



wwPDB X-ray Structure Validation Summary Report

Aug 2, 2014 – 08:34 AM EDT

PDB ID : 4CWU
Title : CRYSTAL STRUCTURE DERIVED MODELS OF ADENOVIRUS CE-
MENT PROTEINS AT 3.8Å
Authors : Reddy, V.S.; Nemerow, G.R.
Deposited on : 2014-04-03
Resolution : 3.80 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

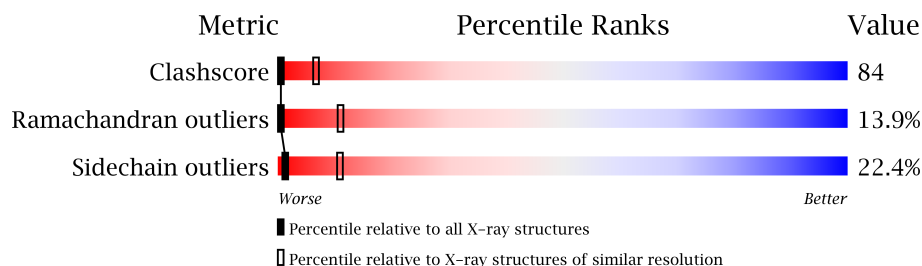
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : **FAILED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1100 (4.10-3.50)
Ramachandran outliers	78287	1050 (4.10-3.50)
Sidechain outliers	78261	1042 (4.10-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	952	
1	B	952	
1	C	952	
1	D	952	
1	E	952	
1	F	952	
1	G	952	
1	H	952	
1	I	952	
1	J	952	
1	K	952	
1	L	952	
2	N	571	
3	O	585	
4	P	140	
4	Q	140	
4	R	140	

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Mol	Chain	Length	Quality of chain
4	S	140	<div><div></div></div>
5	T	368	<div><div></div></div>
6	U	250	<div><div></div></div>
6	V	250	<div><div></div></div>
7	X	227	<div><div></div></div>
7	Y	227	<div><div></div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 98419 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HEXON PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	913	Total	C	N	O	S	0	0	0
			7320	4656	1238	1390	36			
1	B	913	Total	C	N	O	S	0	0	0
			7320	4656	1238	1390	36			
1	C	913	Total	C	N	O	S	0	0	0
			7320	4656	1238	1390	36			
1	D	913	Total	C	N	O	S	0	0	0
			7320	4656	1238	1390	36			
1	E	913	Total	C	N	O	S	0	0	0
			7320	4656	1238	1390	36			
1	F	913	Total	C	N	O	S	0	0	0
			7320	4656	1238	1390	36			
1	G	918	Total	C	N	O	S	0	0	0
			7352	4673	1244	1399	36			
1	H	913	Total	C	N	O	S	0	0	0
			7320	4656	1238	1390	36			
1	I	913	Total	C	N	O	S	0	0	0
			7320	4656	1238	1390	36			
1	J	913	Total	C	N	O	S	0	0	0
			7320	4656	1238	1390	36			
1	K	913	Total	C	N	O	S	0	0	0
			7320	4656	1238	1390	36			
1	L	913	Total	C	N	O	S	0	0	0
			7320	4656	1238	1390	36			

- Molecule 2 is a protein called PENTON PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	440	Total	C	N	O	S	0	0	0
			3524	2230	611	671	12			

- Molecule 3 is a protein called PRE-CAPSID VERTEX PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	O	283	Total	C	N	O	S	0	0	0
			2198	1353	406	433	6			

- Molecule 4 is a protein called HEXON-INTERLACING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	57	Total	C	N	O	S	0	0	0
			394	242	70	80	2			
4	Q	81	Total	C	N	O	S	0	0	0
			573	355	100	116	2			
4	R	49	Total	C	N	O	S	0	0	0
			328	200	56	71	1			
4	S	58	Total	C	N	O	S	0	0	0
			401	245	71	84	1			

- Molecule 5 is a protein called CORE-CAPSID BRIDGING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	T	72	Total	C	N	O	S	0	0	0
			518	319	95	103	1			

- Molecule 6 is a protein called PRE-PROTEIN VI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	U	143	Total	C	N	O	S	0	0	0
			1118	696	201	218	3			
6	V	23	Total	C	N	O		0	0	0
			188	116	29	43				

- Molecule 7 is a protein called PRE-HEXON-LINKING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	X	111	Total	C	N	O	S	0	0	0
			865	549	155	159	2			
7	Y	56	Total	C	N	O	S	0	0	0
			440	274	87	77	2			

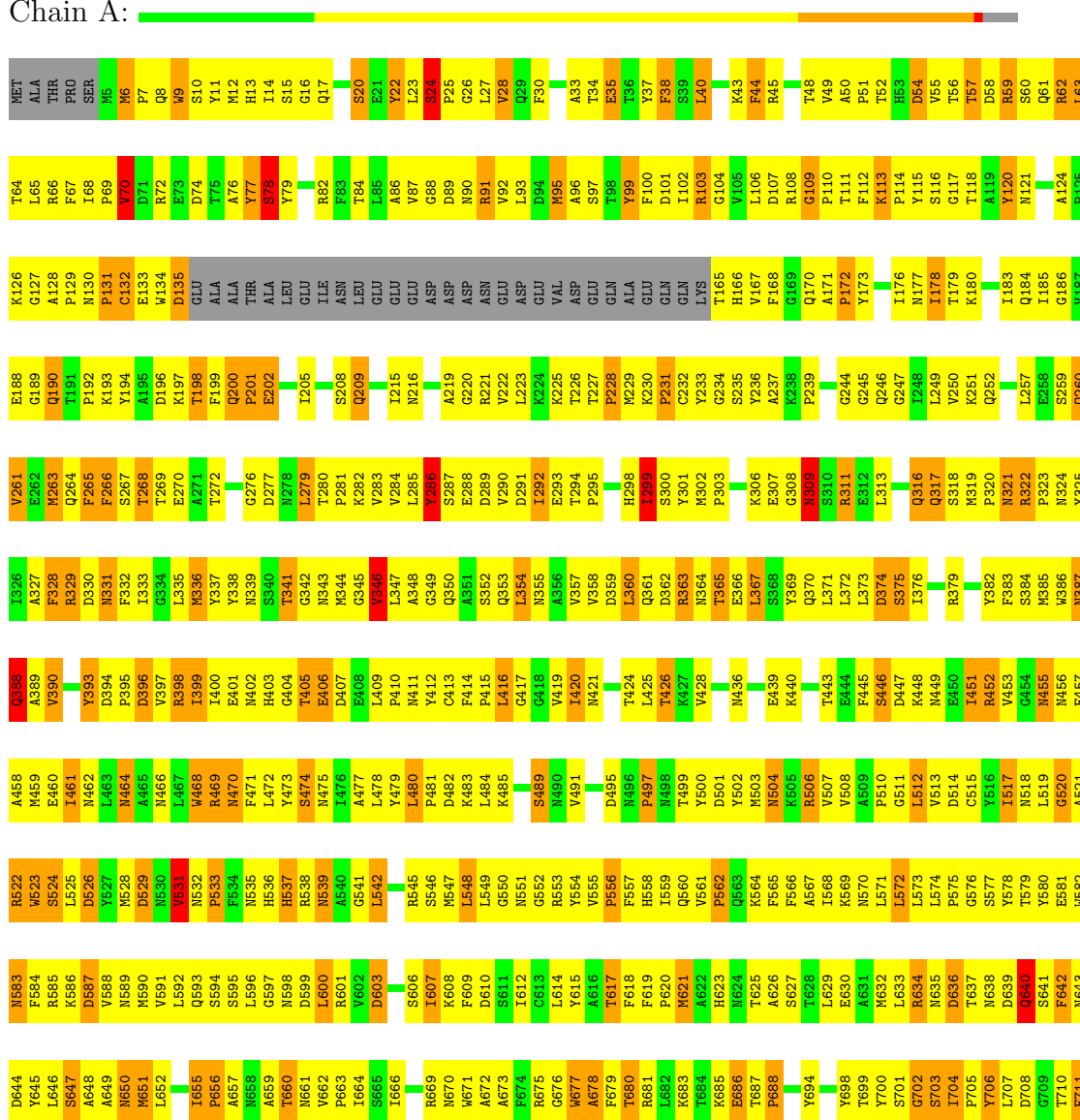
3 Residue-property plots

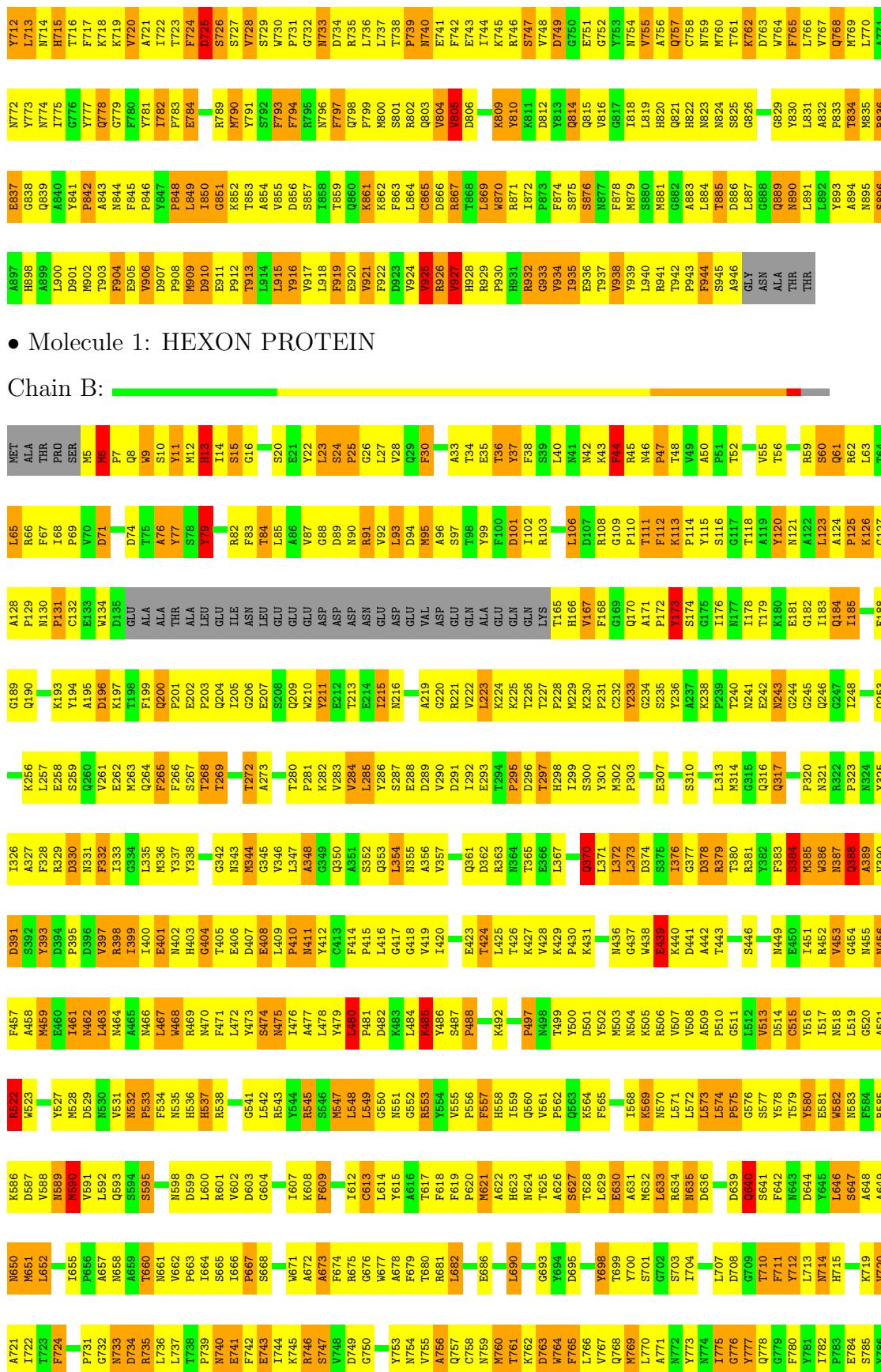
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS failed to run properly.

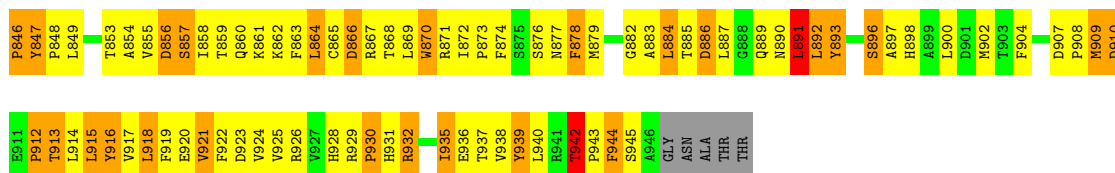
• Molecule 1: HEXON PROTEIN

Chain A:



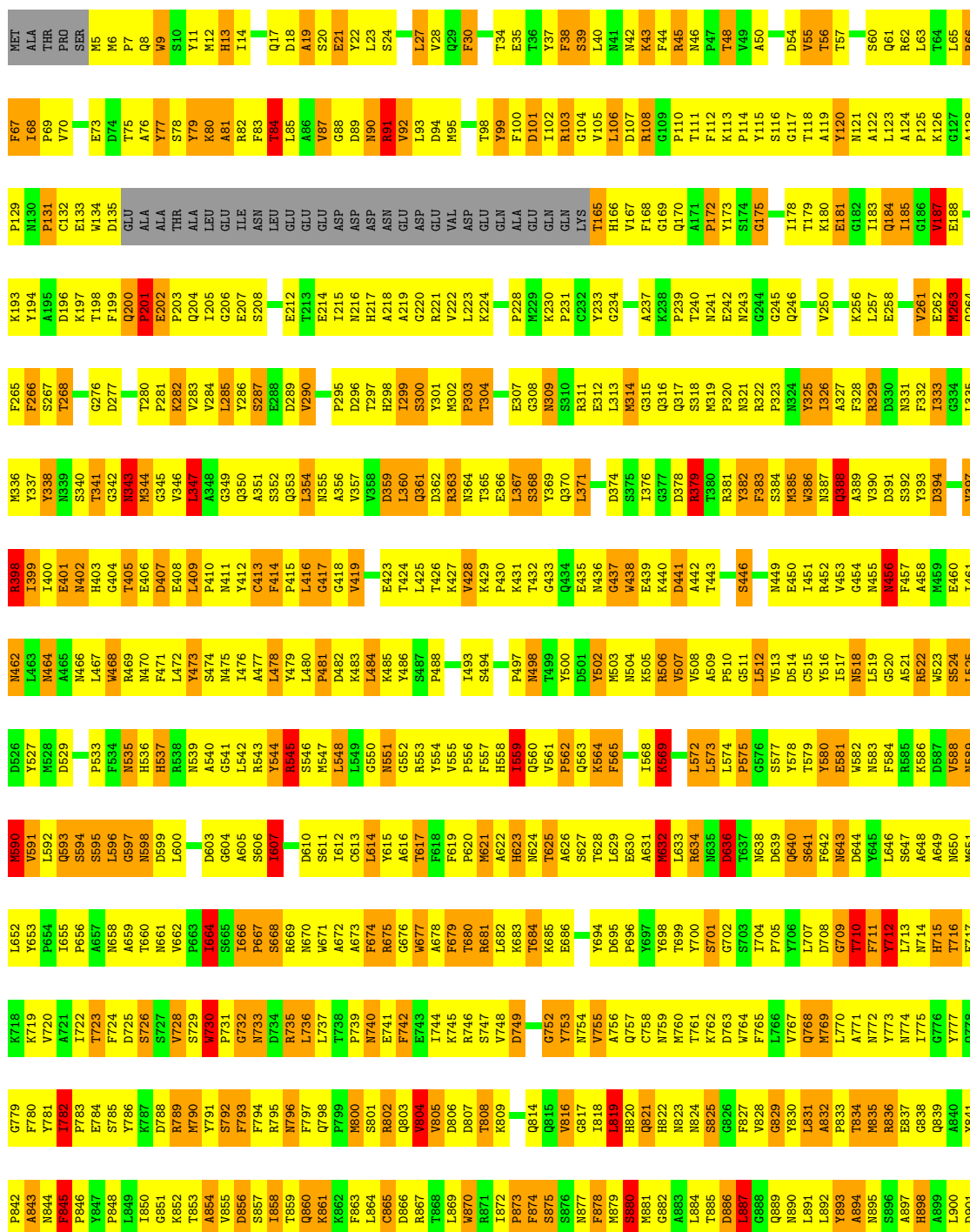






Molecule 1: HEXON PROTEIN

Chain D:



H902	H903	H904	H905	H906	H907	H908	H909	H910	H911	H912	H913	H914	H915	H916	H917	H918	H919	H920	H921	H922	H923	H924	H925	H926	H927	H928	H929	H930

• Molecule 1: HEXON PROTEIN

Chain E:

MET	ALA	THR	PRO	SER	M5	M6	P7	Q8	W9	S10	Y11	M12	H13	I14	S15	G16	Q17	Q18	E21	Y22	L23	S24	P25	G26	L27	V28	GLU	R29	P30																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
R66	F67	L68	P69	N70	D71	R72	E73	T74	T75	A76	Y77	S78	R79	K80	A81	R82	F83	T84	L85	A86	G87	G88	D89	N90	P91	V92	L93	D94	N95	A96	S97	S98	T99	F100	F101	D102	R103	G104	T105	L106	V107	F108	G109	P110	T111	F112	K113	P114	D115	S116	G117	T118	A119	S120	Q121	A122	L123	A124	T125																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
K126	G127	A128	P129	N130	P131	C132	E133	D134	D135	GLU	ALA	ALA	THR	ALA	LEU	GLU	ILE	ASN	LEU	GLU	GLU	GLU	ASP	ASP	ASP	ASN	GLU	GLU	ASP	GLU	VAL	ASP	GLU	GLN	LYS	T165	H166	V167	F168	G169	Q170	A171	P172	K173	P174	N175	I176	T177	K178	E179	E180	E181	A182	Y183	Q184	I185	G186	T187																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
Q190	T191	P192	K193	K194	A195	D196	K197	F198	F199	Q200	Q201	E202	P203	Q204	G205	L206	Q207	Q208	E212	T215	N216	H217	A218	L219	E220	E221	E222	E223	E224	E225	E226	E227	E228	E229	E230	E231	E232	E233	E234	E235	E236	E237	E238	E239	E240	E241	E242	E243	E244	E245	E246	E247	E248	E249	E250	K251																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
Q252	Q253	N254	G255	K256	E257	E258	E259	Q260	V261	E262	M263	Q264	P265	P266	S267	G276	L279	T280	P281	K282	V283	V284	L285	E286	S287	E288	E289	E290	E291	E292	E293	E294	P295	Y301	S302	M303	E304	I305	G308	N309	S310	R311	E312	L313	M314	G315	G316	Q317	S318	M319	P320																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
K321	K322	P323	K324	V325	L326	A327	F328	R329	D330	K331	F332	L333	G334	P335	D336	V337	V338	N339	S340	T341	G342	K343	G344	G345	V346	L347	A348	E349	P410	N411	Y412	C413	F414	L415	L416	G417	G418	V419	I420	N421	T422	E423	L424	T425	T426	K427	V428	K429	P430	K431	T432	G433	Q434	E435	N436	A437	K438	V439	G440	D441																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
R381	Y382	S383	K384	M385	K386	N387	Q388	A389	V390	D391	S392	F393	D394	P395	D396	V397	R398	I399	I400	E401	H402	K403	E406	D407	E408	L409	P410	N411	Y412	C413	F414	L415	L416	G417	G418	V419	I420	N421	T422	E423	L424	T425	T426	K427	V428	K429	P430	K431	T432	G433	Q434	E435	N436	A437	K438	V439	G440	D441																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
A442	S443	K444	N445	E446	L447	R448	L449	V450	V451	V452	G453	N454	F455	A456	M457	E458	L459	N460	L461	N462	L463	A464	A465	N466	L467	V468	R469	N470	F471	L472	Y473	S474	N475	L476	A477	L478	Y479	L480	P481	D482	K483	L484	K485	V486	D487	N488	E489	P490	N491	N492	N493	N494	N495	N496	N497	N498	N499	Y500	D501	Y502	F503	M504	A505	E506	K507	R508	N509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	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	L1129	L1130	L1131	L1132	L1133	L1134	L1135	L1136	L1137	L1138	L1139	L1140	L1141	L1142	L1143	L1144	L1145	L1146	L1147	L1148	L1149	L1150	L1151	L1152	L1153	L1154	L1155	L1156	L1157	L1158	L1159	L1160	L1161	L1162	L1163	L1164	L1165	L1166	L1167	L1168	L1169	L1170	L1171	L1172	L1173	L1174	L1175	L1176	L1177	L1178	L1179	L1180	L1181	L1182	L1183	L1184	L1185	L1186	L1187	L1188	L1189	L1190	L1191	L1192	L1193	L1194	L1195	L1196	L1197	L1198	L1199	L1200	L1201	L1202	L1203	L1204	L1205	L1206	L1207	L1208	L1209	L1210	L1211	L1212	L1213	L1214	L1215	L1216	L1217	L1218	L1219	L1220	L1221	L1222	L1223	L1224	L1225	L1226	L1227	L1228	L1229	L1230	L1231	L1232	L1233	L1234	L1235	L1236	L1237	L1238	L1239	L1240	L1241	L1242	L1243	L1244	L1245	L1246	L1247	L1248	L1249	L1250	L1251	L1252	L1253	L1254	L1255	L1256	L1257	L1258	L1259	L1260	L1261	L1262	L1263	L1264	L1265	L1266	L1267	L1268	L1269	L1270	L1271	L1272	L1273	L1274	L1275	L1276	L1277	L1278	L1279	L1280	L1281	L1282	L1283	L1284	L1285	L1286	L1287	L1288	L1289	L1290	L1291	L1292	L1293	L1294	L1295	L1296	L1297	L1298	L1299	L1300	L1301	L1302	L1303	L1304	L1305	L1306	L1307	L1308	L1309	L1310	L1311	L1312	L1313	L1314	L1315	L1316	L1317	L1318	L1319	L1320	L1321	L1322	L1323	L1324	L1325	L1326	L1327	L1328	L1329	L1330	L1331	L1332	L1333	L1334	L1335	L1336	L1337	L1338	L1339	L1340	L1341	L1342	L1343	L1344	L1345	L1346	L1347	L1348	L1349	L1350	L1351	L1352	L1353	L1354	L1355	L1356	L1357	L1358	L1359	L1360	L1361	L1362	L1363	L1364	L1365	L1366	L1367	L1368	L1369	L1370	L1371	L1372	L1373	L1374	L1375	L1376	L1377	L1378	L1379	L1380	L1381	L1382	L1383	L1384	L1385	L1386	L1387	L1388	L1389	L1390	L1391	L1392	L1393	L1394	L1395	L1396	L1397	L1398	L1399	L1400	L1401	L1402	L1403	L1404	L1405	L1406	L1407	L1408	L1409	L1410	L1411	L1412	L1413	L1414	L1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423	L1424	L1425	L1426	L1427	L1428	L1429	L1430	L1431	L1432	L1433	L1434	L1435	L1436	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447	L1448	L1449	L1450	L1451	L1452	L1453	L1454	L1455	L1456	L1457	L1458	L1459	L1460	L1461	L1462	L1463	L1464	L1465	L1466

A346
GLY
ASN
ALA
THR
THR

• Molecule 1: HEXON PROTEIN

Chain F:

MET	ALA	THR	PRO	SER	W5	P6	M7	Q8	W9	S10	Y11	M12	H13	I14	Q17	D18	A19	S20	E21	Y22	L23	D24	P25	G26	L27	A31	R32	E35	T36	Y37	F38	S39	L40	M41	N42	K43	F44	R45	M46	P47	L48	V49	A50	P51	T52	H53	D54	V55	T56	T57	D58	R59	S60	T64	L65							
R66	F67	T68	P69	W70	D71		A76	Y77	S78	Y79	K80	A81	I82	ASN	LEU	GLU	GLU	ASP	ASP	ASN	GLU	L93	ASP	GLU	VAL	ASP	S97	T98	F100	D101	I102	R103	G104	L105	L106	D107	R108	G109	A110	T111	P112	K113	S114	Y115	S116	G117	T118	A119	M120	M121	A122	I123	T56	T57	D58	R59	S60	T64	L65			
P131	C132	E133	W134	D135	GLU	ALA	ALA	THR	ALA	ALA	LEU	GLU	ILE	ASN	LEU	GLU	GLU	ASP	ASP	ASN	GLU	L93	ASP	GLU	VAL	ASP	S97	T98	GLN	ALA	GLU	T165	F168	G169	Q170	A171	P172	Y173	S174	G175	I176	N177	G178	T179	K180	E181	G182	A183	L184	I185	A124	P125	G127	E188	G189	Q190	T191					
P192	K193	Y194	D196	T198	Q199	F200	E201	E202	P203	Q204	T205	G206	E207	S208	Q209	W210	T213	N216	H217	A218	K219	G220	R221	L223	K224	K225	T226	T227	N228	K229	P230	L231	G232	Y233	G234	S235	T236	K237	K238	P239	T240	E241	N242	K243	G244	G245	Q246	G247	I248	L249	V250	K251	Q252	Q253								
N254	L257	E258	F259	Q260	V261	E262	E263	F264	F265	F266	Q267	T268	T269	E270	A271	L279	T280	P281	V284	L285	Y286	S287	E288	D289	V290	D291	L292	E293	L294	P295	D296	T297	H298	L299	S300	Y301	G302	P303	T304	L305	N309	S310	G311	E312	L313	M314	G315	Q316	Q317	S318	M319	P320	N321	R322	Q323							
K324	T325	I326	A327	F328	R329	D330	K331	F332	I333	G334	L335	K336	Y337	Y338	N339	S340	T341	G342	K343	M344	V346	L347	A348	G349	Q350	A351	S352	K353	L354	K355	A356	V357	Q361	D362	R363	S364	T365	L366	K367	S368	V369	Q370	L371	L372	L373	D374	S375	L376	G377	D378	K379	T380	R381	Y382	F383	S384	D447					
K386	N387	Q388	A389	V390	D391	S392	Y393	D394	P395	D396	Y397	R398	I399	I400	E401	N402	G403	G404	T405	E406	D407	E408	L409	P410	N411	Y412	K413	P414	P415	L416	G417	G418	V419	N420	T421	T422	E423	T424	L425	K426	V428	K429	P430	K431	T432	E435	M436	G437	M438	N504	D441	A442	P445	S446	D447							
K448	M449	E450	I451	R452	V453	G454	N455	N456	F457	A458	M459	E460	I461	N462	L463	N464	A465	L466	K468	N469	N470	F471	L472	Y473	S474	N475	L476	A477	L478	Y479	L480	P481	D482	K483	L484	K485	Y486	S489	N490	V491	D495	N496	P497	N498	T499	Y500	D501	Y502	M503	N504	F505	A507	K508	R509	V508	A509	P510					
G511	L512	Y513	D514	S515	Y516	I517	M518	L519	G520	M521	R522	M523	S524	L525	D526	Y527	M528	V531	N532	P533	H536	H537	R538	N539	A540	G541	L542	R543	Y544	R545	S546	M547	L548	L549	R550	Y551	Y552	V553	P554	P555	P556	F557	H558	L559	Q560	V561	P562	Q563	K564	F565	F566	N567	L568	K569	M570	L571	M632					
L573	L574	P575	G576	S577	Y578	T579	Y580	E581	M582	N583	F584	R585	K586	V587	V588	M589	M590	V591	L592	Q593	S594	S595	L596	G597	N598	D599	L600	R601	V602	D603	G604	A605	S606	L607	K608	F609	S610	L611	L612	L613	L614	Y615	A616	T617	F618	P619	P620	M621	A622	H623	N624	T625	A626	T627	S628	L629	E630	A631	M632			
L633	R634	M635	D636	T637	M638	D639	Q640	S641	F642	N643	D644	Y645	L646	S647	A648	A649	M650	M651	L652	Q653	P654	L655	P656	A657	M658	A659	T660	N661	V662	P663	L664	S665	L666	P667	S668	R669	M670	M671	A672	P674	R675	G676	M677	F678	F679	T680	R681	L682	K683	T684	K685	A686	T687	P688	S689	L690	G691	S692				
G693	Y694	D695	P696	Y697	G698	T699	Y700	S701	G702	N703	I704	Y705	Y706	L707	A708	M709	L710	F711	Y712	L713	M714	H715	T716	F717	K718	W719	V720	A721	I722	V723	F724	S725	S726	Y727	V728	S729	Y730	F731	G732	N733	D734	R735	L736	L737	Y738	P739	N740	E741	F742	E743	I744	Y810	K811	D812	S747	Y813	W748	D749	G750	F751	A815	G817
Y753	N754	T755	A756	Q757	T758	N759	M760	T761	K762	D763	W764	F765	L766	T767	Q768	M769	L770	A771	T772	Y773	M774	T775	G776	T777	Q778	G779	F780	Y784	S785	R789	M790	Y791	T792	A793	F794	R795	N796	F797	Q798	P799	K800	S801	Q803	H804	V805	D806	D807	Y810	T811	D812	S813	Y814	W815	Q816	G817							
L818	L819	H820	R821	Q822	N823	N824	G825	G826	F827	L828	G829	Y830	L831	A832	P833	T834	M835	L836	E837	Y841	P842	A843	N844	R845	P846	Y847	P848	L849	L850	G851	K852	Y853	A854	V855	D856	S857	L858	T859	Q860	R861	K862	F863	L864	T867	L868	L869	R870	R871	S872	T873	R874	S875	S876	R877	F878	P879						
S880	L884	T885	D886	L887	G888	K889	N890	L891	L892	Y893	A894	K895	S896	A897	H898	M899	L900	D901	F904	E905	V906	K909	P910	E911	P912	T913	L914	L915	Y916	V917	L918	F919	A920	V921	F922	D923	Y924	V925	R926	V927	H928	R929	P930	H931	R932	G933	V934	L935	T936	T937	V938	Y939	L940	R941	T942	P943						

F944	S945
A946	GLY
ASN	ALA
THR	THR

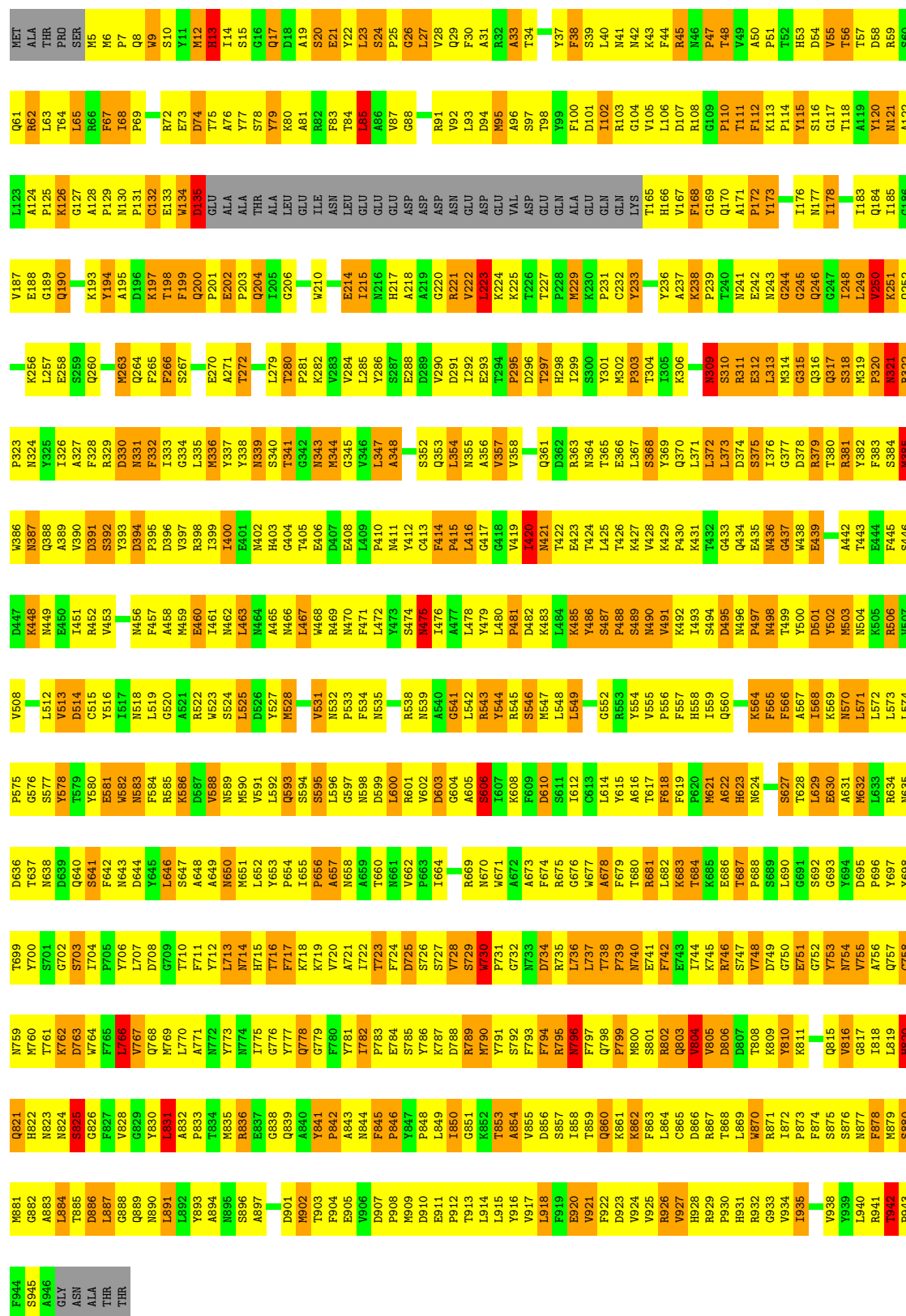
• Molecule 1: HEXON PROTEIN

Chain G:

MET	ALA	THR	PRO	SER	M5	M6	P7	Q8	W9	S10	T75	Y11	M12	H13	I14	G16	Q17	S20	E21	Y22	L23	S24	L27	F30	A31	T34	E35	T36	Y37	F38	S39	L40	K43	F44	R45	R46	P47	T48	V49	A50	P51	F52	H53	D54	V55	T56	T57	D58	R59	S60	Q61	R62	L63	T64																																																											
L85	R66	F67	P68	P69	V70	D71	R72	E73	D74	T75	A76	Y77	S78	H81	Y89	R80	A81	R82	F83	T84	L85	A86	V87	S88	D89	I90	R91	V92	L93	D94	R95	A96	S97	T98	Y99	F100	D101	I102	R103	G104	V105	L106	D107	R108	G109	P110	A50	P51	F52	H53	D54	V55	T56	T57	D58	R59	S60	Q61	R62	L63	T64																																																				
M130	P131	C132	P133	D134	M135	GLU	ALA	ALA	THR	THR	ALA	LEU	GLU	ILE	ASN	LEU	GLU	GLU	GLU	ASP	ASP	ASP	ASN	GLU	ASP	GLU	VAL	ASP	L93	D94	R95	A96	S97	T98	Y99	F100	D101	I102	R103	G104	V105	L106	D107	R108	G109	P110	A50	P51	F52	H53	D54	V55	T56	T57	D58	R59	S60	Q61	R62	L63	T64																																																				
P192	K193	Y194	A195	D196	L197	T198	F199	Q200	P201	E202	P203	Q204	I205	G206	W210	T215	N216	H217	A218	A219	A219	G220	S221	V222	L223	K224	K225	D226	T227	P228	S229	S300	Y301	P302	P303	C232	T233	G234	S235	Y236	A237	K238	P239	T240	G241	E242	N243	G244	G245	O246	G247	N248	R249	P250	K251	K252	Q253	K256	L257																																																						
E258	S259	Q260	V261	E262	M263	Q264	F265	P266	S267	T268	L279	T280	P281	K282	V283	V284	L285	Y286	S287	E288	D289	L292	E293	T294	P295	D296	T297	H298	I299	S300	Y301	P302	P303	T304	G308	N309	S310	R311	K312	L313	M314	G315	Q316	Q317	S318	M319	P320	N321	R322	P323	N324	K325	Y326	I326	A327	F328	R329																																																								
D330	K331	F332	L333	G334	L335	K336	Y337	Y338	N339	S340	T341	G342	K343	K344	G345	V346	L347	A348	G349	Q350	A351	S352	Q353	L354	K355	A356	D359	L360	Q361	R362	R363	T364	E365	L367	S368	Y369	Q370	L371	L372	E373	L374	S375	D378	R379	T380	R381	Y382	F383	S384	K385	N386	Y387	N388	Q389	V390	D391																																																									
P395	D396	V397	R398	L399	T400	E401	H402	H403	G404	S405	T406	D407	E408	L409	N410	N411	Y412	C413	P414	P415	L416	G417	G418	Y419	N420	N421	T424	L425	T426	K427	V428	K429	P430	K431	M436	G437	W438	E439	K440	D441	A442	T443	E444	P445	S446	D447	K448	M449	E450	L451	R452	V453	V454	M455	G457	F457																																																									
A458	M459	E460	L461	N462	L463	N464	A465	N466	L467	N468	R469	N470	F471	L472	R475	L476	A477	L478	Y479	D482	S483	L484	K485	Y486	S487	P488	S489	N490	V491	R492	L493	S494	D495	Y500	D501	Y502	K503	N504	K505	R506	V507	V508	A509	L510	G511	L512	V513	D514	C515	Y516	S517	Y518	L519	E520	A521	R522																																																									
W523	S524	L525	D526	Y527	N528	D529	N530	A531	N532	P533	F534	N535	H536	H537	N538	R539	G540	A541	R542	R543	S544	M545	K546	L547	G548	G549	G550	N551	G552	R553	V554	V555	P556	F557	H558	I559	Q560	V561	P562	Q563	K564	F565	F566	A567	I568	R569	N570	L571	L572	L573	L574	P575	G576	D577	P578	N579	M580	E581	W582	N583																																																					
F584	R585	K586	E587	N588	N589	M590	V591	L592	K593	S594	S595	L596	G597	N598	D599	L600	V601	D602	D603	G604	A605	S606	I607	K608	F609	I612	Y615	Y616	A617	T618	F619	P620	M621	A622	H623	M624	T625	A626	S627	T628	L629	E630	A631	M632	L633	R634	N635	D636	T637	N638	D639	P640	S641	F642	N643	D644	Y645																																																								
L646	S647	A648	M649	N650	L651	P652	P653	P654	L655	P656	A657	M658	P662	P663	T664	S665	T666	P667	S668	R669	S670	W671	A672	A673	F674	R675	E676	W677	A678	F679	T680	R681	L682	E686	T687	P688	S689	L690	G691	S692	G693	Y694	Y698	T699	Y700	S701	G702	S703	T704	P705	Y706	L707	S708	F709	T710	F711																																																									
Y712	L713	M714	H715	T716	F717	K718	K719	W720	T723	F724	W725	S726	S727	V728	W729	M730	Y731	G732	M733	D734	R735	L736	L737	F738	P739	R740	S741	R742	E743	E744	K745	R746	S747	K811	D812	Y813	Q814	G815	L816	G817	T818	L819	H820	Q821	H822	N823	H824	S825	G826	Y830	N831	V832	A833	Q834	M835	L836	N837	Y838	L839	A840	G841	Q842	N843	S844	L845	N846	Y847	R848	L849	S850	Y855	R856	F857	S858	T859	Q860	K861	V862	F863	L864	C865	D866	R867	T868	L869	H870	R871	S872	F873	S874	S875	S876	S877	F878	M879	S880	M881	L884	T885	D886	L887	G888	Q889	N890	L891	A894	N895	S896	A897	H898	A899	L900	D901
H902	T903	F904	E905	V906	D907	P908	H909	D910	P911	E912	T913	L914	L915	Y916	V917	L918	F919	S920	T921	Q922	D923	V924	Y925	R926	Y927	H928	R929	P930	H931	R932	Q933	R934	R935	T937	S938	Y939	L940	R941	T942	P943	F944	S945	N948	A949	T950	T951																																																																			

● Molecule 1: HEXON PROTEIN

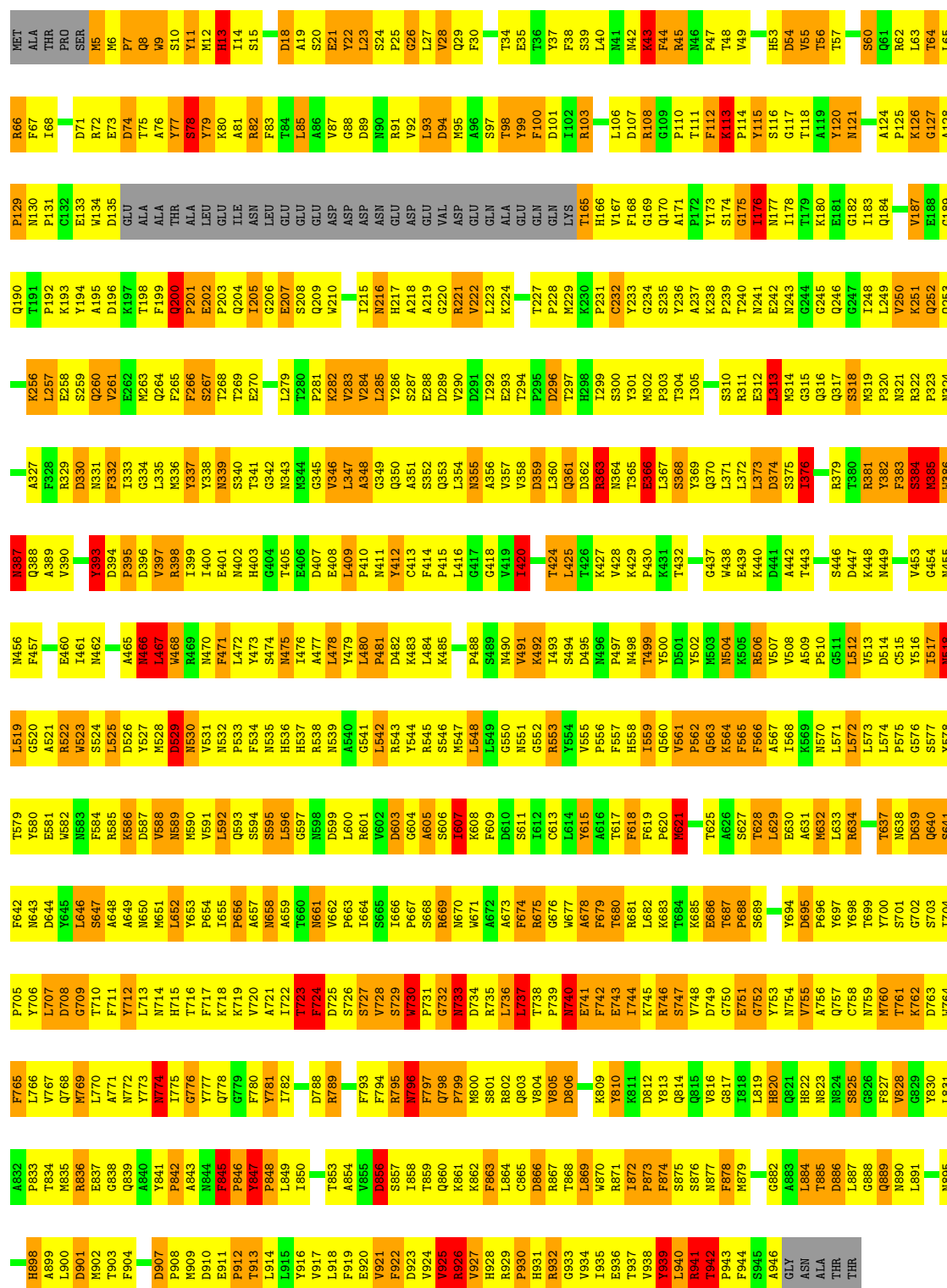
Chain H:



Chain I:



Chain J:



• Molecule 1: HEXON PROTEIN

Chain K:

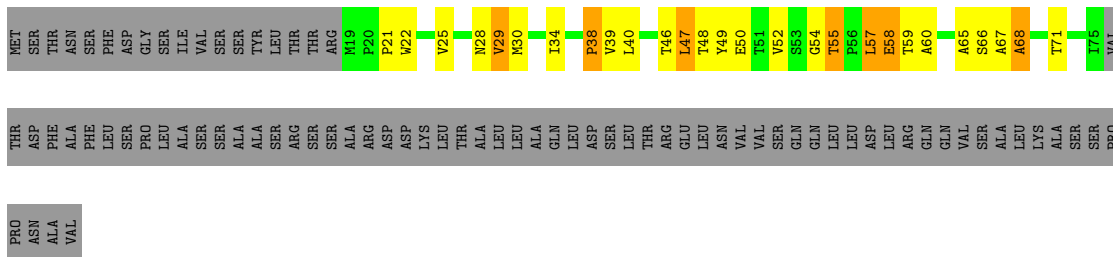
WORLDWIDE
 PDB
PROTEIN DATA BANK



ARG	LYS	PHE	L311	ILE	M471	V102	MET	TS15	T450	K380	ASN	L258	K194	N133	A61	MET
GLU	GLU	THR	H312	ALA	V172	A103	MET	V516	F451	P381	SER	L259	V195	V134	P62	ARG
SER	SER	ASN	L313	PRO	T173	I105	GLN	E517	R452	L382	ALA	G260	G196	M135	L63	ALA
PHE	PHE	ALA	L314	THR	E174	R106	ASP	E518	R453	E384	ALA	T383	Q198	E136	F64	ALA
ARG	ARG	LEU	E318	ASP	T175	S107	THR	M519	Q455	K387	ALA	R263	Q199	M137	D65	MET
PRO	PRO	ASN	E319	SER	P176	G108	ASP	V520	Q456	K388	ALA	R264	G200	F139	T66	TYR
PRO	PRO	PRO	E320	GLY	Q177	M109	PRO	A522	I457	K389	ALA	Q265	V201	T140	T67	GLU
SER	SER	HIS	R321	SER	E179	V110	ASP	L523	M458	K390	MET	P266	L202	N141	R68	GLU
SER	SER	THR	R322	VAL	H180	T112	V10	L524	F460	S390	GLN	F267	L203	K142	Y70	GLY
LEU	LEU	LEU	R323	SER	Y181	T113	R11	H526	P461	R391	PRO	S204	S204	F143	L71	PRO
PRO	PRO	PRO	Y324	ARG	Y182	M113	A12	G527	V462	R392	VAL	D205	D205	K144	V72	PRO
ASP	ASP	ASP	Y325	ASP	P185	L114	A12	G528	V463	R393	GLU	L206	L206	A145	D73	PRO
LEU	LEU	PRO	Q326	ASP	D186	D115	S19	L529	Q464	I394	ASP	G207	G207	R146	D73	SER
GLY	GLY	PHE	Q327	ALA	R116	R117	N22	P530	A465	S395	MET	T274	T274	V147	K75	TYR
ALA	ALA	THR	Q328	ALA	L117	V118	N22	L531	E466	S395	ASN	Y275	Y275	M148	S76	SER
ALA	ALA	THR	Q329	ALA	V118	V118	N22	R532	L467	F400	ASP	D276	D276	V149	D77	VAL
ALA	ALA	THR	Q330	ALA	T191	V121	D25	R533	L468	T401	HIS	D277	D277	R151	T78	VAL
PRO	PRO	GLY	N332	ALA	S192	A122	ASP	S534	P469	Q402	ALA	L278	L278	R151	D78	VAL
ARG	ARG	GLY	L333	ALA	R193	R122	TRP	S535	V470	Q403	ILE	E279	E279	L152	S81	SER
SER	SER	PHE	L334	ALA	Q194	E123	ARG	S536	H471	R404	ARG	G280	G280	P153	L82	ALA
ASP	ASP	GLU	R335	ALA	G195	A124	GLN	G537	S472	S405	GLY	G281	G281	T154	N83	ALA
ALA	ALA	VAL	V336	ALA	L196	V125	VAL	V538	K473	W406	THR	N282	N282	K155	Y84	PRO
SER	SER	PRO	V337	ALA	Q197	A126	MET	Q539	S474	Y407	THR	I283	I283	Q158	Q85	VAL
SER	SER	GLU	V338	ALA	R198	Q127	ASP	R540	F475	L408	PHE	P284	P284	Q158	N86	ALA
PRO	PRO	GLY	P340	ALA	V199	R128	ARG	R541	Y476	A409	ALA	A285	A285	V159	D87	ALA
PHE	PHE	ASN	S341	ALA	N200	E129	ILE	T542	M477	Y410	THR	L286	L286	E160	H88	ALA
PRO	PRO	ASP	A343	ALA	L201	R130	ILE	I543	D478	N411	ARG	L287	L287	L161	F91	GLY
LEU	LEU	PHE	A343	ALA	S202	A131	SER	D545	Q479	D414	GLU	Y289	Y289	K162	L92	SER
ILE	ILE	LEU	M351	ALA	Q209	Q133	THR	A546	V481	P415	GLU	D290	D290	E164	T93	PRO
TRP	TRP	TRP	E352	ALA	GLY	Q134	ALA	R547	Y482	A482	LYS	A291	A291	V165	T94	ASP
SER	SER	ASP	P353	ALA	LEU	Q134	ALA	R548	S483	S483	ASP	Y292	Y292	V166	V95	PHE
LEU	LEU	ASP	M355	ALA	TRP	L137	ARG	R549	I486	R487	GLU	Q293	Q293	E167	Y96	ALA
THR	THR	ILE	G354	ALA	GLY	L137	ASN	T550	T486	T423	GLU	A294	A294	F168	Q97	PRO
PRO	PRO	PRO	M355	ALA	VAL	S139	ASP	C551	R487	L424	ALA	S295	S295	T169	N98	LEU
THR	THR	ASP	TTR	ALA	ALA	A142	ALA	P552	S491	L425	GLU	G229	G229	L170	N99	ASP
ARG	ARG	SER	ALA	ALA	ALA	A142	PHE	P553	S491	L425	ALA	LYS	LYS	P171	ASP	PRO
LEU	LEU	ASN	ALA	ALA	ALA	A142	PHE	P554	L492	T427	ALA	ASP	ASP	E172	PRO	PRO
GLY	GLY	THR	ALA	ALA	ALA	A142	PHE	P555	L492	T427	ALA	ASP	ASP	G173	S107	PHE
LEU	LEU	THR	ALA	ALA	ALA	A142	PHE	P556	T493	P428	ALA	THR	THR	N174	I111	VAL
GLU	GLU	ARG	ALA	ALA	ALA	A142	PHE	P557	H494	D429	GLU	GLU	GLU	Y175	I111	PRO
GLU	GLU	PRO	ALA	ALA	ALA	A142	PHE	P558	V495	V430	ALA	ALA	ALA	S176	N112	PRO
THR	THR	GLN	ALA	ALA	ALA	A142	PHE	P559	F496	T431	ALA	GLN	GLN	E177	L113	ARG
LEU	LEU	PRO	ALA	ALA	ALA	A142	PHE	P560	F499	Q433	PRO	GLY	GLY	T178	D114	TYR
ASN	ASN	GLN	ALA	ALA	ALA	A142	PHE	P561	P500	S434	ALA	GLY	GLY	M179	D115	LEU
ARG	ARG	THR	ALA	ALA	ALA	A142	PHE	P562	E501	E435	ALA	GLY	GLY	T180	R116	ARG
ASP	ASP	LEU	ALA	ALA	ALA	A142	PHE	P563	N502	Q436	ALA	ALA	ALA	I181	S117	PRO
LEU	LEU	LEU	ALA	ALA	ALA	A142	PHE	P564	Q503	Y437	PRO	GLY	GLY	D182	H118	THR
LEU	LEU	THR	ALA	ALA	ALA	A142	PHE	P565	I504	Y438	GLU	GLY	GLY	L183	W119	GLY
LEU	LEU	GLN	ALA	ALA	ALA	A142	PHE	P566	L505	W439	VAL	SER	SER	M184	G120	GLY
ASN	ASN	GLN	ALA	ALA	ALA	A142	PHE	P567	L506	W439	GLU	ASN	ASN	N185	G120	GLY
ALA	ALA	GLU	ALA	ALA	ALA	A142	PHE	P568	R507	L441	LYS	SER	SER	N186	G120	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P569	P508	L441	PRO	SER	SER	A187	T125	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P570	P509	M444	GLN	GLY	GLY	V188	T125	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P571	P510	M444	GLN	GLY	GLY	V188	T125	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P572	P511	Q446	GLY	GLY	GLY	E189	T129	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P573	P512	Q446	GLY	GLY	GLY	H191	N130	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P574	P513	Q446	GLY	GLY	GLY	Y192	M131	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P575	P514	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P576	P515	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P577	P516	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P578	P517	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P579	P518	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P580	P519	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P581	P520	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P582	P521	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P583	P522	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P584	P523	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P585	P524	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P586	P525	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P587	P526	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P588	P527	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P589	P528	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P590	P529	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P591	P530	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P592	P531	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P593	P532	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P594	P533	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P595	P534	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P596	P535	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P597	P536	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P598	P537	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P599	P538	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P600	P539	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P601	P540	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P602	P541	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P603	P542	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P604	P543	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P605	P544	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P606	P545	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P607	P546	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P608	P547	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P609	P548	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P610	P549	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P611	P550	Q446	GLY	GLY	GLY	E189	P132	GLY
LEU	LEU	GLU	ALA	ALA	ALA	A142	PHE	P612	P551	Q446	GLY	GLY	GLY	E189	P132	GLY
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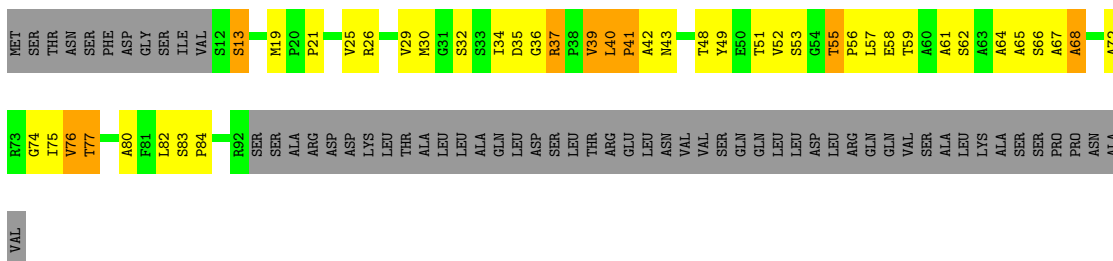
- Molecule 4: HEXON-INTERLACING PROTEIN

Chain P:



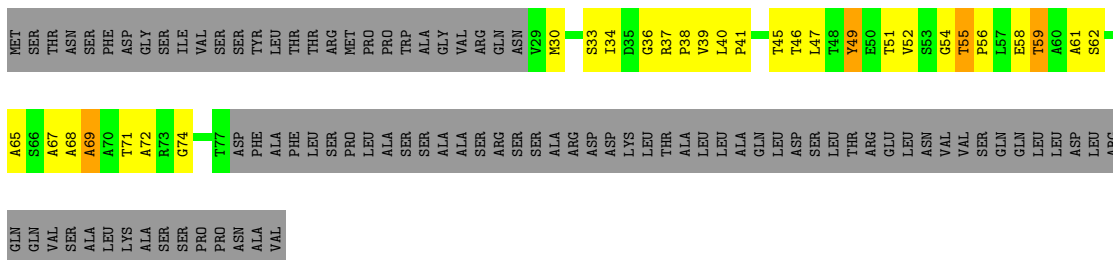
- Molecule 4: HEXON-INTERLACING PROTEIN

Chain Q:



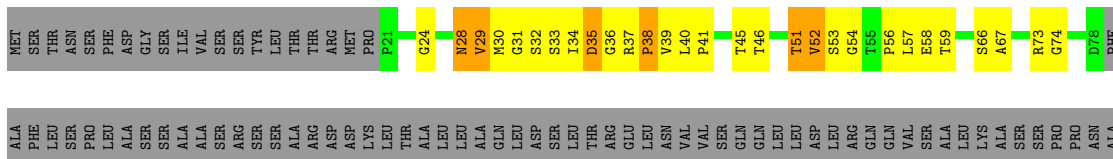
- Molecule 4: HEXON-INTERLACING PROTEIN

Chain R:



- Molecule 4: HEXON-INTERLACING PROTEIN

Chain S:



4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	853.79Å 854.45Å 865.39Å 60.40° 60.42° 61.98°	Depositor
Resolution (Å)	15.00 – 3.80	Depositor
% Data completeness (in resolution range)	17.0 (15.00-3.80)	Depositor
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 3.78Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.368 , 0.382	Depositor
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.040	Xtriage
Estimated twinning fraction	0.229 for h-l,h,h-k 0.229 for k,k-l,-h+k 0.230 for -k+l,l,-h+l 0.230 for k-l,-h+k,k 0.229 for h-k,h-l,h 0.229 for l,-h+l,-k+l 0.229 for l,h,k 0.229 for k,l,h 0.229 for h-k,-k+l,-k 0.229 for h-l,-l,k-l 0.229 for -k,h-k,-k+l 0.229 for -h+k,-h,-h+l 0.230 for -l,k-l,h-l 0.230 for -h+l,-h+k,-h 0.236 for h,h-k,h-l 0.236 for -h+k,k,k-l 0.236 for -l,-k,-h 0.246 for -k,-h,-l 0.236 for -h+l,-k+l,l 0.236 for k-l,h-l,-l 0.236 for -h,-h+l,-h+k 0.236 for -h,-l,-k 0.236 for -k+l,-k,h-k	Xtriage
L-test for twinning	$\langle L \rangle = 0.24$, $\langle L^2 \rangle = 0.09$	Xtriage
Outliers	0 of 8368449 reflections	Xtriage
Total number of atoms	98419	wwPDB-VP

Continued on next page...

¹Intensities estimated from amplitudes.

Continued from previous page...

Property	Value	Source
Average B, all atoms (\AA^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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	A	0.58	0/7519	0.77	0/10227
1	B	0.58	0/7519	0.78	7/10227 (0.1%)
1	C	0.58	0/7519	0.80	5/10227 (0.0%)
1	D	0.59	0/7519	0.81	4/10227 (0.0%)
1	E	0.58	0/7519	0.79	3/10227 (0.0%)
1	F	0.61	4/7519 (0.1%)	0.82	13/10227 (0.1%)
1	G	0.59	1/7551 (0.0%)	0.78	4/10270 (0.0%)
1	H	0.59	0/7519	0.81	6/10227 (0.1%)
1	I	0.59	0/7519	0.79	4/10227 (0.0%)
1	J	0.59	0/7519	0.81	8/10227 (0.1%)
1	K	0.58	0/7519	0.80	9/10227 (0.1%)
1	L	0.58	0/7519	0.79	7/10227 (0.1%)
2	N	0.63	1/3609 (0.0%)	0.83	5/4917 (0.1%)
3	O	0.63	0/2227	0.82	2/3022 (0.1%)
4	P	0.69	0/401	0.84	0/551
4	Q	0.72	0/584	0.83	0/801
4	R	0.59	0/331	0.79	0/455
4	S	0.66	0/407	0.75	0/559
5	T	0.64	0/526	0.85	1/718 (0.1%)
6	U	0.65	1/1144 (0.1%)	0.78	1/1546 (0.1%)
6	V	0.86	0/191	0.93	0/259
7	X	0.65	0/891	0.82	0/1220
7	Y	0.58	0/451	0.74	0/616
All	All	0.59	7/101022 (0.0%)	0.80	79/137431 (0.1%)

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	1
1	B	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	3
1	E	0	3
1	F	0	2
1	H	0	2
1	I	0	1
1	J	0	1
1	K	0	1
7	X	0	1
All	All	0	18

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	943	PRO	CG-CD	9.19	1.80	1.50
1	G	847	TYR	CB-CG	6.97	1.62	1.51
1	F	943	PRO	CA-CB	6.63	1.66	1.53
1	F	943	PRO	CA-C	-5.97	1.41	1.52
1	F	9	TRP	CB-CG	-5.40	1.40	1.50

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	730	TRP	N-CA-C	9.21	135.87	111.00
1	F	942	THR	N-CA-C	9.05	135.44	111.00
1	J	845	PHE	N-CA-C	8.98	135.25	111.00
1	F	942	THR	C-N-CD	8.93	147.15	128.40
1	B	24	SER	N-CA-C	-8.57	87.86	111.00

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	781	TYR	Sidechain
1	B	11	TYR	Sidechain
1	B	120	TYR	Sidechain
1	B	77	TYR	Sidechain
1	D	730	TRP	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7320	0	7029	1354	0
1	B	7320	0	7029	1209	0
1	C	7320	0	7029	1270	0
1	D	7320	0	7029	1322	0
1	E	7320	0	7029	1450	0
1	F	7320	0	7029	1452	0
1	G	7352	0	7057	1460	0
1	H	7320	0	7029	1469	0
1	I	7320	0	7029	1579	0
1	J	7320	0	7029	1480	0
1	K	7320	0	7029	1381	0
1	L	7320	0	7029	1455	0
2	N	3524	0	3456	486	0
3	O	2198	0	2175	152	0
4	P	394	0	391	51	0
4	Q	573	0	568	59	0
4	R	328	0	330	55	0
4	S	401	0	396	32	0
5	T	518	0	516	45	0
6	U	1118	0	1083	71	0
6	V	188	0	176	18	0
7	X	865	0	847	46	0
7	Y	440	0	442	45	0
All	All	98419	0	94756	16163	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 84.

The worst 5 of 16163 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:943:PRO:CG	1:F:943:PRO:CD	1.81	1.43
1:I:731:PRO:HA	1:I:735:ARG:NH2	1.41	1.33
1:D:246:GLN:HE21	1:E:844:ASN:ND2	1.33	1.27
1:L:942:THR:HB	1:L:943:PRO:CD	1.65	1.24
1:B:132:CYS:SG	1:B:223:LEU:HB2	1.79	1.23

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	911/952 (96%)	597 (66%)	218 (24%)	96 (10%)	1	18
1	B	911/952 (96%)	596 (65%)	204 (22%)	111 (12%)	1	14
1	C	911/952 (96%)	625 (69%)	194 (21%)	92 (10%)	1	20
1	D	911/952 (96%)	524 (58%)	241 (26%)	146 (16%)	0	7
1	E	911/952 (96%)	541 (59%)	241 (26%)	129 (14%)	0	10
1	F	911/952 (96%)	516 (57%)	254 (28%)	141 (16%)	0	8
1	G	916/952 (96%)	548 (60%)	230 (25%)	138 (15%)	0	8
1	H	911/952 (96%)	539 (59%)	245 (27%)	127 (14%)	0	11
1	I	911/952 (96%)	500 (55%)	274 (30%)	137 (15%)	0	9
1	J	911/952 (96%)	518 (57%)	253 (28%)	140 (15%)	0	8
1	K	911/952 (96%)	509 (56%)	247 (27%)	155 (17%)	0	6
1	L	911/952 (96%)	519 (57%)	251 (28%)	141 (16%)	0	8
2	N	438/571 (77%)	244 (56%)	127 (29%)	67 (15%)	0	8
3	O	277/585 (47%)	180 (65%)	83 (30%)	14 (5%)	3	43
4	P	55/140 (39%)	31 (56%)	17 (31%)	7 (13%)	0	14
4	Q	79/140 (56%)	47 (60%)	24 (30%)	8 (10%)	1	20
4	R	47/140 (34%)	28 (60%)	14 (30%)	5 (11%)	1	18
4	S	56/140 (40%)	36 (64%)	17 (30%)	3 (5%)	3	42
5	T	68/368 (18%)	35 (52%)	20 (29%)	13 (19%)	0	4
6	U	137/250 (55%)	92 (67%)	36 (26%)	9 (7%)	2	36
6	V	21/250 (8%)	14 (67%)	3 (14%)	4 (19%)	0	4
7	X	107/227 (47%)	69 (64%)	24 (22%)	14 (13%)	0	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	Y	54/227 (24%)	35 (65%)	13 (24%)	6 (11%)	1	17
All	All	12276/14462 (85%)	7343 (60%)	3230 (26%)	1703 (14%)	0	11

5 of 1703 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	MET
1	A	49	VAL
1	A	59	ARG
1	A	78	SER
1	A	109	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 X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	797/829 (96%)	624 (78%)	173 (22%)	1	11
1	B	797/829 (96%)	637 (80%)	160 (20%)	2	14
1	C	797/829 (96%)	608 (76%)	189 (24%)	1	9
1	D	797/829 (96%)	625 (78%)	172 (22%)	1	12
1	E	797/829 (96%)	604 (76%)	193 (24%)	1	9
1	F	797/829 (96%)	604 (76%)	193 (24%)	1	9
1	G	800/829 (96%)	616 (77%)	184 (23%)	1	10
1	H	797/829 (96%)	606 (76%)	191 (24%)	1	9
1	I	797/829 (96%)	592 (74%)	205 (26%)	1	8
1	J	797/829 (96%)	620 (78%)	177 (22%)	1	11
1	K	797/829 (96%)	620 (78%)	177 (22%)	1	11
1	L	797/829 (96%)	606 (76%)	191 (24%)	1	9
2	N	399/489 (82%)	304 (76%)	95 (24%)	1	9
3	O	239/500 (48%)	215 (90%)	24 (10%)	11	53
4	P	40/112 (36%)	34 (85%)	6 (15%)	4	31
4	Q	60/112 (54%)	50 (83%)	10 (17%)	3	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	R	34/112 (30%)	30 (88%)	4 (12%)	8	43
4	S	41/112 (37%)	33 (80%)	8 (20%)	2	16
5	T	53/315 (17%)	41 (77%)	12 (23%)	1	10
6	U	123/210 (59%)	108 (88%)	15 (12%)	7	42
6	V	22/210 (10%)	17 (77%)	5 (23%)	1	10
7	X	96/186 (52%)	87 (91%)	9 (9%)	13	56
7	Y	47/186 (25%)	42 (89%)	5 (11%)	10	49
All	All	10721/12492 (86%)	8323 (78%)	2398 (22%)	1	11

5 of 2398 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	20	SER
1	H	392	SER
2	N	99	ASN
1	G	210	TRP
1	G	736	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 422 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	455	ASN
1	H	640	GLN
1	L	821	GLN
1	G	558	HIS
1	H	17	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.