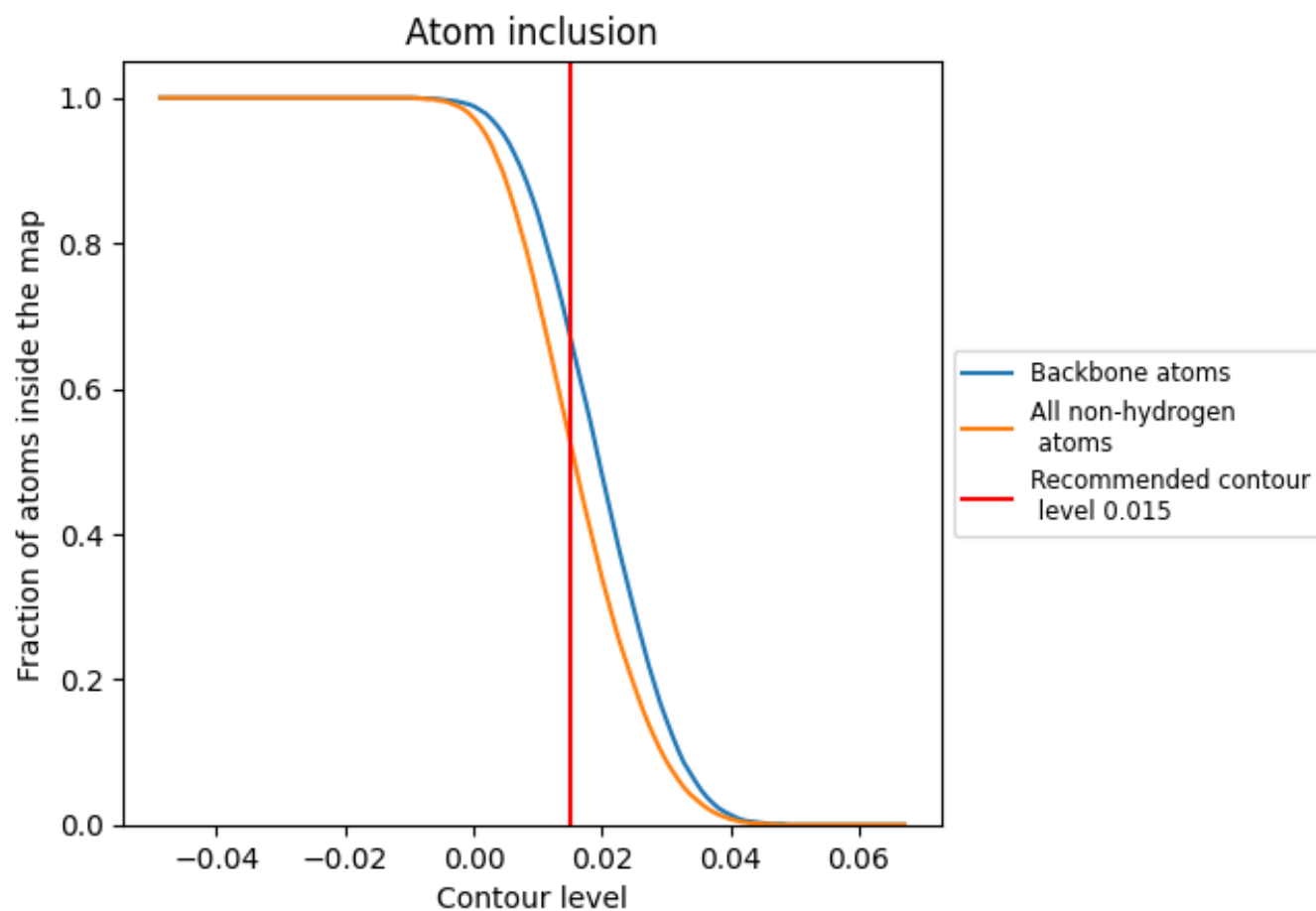
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 53% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ





The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5290	 0.4610
0	 0.2440	 0.4680
1	 0.6220	 0.5020
2	 0.4350	 0.4980
3	 0.3900	 0.4510
4	 0.5000	 0.4060
5	 0.5420	 0.4650
6	 0.6150	 0.5350
7	 0.5770	 0.4950
8	 0.5100	 0.4680
9	 0.5770	 0.5150
A	 0.5140	 0.4630
B	 0.4800	 0.4610
C	 0.5110	 0.4660
D	 0.5410	 0.4650
E	 0.5330	 0.4640
F	 0.5610	 0.4760
G	 0.5750	 0.4760
H	 0.5610	 0.4720
I	 0.5580	 0.4650
J	 0.5380	 0.4650
K	 0.5430	 0.4590
L	 0.5490	 0.4680
M	 0.2800	 0.3230
N	 0.5770	 0.4360
O	 0.4840	 0.4540
P	 0.4560	 0.4440
Q	 0.4710	 0.4460
R	 0.5000	 0.4750
S	 0.5270	 0.4830
T	 0.5990	 0.4750
U	 0.6330	 0.4950
V	 0.7800	 0.5380
W	 0.7780	 0.4850
X	 0.0000	 0.0520



*Continued on next page...*

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Chain	Atom inclusion	Q-score
Y	 0.6000	 0.5160
Z	 0.5780	 0.4700