



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:35 PM BST

PDB ID : 3J9K  
EMDB ID: : EMD-2870  
Title : Structure of Dark apoptosome in complex with Dronc CARD domain  
Authors : Pang, Y.; Bai, X.; Yan, C.; Hao, Q.; Chen, Z.; Wang, J.; Scheres, S.H.W.; Shi, Y.  
Deposited on : 2015-02-04  
Resolution : 4.10 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

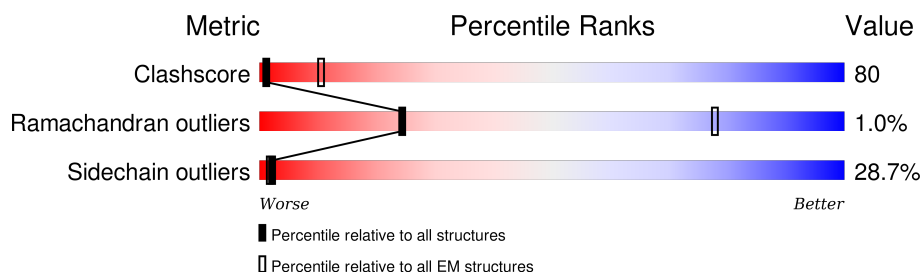
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.10 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.




















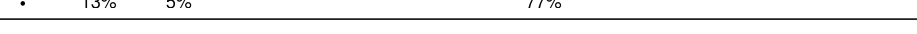





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1102	49% 34% 13% . .
1	C	1102	50% 34% 13% . .
1	E	1102	50% 33% 13% . .
1	G	1102	51% 33% 13% . .
1	I	1102	50% 33% 13% . .
1	K	1102	50% 33% 13% . .
1	M	1102	51% 33% 13% . .
1	O	1102	50% 33% 13% . .
1	Q	1102	50% 33% 13% . .

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Mol	Chain	Length	Quality of chain
1	S	1102	
1	U	1102	
1	W	1102	
1	Y	1102	
1	a	1102	
1	c	1102	
1	e	1102	
2	B	450	
2	D	450	
2	F	450	
2	H	450	
2	J	450	
2	L	450	
2	N	450	
2	P	450	
2	R	450	
2	T	450	
2	V	450	
2	X	450	
2	Z	450	
2	b	450	
2	d	450	
2	f	450	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 126512 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 Apaf-1 related killer DARK.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	C	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	E	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	G	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	I	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	K	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	M	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	O	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	Q	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	S	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	U	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	W	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	Y	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	a	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	c	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	e	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		

- Molecule 2 is a protein called Caspase Nc.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	D	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	F	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	H	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	J	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	L	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	N	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	P	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	R	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	T	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	V	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	X	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	Z	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	b	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	d	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	f	102	Total	C	N	O	S	0	0
			840	522	160	152	6		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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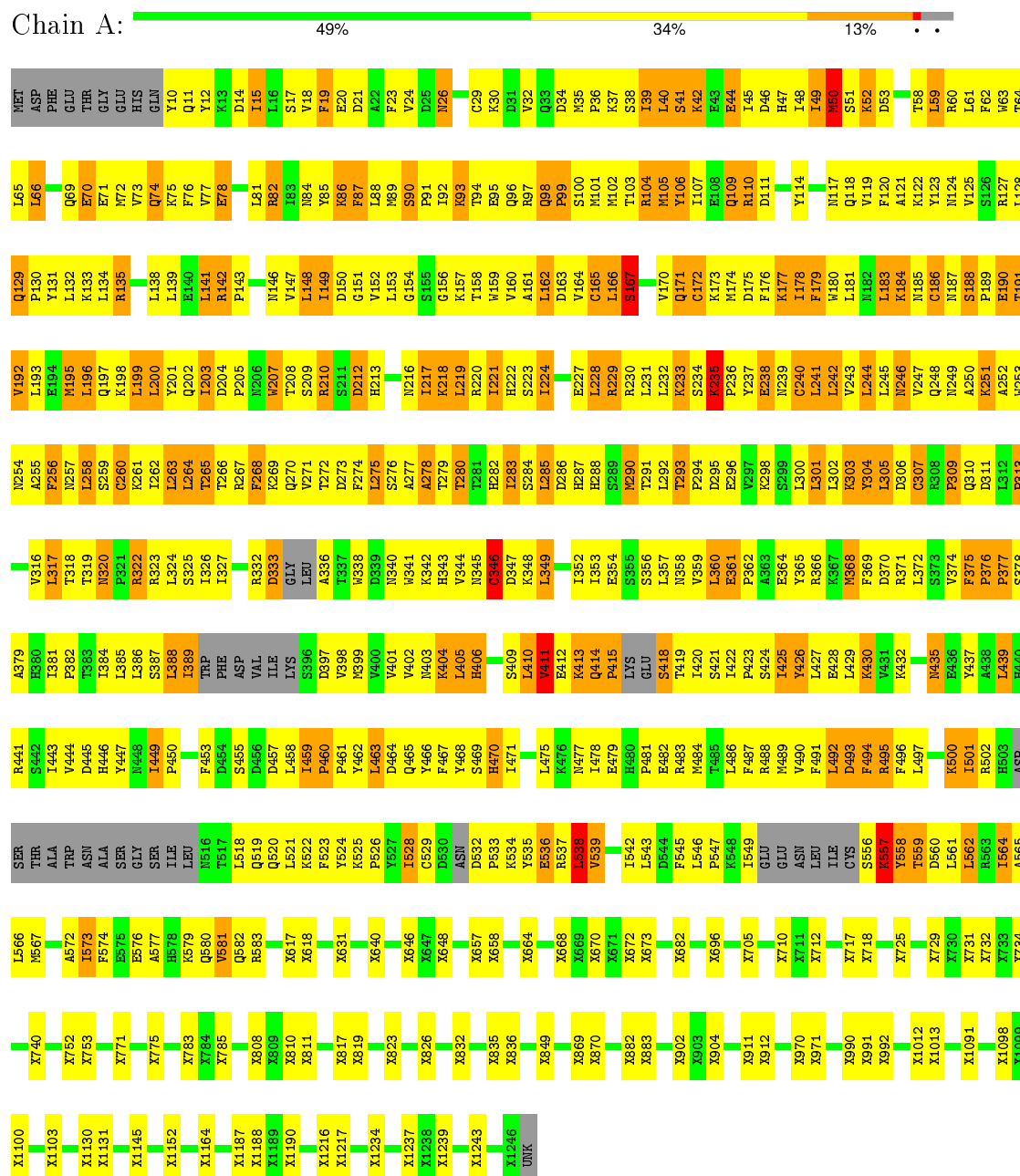
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Mol	Chain	Residues	Atoms					AltConf
3	c	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	e	1	Total	C	N	O	P	0
			27	10	5	10	2	

### 3 Residue-property plots

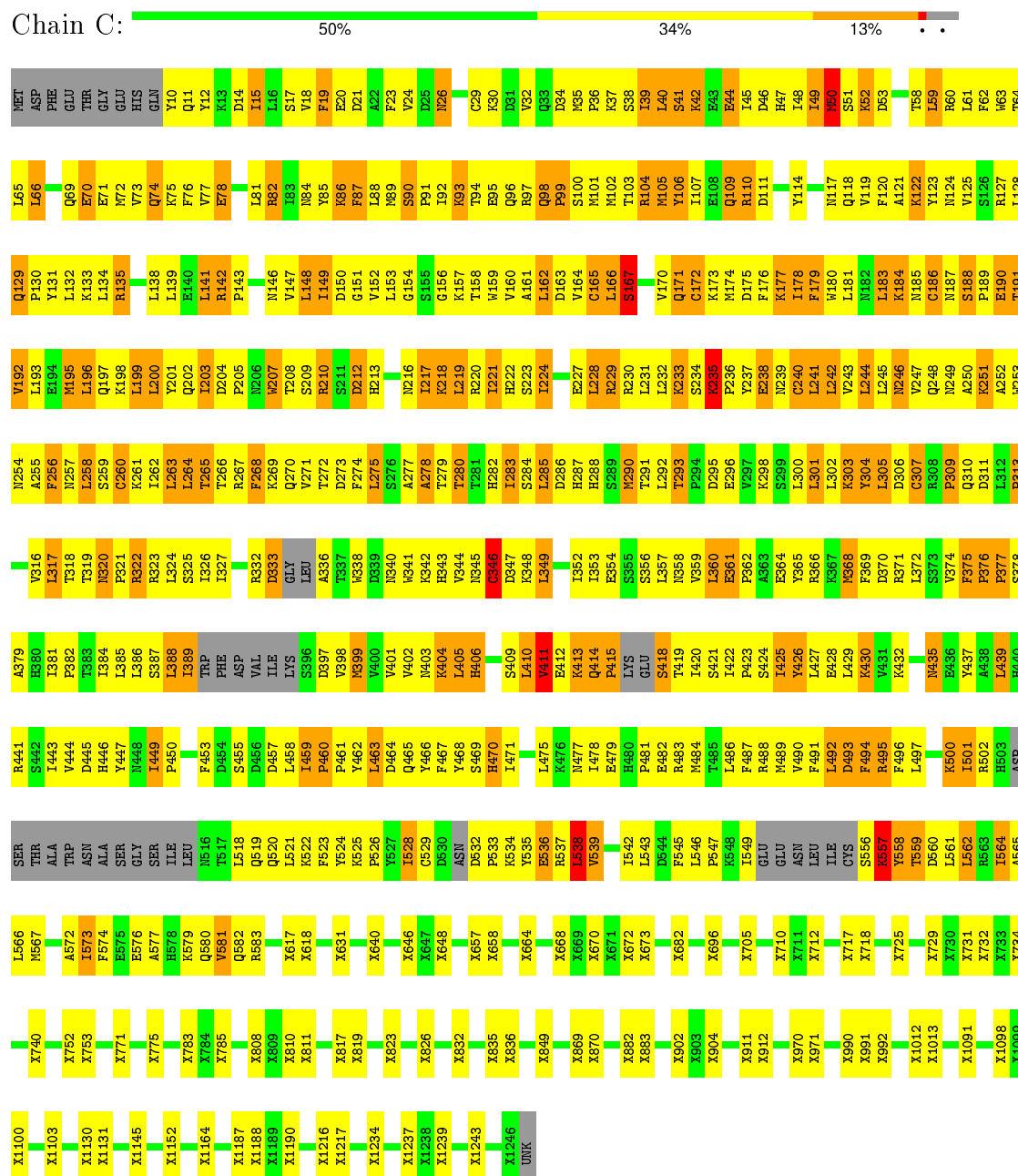
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric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

- Molecule 1: Apaf-1 related killer DARK

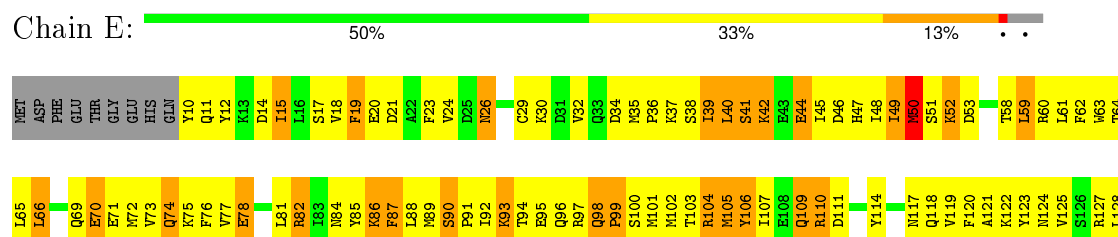




• Molecule 1: Apaf-1 related killer DARK

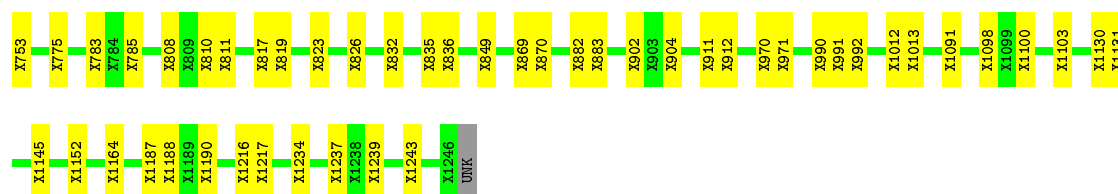


• Molecule 1: Apaf-1 related killer DARK



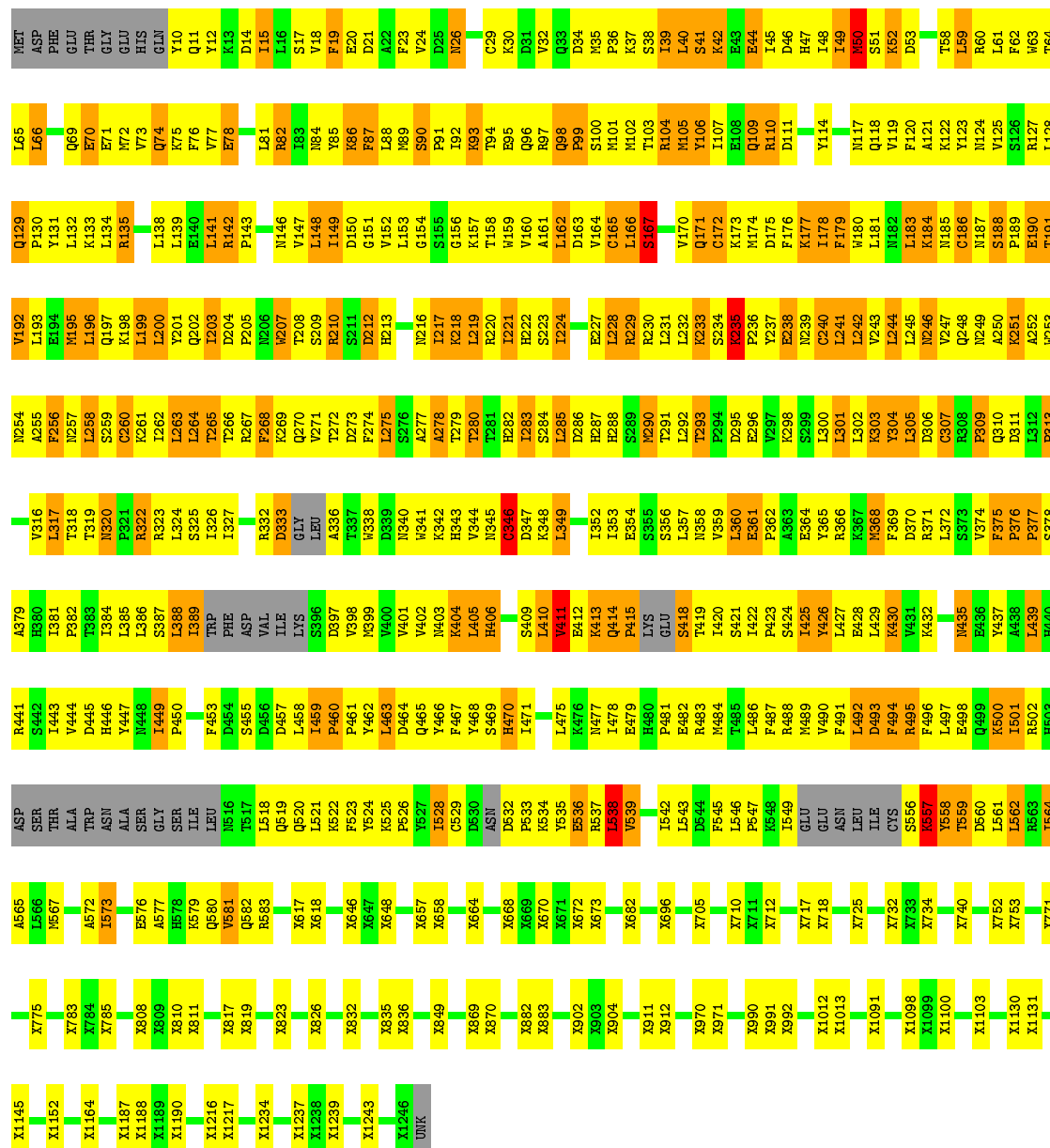
Q129	P130	Y131	L132	K133	L134	R135	L138	L139	Q201	Q202	L203	L204	R205	P206	L207	L208	S209	L210	R211	L212	H213	N216	L217	K218	L219	R220	L221	R222	S223	L224	E227	L228	R229	R230	L231	L232	S233	S234	K235	P236	M237	F238	L239	C240	L241	F242	L243	L244	L245	N246	L247	Q248	L249	S250	P251	L252	L253	L254	A255	F256	E257	L258	L259	L260	K261	L262	L263	L264	T265	T266	R267	F268	Q269	L270	Q271	L272	L273	L274	L275	L276	L277	A278	T279	T280	L281	T282	L283	L284	S285	L286	L287	L288	S289	N290	T291	L292	T293	P294	D295	E296	P297	K298	S299	L300	Y301	L302	L303	Y304	L305	D306	R307	L308	L309	L310	D311	Q312	L313	L314	L315	L316	L317	L318	L319	L320	L321	L322	L323	L324	L325	L326	L327	L328	L329	L330	L331	L332	L333	L334	L335	L336	L337	L338	L339	L340	L341	L342	L343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354	L355	L356	L357	L358	L359	L360	L361	L362	L363	L364	L365	L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	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	L1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• Molecule 1: Apaf-1 related killer DARK

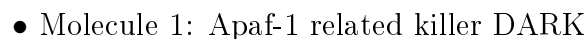
Chain K: 50% 33% 13% . .



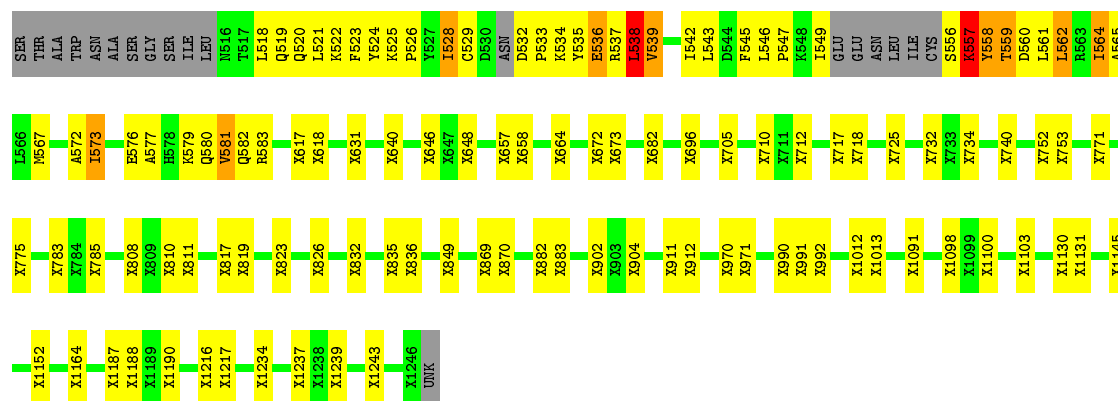
• Molecule 1: Apaf-1 related killer DARK

Chain M: 51% 33% 13% . .

Y192	V193	V194	V195	V196	V197	V198	V199	V200	V201	V202	V203	V204	V205	V206	V207	V208	V209	V210	V211	V212	V213	V214	V215	V216	V217	V218	V219	V220	V221	V222	V223	V224	V225	V226	V227	V228	V229	V230	V231	V232	V233	V234	V235	V236	V237	V238	V239	V240	V241	V242	V243	V244	V245	V246	V247	V248	V249	V250	V251	V252	V253	V254	V255	V256	V257	V258	V259	V260	V261	V262	V263	V264	V265	V266	V267	V268	V269	V270	V271	V272	V273	V274	V275	V276	V277	V278	V279	V280	V281	V282	V283	V284	V285	V286	V287	V288	V289	V290	V291	V292	V293	V294	V295	V296	V297	V298	V299	V300	V301	V302	V303	V304	V305	V306	V307	V308	V309	V310	V311	V312	V313	V314	V315	V316	V317	V318	V319	V320	V321	V322	V323	V324	V325	V326	V327	V328	V329	V330	V331	V332	V333	V334	V335	V336	V337	V338	V339	V340	V341	V342	V343	V344	V345	V346	V347	V348	V349	V350	V351	V352	V353	V354	V355	V356	V357	V358	V359	V360	V361	V362	V363	V364	V365	V366	V367	V368	V369	V370	V371	V372	V373	V374	V375	V376	V377	V378	V379	V380	V381	V382	V383	V384	V385	V386	V387	V388	V389	V390	V391	V392	V393	V394	V395	V396	V397	V398	V399	V400	V401	V402	V403	V404	V405	V406	V407	V408	V409	V410	V411	V412	V413	V414	V415	V416	V417	V418	V419	V420	V421	V422	V423	V424	V425	V426	V427	V428	V429	V430	V431	V432	V433	V434	V435	V436	V437	V438	V439	V440	V441	V442	V443	V444	V445	V446	V447	V448	V449	V450	V451	V452	V453	V454	V455	V456	V457	V458	V459	V460	V461	V462	V463	V464	V465	V466	V467	V468	V469	V470	V471	V472	V473	V474	V475	V476	V477	V478	V479	V480	V481	V482	V483	V484	V485	V486	V487	V488	V489	V490	V491	V492	V493	V494	V495	V496	V497	V498	V499	V500	V501	V502	V503	V504	V505	V506	V507	V508	V509	V510	V511	V512	V513	V514	V515	V516	V517	V518	V519	V520	V521	V522	V523	V524	V525	V526	V527	V528	V529	V530	V531	V532	V533	V534	V535	V536	V537	V538	V539	V540	V541	V542	V543	V544	V545	V546	V547	V548	V549	V550	V551	V552	V553	V554	V555	V556	V557	V558	V559	V560	V561	V562	V563	V564	V565	V566	V567	V568	V569	V570	V571	V572	V573	V574	V575	V576	V577	V578	V579	V580	V581	V582	V583	V584	V585	V586	V587	V588	V589	V590	V591	V592	V593	V594	V595	V596	V597	V598	V599	V600	V601	V602	V603	V604	V605	V606	V607	V608	V609	V610	V611	V612	V613	V614	V615	V616	V617	V618	V619	V620	V621	V622	V623	V624	V625	V626	V627	V628	V629	V630	V631	V632	V633	V634	V635	V636	V637	V638	V639	V640	V641	V642	V643	V644	V645	V646	V647	V648	V649	V650	V651	V652	V653	V654	V655	V656	V657	V658	V659	V660	V661	V662	V663	V664	V665	V666	V667	V668	V669	V670	V671	V672	V673	V674	V675	V676	V677	V678	V679	V680	V681	V682	V683	V684	V685	V686	V687	V688	V689	V690	V691	V692	V693	V694	V695	V696	V697	V698	V699	V700	V701	V702	V703	V704	V705	V706	V707	V708	V709	V710	V711	V712	V713	V714	V715	V716	V717	V718	V719	V720	V721	V722	V723	V724	V725	V726	V727	V728	V729	V730	V731	V732	V733	V734	V735	V736	V737	V738	V739	V740	V741	V742	V743	V744	V745	V746	V747	V748	V749	V750	V751	V752	V753	V754	V755	V756	V757	V758	V759	V760	V761	V762	V763	V764	V765	V766	V767	V768	V769	V770	V771	V772	V773	V774	V775	V776	V777	V778	V779	V780	V781	V782	V783	V784	V785	V786	V787	V788	V789	V790	V791	V792	V793	V794	V795	V796	V797	V798	V799	V800	V801	V802	V803	V804	V805	V806	V807	V808	V809	V810	V811	V812	V813	V814	V815	V816	V817	V818	V819	V820	V821	V822	V823	V824	V825	V826	V827	V828	V829	V830	V831	V832	V833	V834	V835	V836	V837	V838	V839	V840	V841	V842	V843	V844	V845	V846	V847	V848	V849	V850	V851	V852	V853	V854	V855	V856	V857	V858	V859	V860	V861	V862	V863	V864	V865	V866	V867	V868	V869	V870	V871	V872	V873	V874	V875	V876	V877	V878	V879	V880	V881	V882	V883	V884	V885	V886	V887	V888	V889	V890	V891	V892	V893	V894	V895	V896	V897	V898	V899	V900	V901	V902	V903	V904	V905	V906	V907	V908	V909	V910	V911	V912	V913	V914	V915	V916	V917	V918	V919	V920	V921	V922	V923	V924	V925	V926	V927	V928	V929	V930	V931	V932	V933	V934	V935	V936	V937	V938	V939	V940	V941	V942	V943	V944	V945	V946	V947	V948	V949	V950	V951	V952	V953	V954	V955	V956	V957	V958	V959	V960	V961	V962	V963	V964	V965	V966	V967	V968	V969	V970	V971	V972	V973	V974	V975	V976	V977	V978	V979	V980	V981	V982	V983	V984	V985	V986	V987	V988	V989	V990	V991	V992	V993	V994	V995	V996	V997	V998	V999	V1000	V1001	V1002	V1003	V1004	V1005	V1006	V1007	V1008	V1009	V1010	V1011	V1012	V1013	V1014	V1015	V1016	V1017	V1018	V1019	V1020	V1021	V1022	V1023	V1024	V1025	V1026	V1027	V1028	V1029	V1030	V1031	V1032	V1033	V1034	V1035	V1036	V1037	V1038	V1039	V1040	V1041	V1042	V1043	V1044	V1045	V1046	V1047	V1048	V1049	V1050	V1051	V1052	V1053	V1054	V1055	V1056	V1057	V1058	V1059	V1060	V1061	V1062	V1063	V1064	V1065	V1066	V1067	V1068	V1069	V1070	V1071	V1072	V1073	V1074	V1075	V1076	V1077	V1078	V1079	V1080	V1081	V1082	V1083	V1084	V1085	V1086	V1087	V1088	V1089	V1090	V1091	V1092	V1093	V1094	V1095	V1096	V1097	V1098	V1099	V1100	V1101	V1102	V1103	V1104	V1105	V1106	V1107	V1108	V1109	V1110	V1111	V1112	V1113	V1114	V1115	V1116	V1117	V1118	V1119	V1120	V1121	V1122	V1123	V1124	V1125	V1126	V1127	V1128	V1129	V1130	V1131	V1132	V1133	V1134	V1135	V1136	V1137	V1138	V1139	V1140	V1141	V1142	V1143	V1144	V1145	V1146	V1147	V1148	V1149	V1150	V1151	V1152	V1153	V1154	V1155	V1156	V1157	V1158	V1159	V1160	V1161	V1162	V1163	V1164	V1165	V1166	V1167	V1168	V1169	V1170	V1171	V1172	V1173	V1174	V1175	V1176	V1177	V1178	V1179	V1180	V1181	V1182	V1183	V1184	V1185	V1186	V1187	V1188	V1189	V1190	V1191	V1192	V1193	V1194	V1195	V1196	V1197	V1198	V1199	V1200	V1201	V1202	V1203	V1204	V1205	V1206	V1207	V1208	V1209	V1210	V1211	V1212	V1213	V1214	V1215	V1216	V1217	V1218	V1219	V1220	V1221	V1222	V1223	V1224	V1225	V1226	V1227	V1228	V1229	V1230	V1231	V1232	V1233	V1234	V1235	V1236	V1237	V1238	V1239	V1240	V1241	V1242	V1243	V1244	V1245	V1246	V1247	V1248	V1249	V1250	V1251	V1252	V1253	V1254	V1255	V1256	V1257	V1258	V1259	V1260	V1261	V1262	V1263	V1264	V1265	V1266	V1267	V1268	V1269	V1270	V1271	V1272	V1273	V1274	V1275	V1276	V1277	V1278	V1279	V1280	V1281	V1282	V1283	V1284	V1285	V1286	V1287	V1288	V1289	V1290	V1291	V1292	V1293	V1294	V1295	V1296	V1297	V1298	V1299	V1300	V1301	V1302	V1303	V1304	V1305	V1306	V1307	V1308	V1309	V1310	V1311	V1312	V1313	V1314	V1315	V1316	V1317	V1318	V1319	V1320	V1321	V1322	V1323	V1324	V1325	V1326	V1327	V1328	V1329	V1330	V1331	V1332	V1333	V1334	V1335	V1336	V1337	V1338	V1339	V1340	V1341	V1342	V1343	V1344	V1345	V1346	V1347	V1348	V1349	V1350	V1351	V1352	V1353	V1354	V1355	V1356	V1357	V1358	V1359	V1360	V1361	V1362	V1363	V1364	V1365	V1366	V1367	V1368	V1369	V1370	V1371	V1372	V1373	V1374	V1375	V1376	V1377	V1378	V1379	V1380	V1381	V1382	V1383	V1384	V1385	V1386	V1387	V1388	V1389	V1390	V1391	V1392	V1393	V1394	V1395	V1396	V1397	V1398	V1399	V1400	V1401	V1402	V1403	V1404	V1405	V1406	V1407	V1408	V1409	V1410	V1411	V1412	V1413	V1414	V1415	V1416	V1417	V1418	V1419	V1420	V1421	V1422	V1423	V1424	V1425	V1426	V1427	V1428	V1429	V1430	V1431	V1432	V1433	V1434	V1435	V1436	V1437	V1438	V1439	V1440	V1441	V1442	V1443	V1444	V1445	V1446	V1447	V1448	V1449	V1450	V1451	V1452	V1453	V1454	V1455	V1456	V1457	V1458	V1459	V1460	V1461	V1462	V1463	V1464	V1465	V1466	V1467	V1468	V1469	V1470	V1471	V1472	V1473	V1474	V1475	V1476	V1477	V1478	V1479	V1480	V1481	V1482	V1483	V1484	V1485	V1486	V1487	V1488	V1489	V1490	V1491	V1492	V1493	V1494	V1495	V1496	V1497	V1498	V1499	V1500	V1501	V1502	V1503	V1504	V1505	V1506	V1507	V1508	V1509	V1510	V1511	V1512	V1513	V1514	V1515	V1516	V1517	V1518	V1519	V1520	V1521	V1522	V1523	V1524	V1525	V1526	V1527	V1528	V1529	V1530	V1531	V1532	V1533	V1534	V1535	V1536	V1537	V1538	V1539	V1540	V1541	V1542	V1543	V1544	V1545	V1546	V1547	V1548	V1549	V1550	V1551	V1552	V1553	V1554	V1555	V1556	V1557	V1558	V1559	V1560	V1561	V1562	V1563	V1564	V1565	V1566	V1567	V1568	V1569	V1570	V1571	V1572	V1573	V1574	V1575	V1576	V1577	V1578	V1579	V1580	V1581	V1582	V1583	V1584	V1585	V1586	V1587	V1588	V1589	V1590	V1591	V1592	V1593	V1594	V1595	V1596	V1597	V1598	V1599	V1600	V1601	V1602	V1603	V1604	V1605	V1606	V1607	V1608	V1609	V1610	V1611	V1612	V1613	V1614	V1615	V1616	V1617	V1618	V1619	V1620	V1621	V1622	V1623	V1624	V1625	V1626	V1627	V1628	V1629	V1630	V1631	V1632	V1633	V1634	V1635	V1636	V1637	V1638	V1639	V1640	V1641	V164
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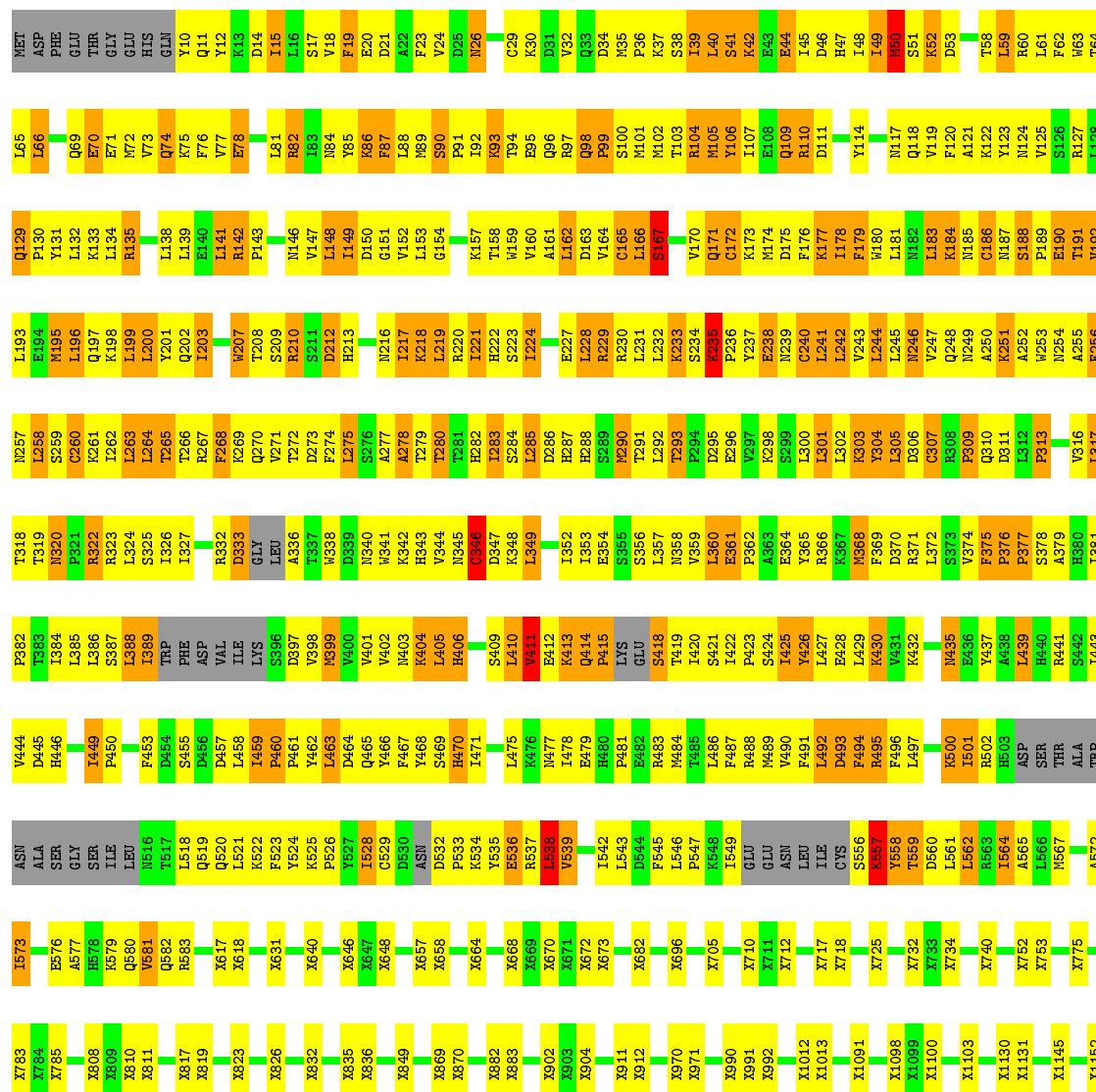


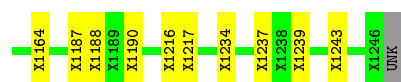
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I443	L317	T318	F256	E194	V131		PHE
V444	P382	T319	N257	M195	L132	O69	GLU
D445	T383	T319	L258	L196	L133	E70	THR
K446	L384	K320	S259	Q197	L134	E71	GLY
V447	L385	F321	C260	L198	R135	M72	GLU
M448	L386	R322	K261	L199		V73	HIS
I449	S387	R323	L262	L200	L138	Q74	GLN
P450	L388	L324	L263	Y201	L139	K75	Y10
F453	T389	S325	L264	Q202	E140	F76	Q11
D454	PHE	L326	T265	L203	L141	V77	Y12
S455	ASP	L327	T266	D204	R142	E78	K13
D456	VAL	R332	F268	P205	P143		D14
L457	ILE	D333	K269	M206	L146	L81	I15
L458	LYS	GLY	Q270	T208	V147	B82	L16
I459	S386	LEU	V271	S209	L148	B84	S17
P460	D397	T336	T272	R210	L149	B85	F19
P461	V388	F337	D273	S211	D150	K86	E20
Y462	K399	K338	F274	D212	G151	F87	D21
L463	V400	D339	L275	B213	V152	L88	A22
D464	V401	K340	S276		L153	K89	F23
Q465	V402	K341	A277	M216	G154	S90	V24
Y466	M403	K342	A278	L217	S155	P91	D25
F467	F404	F343	T279	K218	G156	L92	M26
Y468	L405	V344	T280	L219	K157	R93	
S469	H406	K345	T281	R220	T158	T94	C29
H470		G346	H282	T221	H159	E95	K30
I471	S409	D347	L283	R222	V160	Q96	D31
	L410	K348	S284	S223	L162	R97	V32
L475	V411	L349	L285	T224	A163		
K476			D286		D163	Q98	Q33
M477	E413	L352	H287	E227	V164	P99	D34
L478	D414	L353	H288	L228	G165	M01	M35
E479	P415	E354	S289	R229	L166	M02	P36
H480	LYS	S355	M290	R230	E167	T103	K37
P481	GLU	L356	T291	L231			S38
E482	L418	L357	L292	L232	V170	M04	I39
K483	T419	K358	T293	K233	Q171	M05	L40
M484	T420	V359	P294	S234	C172	I106	S41
H485	S421	L360	D295	E235	K173	E108	K42
L486	L422	E361	E296	F236	M174	Q109	E43
F487	P423	P362	V297	T237	D175	R110	E44
K488	S424	F369	K298	E238	F176	D111	I45
M489	L425	E364	S299	M239	K177		H46
V490	V426	K365	K301	C240	L178	Y114	H47
F491	L427	R366	L301	L241	F179		I48
L492	E428	K367	L302	L242			I49
D493	L429	K368	K303	V243	H180	M117	M50
F494	F430	F369	Y304	L244	L181	Q118	S51
K495	V431	D370	L305	L245	H182	V119	K52
F496	H432	K371	D306	M246	L183	F120	D53
L497		L372	C307	V247	L184	A121	
		S373	C308	Q248	H185	K122	T88
K500	E436	V374	P309	M249	G186	M123	L59
I501	V437	F375	Q310	A250	N187	Y123	R60
R502	A438	P376	D311	K251	S188	V125	L61
H503	L439	E377	L312	E252	P189	S126	F62
F504	H440	E377	R312	A253	P190	L127	H63
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• Molecule 1: Apaf-1 related killer DARK

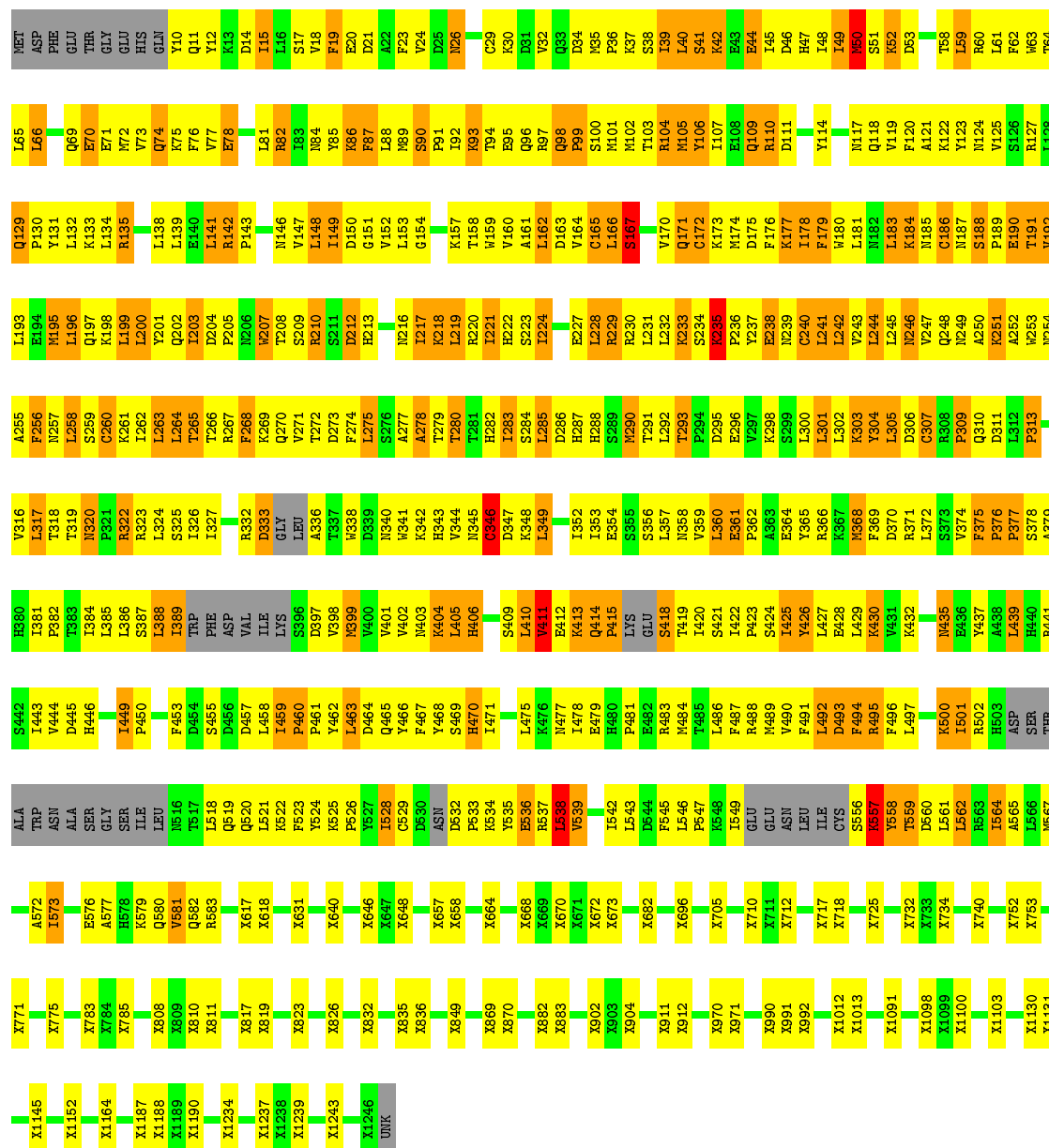
Chain S: 51% 33% 13%





• Molecule 1: Apaf-1 related killer DARK

Chain U: 51% 33% 13% . .



• Molecule 1: Apaf-1 related killer DARK

Chain W: 50% 33% 13% . .



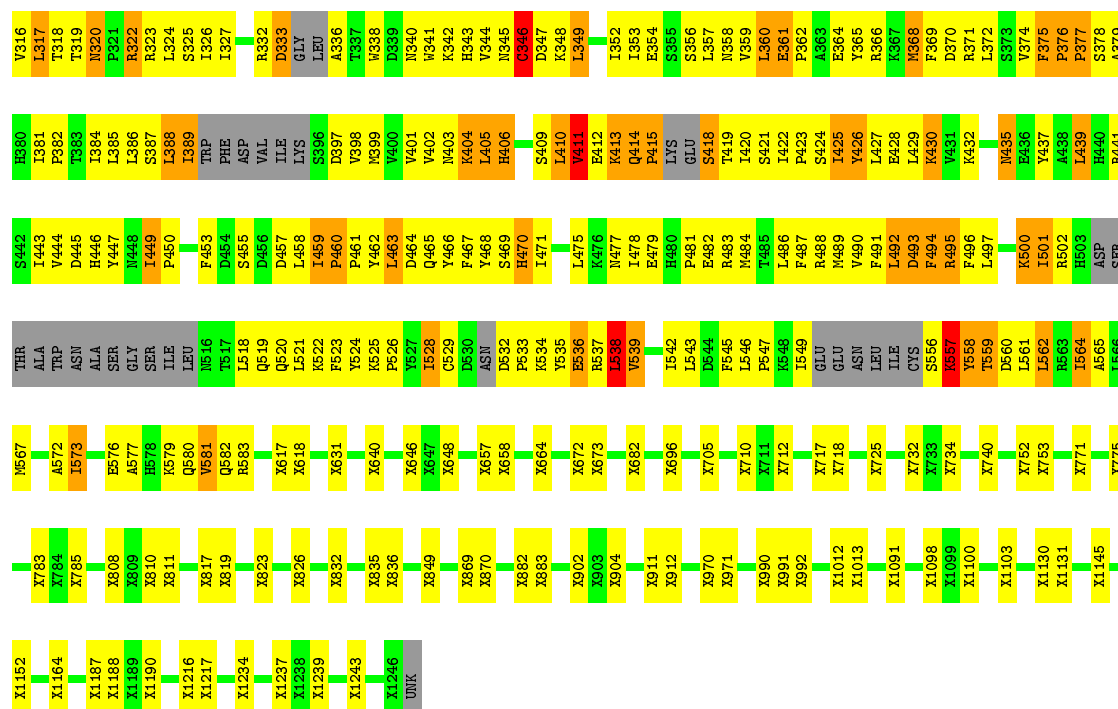


L65	L66	Q129	L193	A255	V316	H380	S442	ALA	X775	X1145
L69	Q69	P130	E194	F256	L317	I381	I443	TRP	X783	X1152
E70	L196	Y131	M195	N257	T318	P382	V444	ASN	X785	X1164
E71	L196	L133	L196	L258	T319	T383	H446	GLY	X785	X1187
E71	Q197	K133	Q197	S259	K321	I384	T449	GLY	X808	X1188
E72	K198	L134	K198	C260	R322	L385	P450	SER	X809	X1189
E72	L199	R135	L199	K261	R323	L386	T450	GLY	X811	X1190
E73	L200	L138	L200	L262	R324	S387	P451	ILE	X817	X1216
Q74	L201	L139	L201	L263	R325	P388	F453	LEU	X819	X1217
E76	Q202	E140	Q202	L264	L326	L388	P453	TRP	X823	X1234
E77	L139	L141	L139	T265	I327	TRP	F454	ASP	X826	X1237
E78	L205	L142	L205	T266	L327	PHE	D455	ASP	X832	X1238
	P143	P143	P205	R267		ASP	D456	ASP	X833	X1239
			R206	R268	R332	VAL	D457	Q520	X840	X1243
L81	L82	N146	R207	R269	R333	ILE	D458	L521	X846	X1246
L83	L83	N147	T208	Q270	GLY	LYS	L459	K522	X848	UNK
N84	L148	L147	S209	V271	LEU	S386	L460	F523	X861	
E85	I149	I149	R210	T272	A336	D387	P461	Y524	X863	
K86	D150	D150	S211	D273	T337	V398	Y462	K525	X864	
E87	G151	G151	D212	D274	K338	K399	L463	P526	X869	
L88	V152	V152	D213	L275	K339	V400	Q465	F527	X870	
L89	L153	L153	N216	A277	K341	V401	Q466	I528	X871	
S90	G154	G154	T217	T278	K342	N403	F467	C529	X873	
P91			K218	T279	K343	K404	Y468	ASN	X882	
I92			L219	T280	V344	L405	S469	D530	X883	
K93	K157	K157	T220	T281	R345	H406	H470	D532	X902	
T94	M158	M158	R221	H382	C346		L471	P533	X903	
E95	V160	V160	R222	T283	K347	S409	L475	K534	X904	
Q96	A161	A161	S223	S284	K348	L410	L476	Y535	X911	
R97	L162	L162	T224	K285	L349	V411	K477	R537	X912	
Q98	D163	D163		D286		E412	H478	L538	X970	
P99	V164	V164	E227	H287		K413	P479	V539	X971	
S100	C165	C165	R228	H288		Q414	H480	I542	X990	
M101	L166	L166	R229	S289		P415	T485	L546	X991	
M102	S167	S167	R230	K290		L543	P481	P547	X992	
T103			L231	M290		GLY	H482	L548	X1012	
R104	V170	V170	L232	T291		S418	R483	I549	X1013	
M105	Q171	Q171	L233	L292		L419	P484	GLY	X1091	
Y106	C172	C172	R233	T293		L420	H485	ASN	X1098	
I107	K173	K173	S234	P294		L427	L486	LEU	X1100	
E108	M174	M174	K235	D295		E422	L487	ILE	X1103	
Q109	D175	D175	P236	E296		K423	P488	CYS	X1131	
R110	F176	F176	Y237	K297		S424	H489	GLY	X130	
D111	K177	K177	E238	K298		L425	V490	ASN	X153	
			N239	S299		I426	F491	LEU	X156	
Y114	L178	L178	C240	L300		L492	L492	ILE	X157	
N117	F179	F179	L241	L301		D493	P494	CYS	X175	
Q118	M180	M180	L242	L302		K367	F495		X178	
F119	L181	L181	V243	Y304		F369	R496		X179	
F120	L182	L182	L244	L305		D370	L497		X188	
K183	K184	K184	L245	L306		R371			X189	
N185	A121	A121	N246	D306		K372			X190	
K186	Q248	Q248	V247	C307		S373			X191	
N187	N249	N249	Q248	K308		V374			X192	
N123	N187	N187	Q249	Q309		P375				
N124	S188	S188	A250	Q310		P376				
V125	P189	P189	K251	D311		P377				
S126	E190	E190	A252	L312		S378				
R127	T191	T191	W253	P313		H441				
L128	V192	V192	N254			R441				

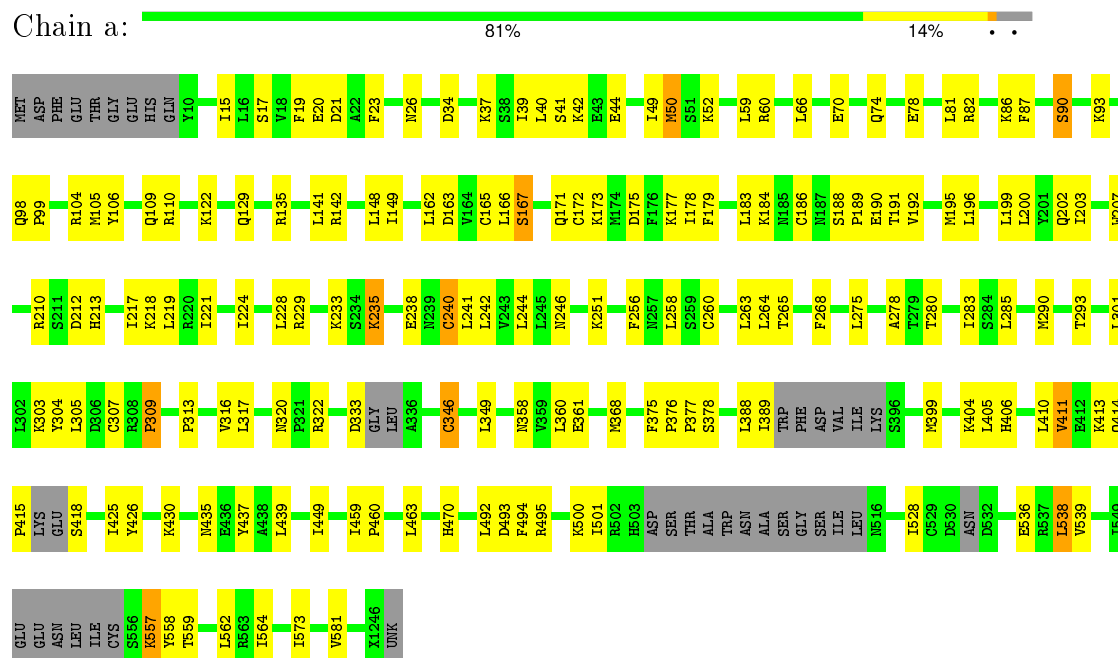
• Molecule 1: Apaf-1 related killer DARK

Chain Y:  50% 33% 13% • •

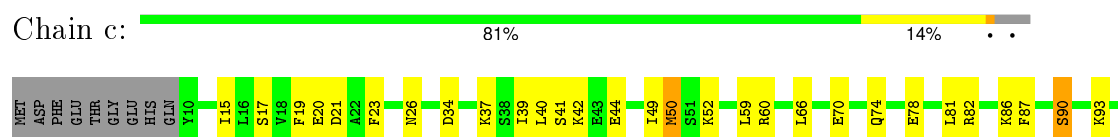
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GLY	GLY	Q69	Y131	M195	N257	THR	THR	Q69	Y131	M195	N257
GLY	GLY	E70	L132	L196	L258	GLY	GLY	E70	L132	L196	L258
GLY	GLY	E71	K133	Q197	S259	GLY	GLY	E71	K133	Q197	S259
GLY	GLY	E72	L134	K198	C260	GLY	GLY	E72	L134	K198	C260
GLY	GLY	E73	R135	L199	K261	GLY	GLY	E73	R135	L199	K261
GLY	GLY	Q74	L138	L200	L262	GLY	GLY	Q74	L138	L200	L262
GLY	GLY	E76	L139	L201	L263	GLY	GLY	E76	L139	L201	L263
GLY	GLY	F76	E140	Q202	L264	GLY	GLY	F76	E140	Q202	L264
GLY	GLY	V77	L141	D204	T266	GLY	GLY	V77	L141	D204	T266
GLY	GLY	E78	L142	P205	R267	GLY	GLY	E78	L142	P205	R267
GLY	GLY		P143	P206	F268	GLY	GLY		P143	P206	F268
GLY	GLY	L81	N146	R207	R269	GLY	GLY	L81	N146	R207	R269
GLY	GLY	R82	V147	T208	Q270	GLY	GLY	R82	V147	T208	Q270
GLY	GLY	L83	L148	S209	V271	GLY	GLY	L83	L148	S209	V271
GLY	GLY	N84	L149	R210	T272	GLY	GLY	N84	L149	R210	T272
GLY	GLY	E85	I149	S211	D273	GLY	GLY	E85	I149	S211	D273
GLY	GLY	K86	D150	D212	L274	GLY	GLY	K86	D150	D212	L274
GLY	GLY	E87	G151	D213	L275	GLY	GLY	E87	G151	D213	L275
GLY	GLY	L88	V152	N216	A277	GLY	GLY	L88	V152	N216	A277
GLY	GLY	M89	L153	T217	T278	GLY	GLY	M89	L153	T217	T278
GLY	GLY	S90	G154	K218	T279	GLY	GLY	S90	G154	K218	T279
GLY	GLY	P91		L219	T280	GLY	GLY	P91		L219	T280
GLY	GLY	I92	K157	R220	T281	GLY	GLY	I92	K157	R220	T281
GLY	GLY	K93	M158	R221	H282	GLY	GLY	K93	M158	R221	H282
GLY	GLY	T94	V160	R222	T283	GLY	GLY	T94	V160	R222	T283
GLY	GLY	E95	A161	S223	S284	GLY	GLY	E95	A161	S223	S284
GLY	GLY	Q96	L162	R224	L285	GLY	GLY	Q96	L162	R224	L285
GLY	GLY	R97	D163	T224	L286	GLY	GLY	R97	D163	T224	L286
GLY	GLY	Q98	P99	E227	D286	GLY	GLY	Q98	P99	E227	D286
GLY	GLY	P99	V164	R228	H287	GLY	GLY	P99	V164	R228	H287
GLY	GLY	S100	C165	L228	H288	GLY	GLY	S100	C165	L228	H288
GLY	GLY	M101	L166	R229	S289	GLY	GLY	M101	L166	R229	S289
GLY	GLY	M102	S167	R230	M290	GLY	GLY	M102	S167	R230	M290
GLY	GLY	T103		L231	T291	GLY	GLY	T103		L231	T291
GLY	GLY	R104	V170	L232	L292	GLY	GLY	R104	V170	L232	L292
GLY	GLY	M105	Q171	R233	T293	GLY	GLY	M105	Q171	R233	T293
GLY	GLY	Y106	C172	S234	P294	GLY	GLY	Y106	C172	S234	P294
GLY	GLY	I107	K173	K235	D295	GLY	GLY	I107	K173	K235	D295
GLY	GLY	E108	M174	P236	E296	GLY	GLY	E108	M174	P236	E296
GLY	GLY	Q109	D175	Y237	V297	GLY	GLY	Q109	D175	Y237	V297
GLY	GLY	R110	F176	E238	K298	GLY	GLY	R110	F176	E238	K298
GLY	GLY	D111	K177	N239	S299	GLY	GLY	D111	K177	N239	S299
GLY	GLY		L178	C240	L300	GLY	GLY		L178	C240	L300
GLY	GLY	Y114	F179	L241	L301	GLY	GLY	Y114	F179	L241	L301
GLY	GLY	N117	M180	L242	L302	GLY	GLY	N117	M180	L242	L302
GLY	GLY	Q118	L181	V243	K303	GLY	GLY	Q118	L181	V243	K303
GLY	GLY	F119	L182	L244	Y304	GLY	GLY	F119	L182	L244	Y304
GLY	GLY	F120	L183	L245	L305	GLY	GLY	F120	L183	L245	L305
GLY	GLY	K184	K184	N246	D306	GLY	GLY	K184	K184	N246	D306
GLY	GLY	A121	N185	V247	C307	GLY	GLY	A121	N185	V247	C307
GLY	GLY	K122	C186	Q248	R308	GLY	GLY	K122	C186	Q248	R308
GLY	GLY	N187	N187	N249	P309	GLY	GLY	N187	N187	N249	P309
GLY	GLY	N124	S188	A250	Q310	GLY	GLY	N124	S188	A250	Q310
GLY	GLY	V125	P189	K251	D311	GLY	GLY	V125	P189	K251	D311
GLY	GLY	S126	E190	A252	L312	GLY	GLY	S126	E190	A252	L312
GLY	GLY	R127	T191	W253	P313	GLY	GLY	R127	T191	W253	P313
GLY	GLY	L128	V192	N254		GLY	GLY	L128	V192	N254	



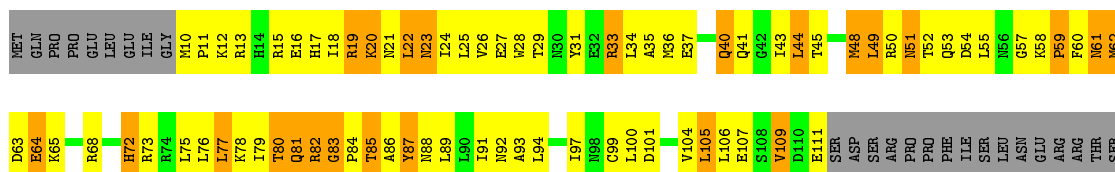
### • Molecule 1: Apaf-1 related killer DARK



### • Molecule 1: Apaf-1 related killer DARK



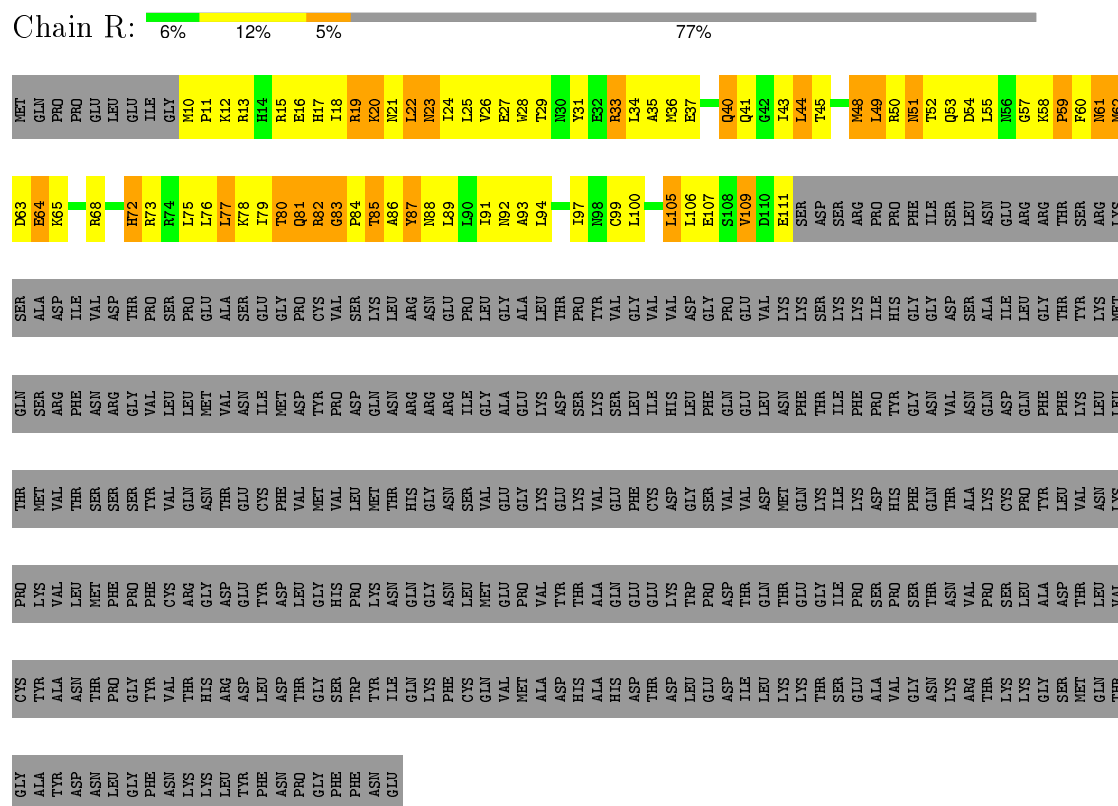




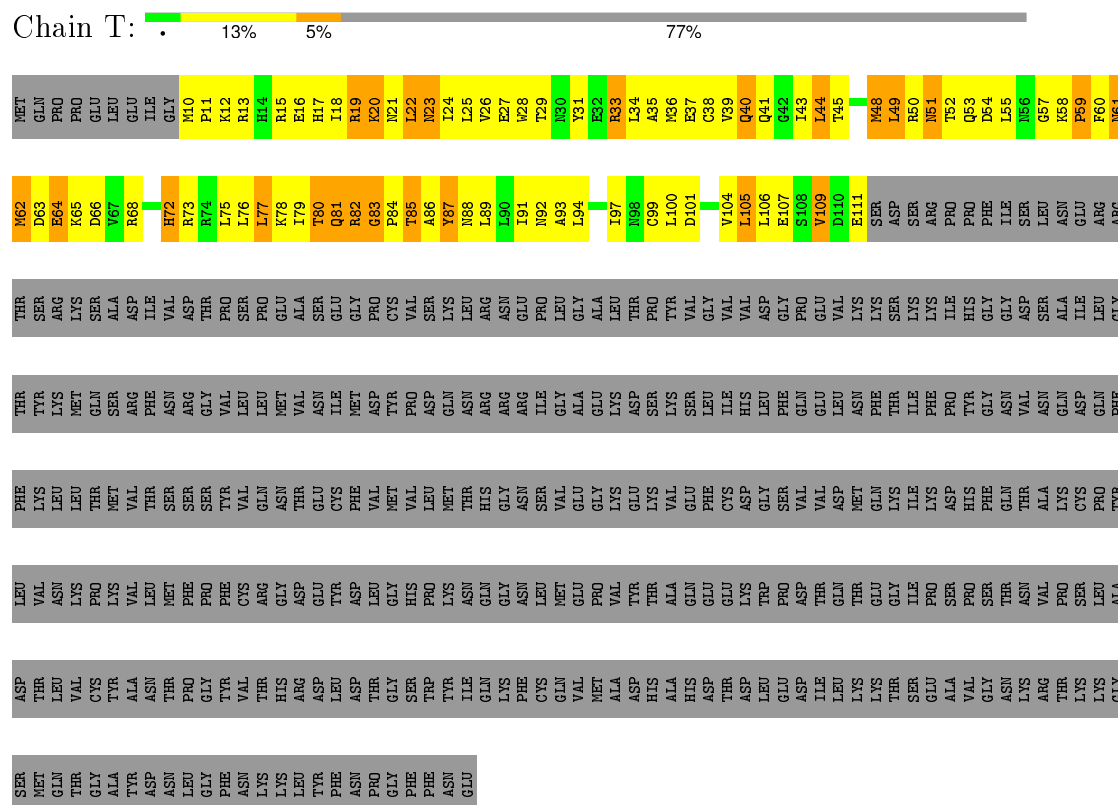






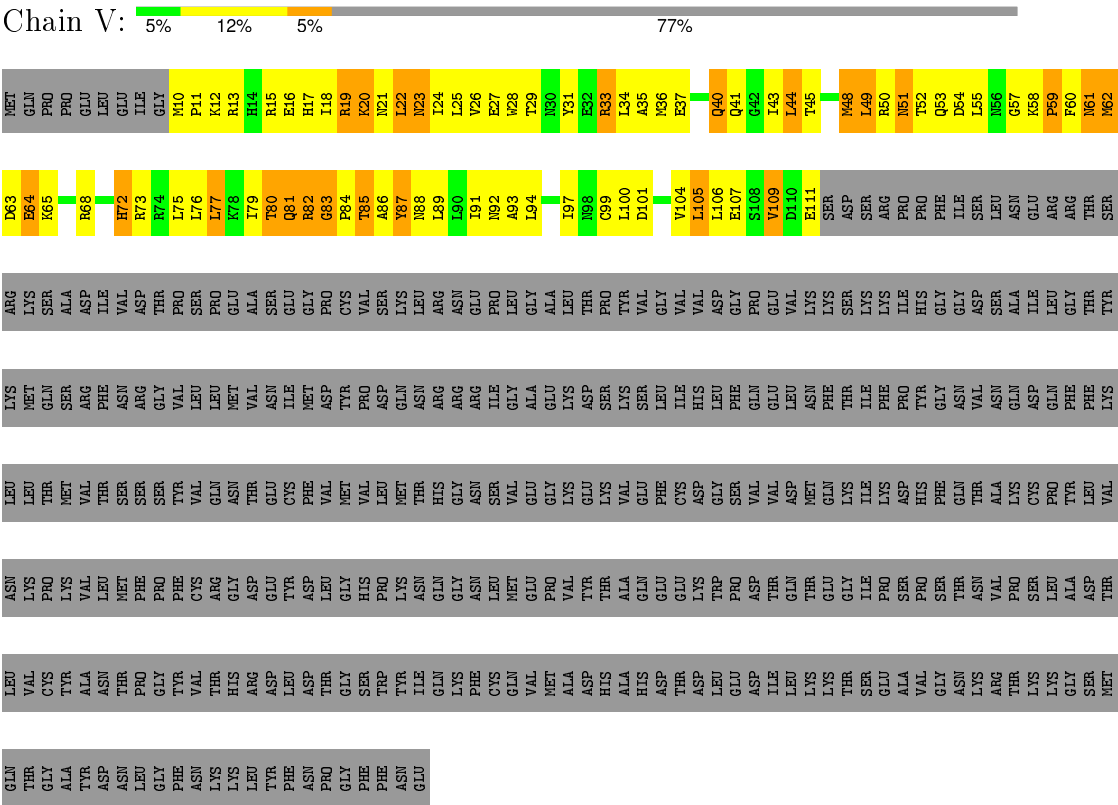


- Molecule 2: Caspase Nc

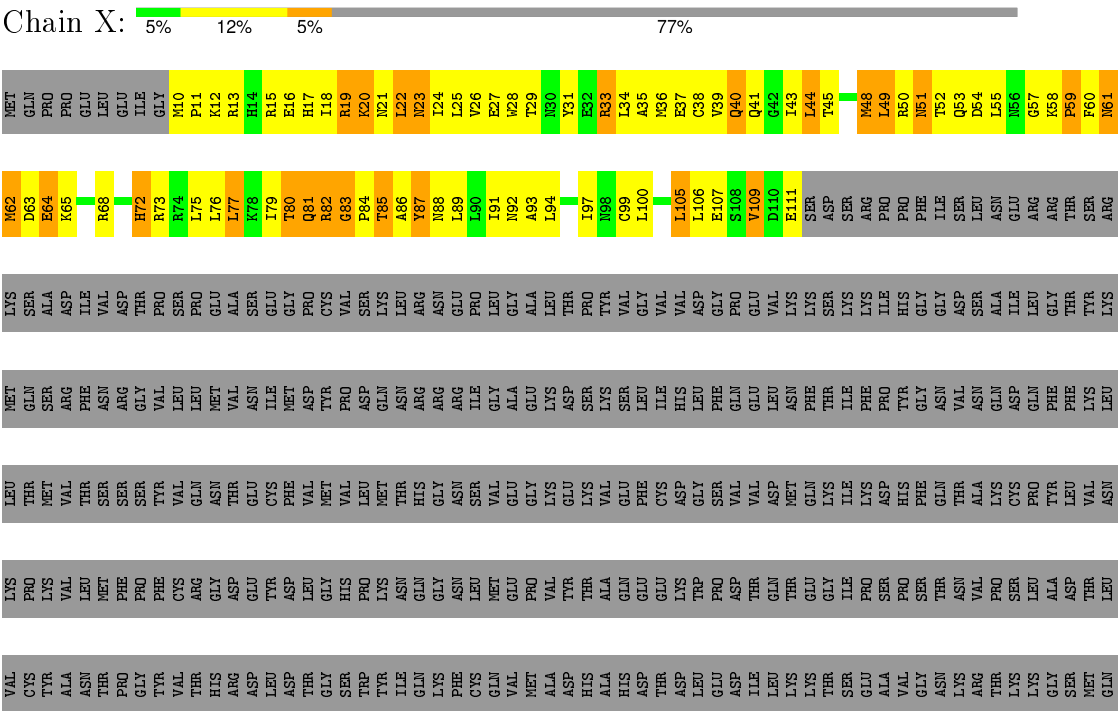




● Molecule 2: Caspase Nc



● Molecule 2: Caspase Nc





ILE	LEU	LYS	LYS	THR	THR	GLU	ALA	VAL	GLY	ASN	LYS	ARG	THR	LYS	LYS	GLY	SER	SER	MET	GLN	THR	GLY	ALA	TYR	ASP	ASN	LEU	GLY	PHE	ASN	LYS	LYS	LEU	LEU	TYR	PHE	ASN	PRO	GLY	PHE	PHE	ASN	GLU
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● Molecule 2: Caspase Nc



MET	GLN	PRO	PRO	GLU	LEU	ILE	GLY	M10	P11	K12	R13	R19	K20	N21	L22	N23	E27	R33	Q40	L44	M48	L49	R50	N51	D54	P59	F60	N61	M62	D63	E64	H72	R73	L77	T80	Q81	R82	G83	P84	T85	A86	Y87	L100	L105
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V109	D110	E111	SER	ASP	SER	ARG	PRO	PRO	PHE	ILE	SER	ASN	GLU	ARG	ARG	THR	SER	ARG	ILE	VAL	ASP	PRO	SER	PRO	GLU	ALA	GLY	PRO	CYS	VAL	SER	LYS	LEU	ARG	ASN	GLU	PRO	ILE	GLY	ALA	LEU	THR	PRO	TYR	VAL	GLY	VAL	ASP	PRO
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GLU	VAL	LYS	LYS	SER	LYS	LYS	ILE	HIS	GLY	GLY	ASP	ALA	ILE	GLY	GLY	THR	LYS	LYS	ARG	ASN	ARG	VAL	LEU	LEU	GLY	ASN	ILE	GLY	ASP	TYR	PRO	GLN	LEU	ASN	ARG	ARG	ASN	GLU	PRO	ILE	GLY	ALA	GLY	LYS	ASP	SER	LYS	THR	ILE	HIS	LEU	PHE	GLY	GLN
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GLU	LEU	ASN	PHE	THR	ILE	PHE	PRO	TYR	GLY	ASN	VAL	GLN	ASP	GLN	GLY	PHE	LYS	LEU	THR	VAL	SER	SER	TYR	VAL	GLN	ASN	THR	PHE	VAL	GLY	LEU	GLY	ASN	GLY	ASN	GLY	ASN	LEU	SER	VAL	GLY	GLY	LYS	ASP	GLY	ASP	GLY	THR	SER	VAL
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VAL	ASP	MET	GLN	LYS	ILE	LYS	ASP	HIS	PHE	ILE	THR	LYS	CYS	PRO	TYR	VAL	ASN	VAL	LEU	MET	PHE	PRO	PHE	CYS	ARG	GLY	ASP	ASP	GLY	GLY	HIS	PRO	LYS	ASN	GLN	GLY	ASN	LEU	MET	GLN	VAL	GLY	VAL	THR	LYS	TRP	PRO	ASP
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THR	GLN	THR	GLY	THR	ILE	PRO	PRO	PRO	SER	ASN	VAL	PRO	SER	LEU	ALA	ASP	THR	VAL	ASN	THR	PRO	TYR	THR	THR	HIS	ANG	ASP	ASP	THR	GLY	SER	TRP	TYR	ILE	ILE	GLN	LYS	PHE	CYS	GLN	VAL	GLY	VAL	ALA	ASP	ASP	THR	ASP	LEU	GLY	ASP
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ILE	LEU	LYS	LYS	THR	SER	GLU	ALA	VAL	ASN	ARG	THR	LYS	LYS	GLY	ALA	TYR	ASN	ASP	ASN	LEU	GLY	PHE	ASN	LYS	LYS	LEU	TYR	PHE	ASN	PRO	GLY	PHE	PHE	ASN	GLU
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● Molecule 2: Caspase Nc



MET	GLN	PRO	PRO	GLU	LEU	ILE	GLY	M10	P11	K12	R13	R19	K20	N21	L22	N23	E27	R33	Q40	L44	M48	L49	R50	N51	D54	P59	F60	N61	M62	D63	E64	H72	R73	L77	T80	Q81	R82	G83	P84	T85	A86	Y87	L100	L105
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V109	D110	E111	SER	ASP	SER	ARG	PRO	PRO	PHE	ILE	SER	ASN	GLU	ARG	ARG	THR	SER	ARG	ILE	VAL	ASP	PRO	CYS	VAL	GLY	PRO	CYS	VAL	SER	VAL	SER	LYS	LEU	ARG	ASN	GLU	PRO	ILE	GLY	ALA	LEU	THR	PRO	TYR	VAL	GLY	VAL	ASP	PRO
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GLU	VAL	LYS	LYS	SER	LYS	LYS	ILE	HIS	GLY	GLY	ASP	ALA	ILE	GLY	GLY	THR	LYS	LYS	MET	GLN	ARG	ASN	VAL	LEU	LEU	GLY	ASN	ASP	ASP	TYR	PRO	GLN	ASN	ARG	ARG	ASN	GLY	ASN	LEU	ILE	GLY	ALA	GLY	LYS	ASP	SER	LYS	THR	ILE	HIS	LEU	PHE	GLN
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GLU	LEU	ASN	PHE	THR	ILE	PHE	PRO	TYR	GLY	ASN	VAL	GLN	ASP	GLN	GLY	PHE	LYS	LEU	THR	VAL	SER	SER	TYR	VAL	GLN	ASN	THR	PHE	VAL	GLY	LEU	GLY	ASN	HIS	GLY	ASN	GLY	ASN	LEU	VAL	GLY	VAL	GLY	LYS	GLU	ASP	GLY	THR	SER	VAL
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VAL	ASP	MET	GLN	LYS	ILE	LYS	ASP	HIS	PHE	GLN	THR	LYS	CYS	PRO	TYR	VAL	ASN	VAL	LEU	MET	PHE	PRO	PHE	CYS	ARG	GLY	ASP	ASP	TYR	GLY	HIS	PRO	LYS	ASN	GLN	GLY	ASN	LEU	MET	GLN	VAL	GLY	VAL	THR	LYS	TRP	PRO	ASP
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THR	GLN	THR	GLY	THR	ILE	PRO	PRO	SER	THR	ASN	VAL	PRO	SER	LEU	ALA	ASP	THR	VAL	ASN	THR	PRO	GLY	TYR	VAL	THR	HIS	ARG	ASP	LEU	THR	GLY	TRP	TYR	ILE	GLN	LYS	PHE	CYS	GLN	VAL	VAL	ALA	ASP	HIS	ASP	HIS	THR	ASP	GLY	LEU	GLY	ASP
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ILE	LEU	LYS	LYS	THR	SER	GLU	ALA	VAL	ASN	ARG	THR	LYS	LYS	GLY	SER	MET	GLN	THR	GLY	TYR	ASN	ASP	ASN	LEU	PHE	ASN	LYS	LYS	LEU	TYR	PHE	ASN	PRO	GLY	PHE	PHE	ASN	GLU
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## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	11359	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	28	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	6400	Depositor
Magnification	78000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 2$	RMSZ	# $ Z  > 2$
1	A	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	C	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	E	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	G	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	I	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	K	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	M	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	O	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	Q	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	S	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	U	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	W	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	Y	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	a	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	c	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	e	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
2	B	0.47	0/850	0.72	1/1146 (0.1%)
2	D	0.47	0/850	0.72	1/1146 (0.1%)
2	F	0.47	0/850	0.72	1/1146 (0.1%)
2	H	0.47	0/850	0.72	1/1146 (0.1%)
2	J	0.47	0/850	0.72	1/1146 (0.1%)
2	L	0.47	0/850	0.72	1/1146 (0.1%)
2	N	0.47	0/850	0.72	1/1146 (0.1%)
2	P	0.47	0/850	0.72	1/1146 (0.1%)
2	R	0.47	0/850	0.72	1/1146 (0.1%)
2	T	0.47	0/850	0.72	1/1146 (0.1%)
2	V	0.47	0/850	0.72	1/1146 (0.1%)
2	X	0.47	0/850	0.72	1/1146 (0.1%)
2	Z	0.47	0/850	0.72	1/1146 (0.1%)
2	b	0.47	0/850	0.72	1/1146 (0.1%)
2	d	0.47	0/850	0.72	1/1146 (0.1%)
2	f	0.47	0/850	0.72	1/1146 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
All	All	0.63	80/86592 (0.1%)	0.93	352/117008 (0.3%)

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	7
1	C	0	7
1	E	0	7
1	G	0	7
1	I	0	7
1	K	0	7
1	M	0	7
1	O	0	7
1	Q	0	7
1	S	0	7
1	U	0	7
1	W	0	7
1	Y	0	7
1	a	0	7
1	c	0	7
1	e	0	7
All	All	0	112

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	PRO	N-CD	5.32	1.55	1.47
1	E	189	PRO	N-CD	5.32	1.55	1.47
1	I	189	PRO	N-CD	5.32	1.55	1.47
1	M	189	PRO	N-CD	5.32	1.55	1.47
1	Q	189	PRO	N-CD	5.32	1.55	1.47

The worst 5 of 352 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	CYS	CA-CB-SG	-9.44	97.02	114.00
1	E	240	CYS	CA-CB-SG	-9.44	97.02	114.00
1	I	240	CYS	CA-CB-SG	-9.44	97.02	114.00
1	M	240	CYS	CA-CB-SG	-9.44	97.02	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	240	CYS	CA-CB-SG	-9.44	97.02	114.00

There are no chirality outliers.

5 of 112 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	278	ALA	Peptide
1	A	346	CYS	Mainchain
1	A	410	LEU	Peptide
1	A	50	MET	Peptide
1	A	66	LEU	Mainchain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7040	0	5126	1313	0
1	C	7040	0	5126	1322	0
1	E	7040	0	5126	1321	0
1	G	7040	0	5126	1249	0
1	I	7040	0	5126	1264	0
1	K	7040	0	5126	1264	0
1	M	7040	0	5126	1264	0
1	O	7040	0	5126	1249	0
1	Q	7040	0	5126	1249	0
1	S	7040	0	5126	1250	0
1	U	7040	0	5126	1258	0
1	W	7040	0	5126	1267	0
1	Y	7040	0	5126	1247	0
1	a	7040	0	5126	0	0
1	c	7040	0	5126	0	0
1	e	7040	0	5126	0	0
2	B	840	0	863	139	0
2	D	840	0	863	137	0
2	F	840	0	863	137	0
2	H	840	0	863	128	0
2	J	840	0	863	127	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	840	0	863	124	0
2	N	840	0	863	125	0
2	P	840	0	863	129	0
2	R	840	0	863	126	0
2	T	840	0	863	128	0
2	V	840	0	863	128	0
2	X	840	0	863	125	0
2	Z	840	0	863	126	0
2	b	840	0	863	0	0
2	d	840	0	863	0	0
2	f	840	0	863	0	0
3	A	27	0	12	4	0
3	C	27	0	12	6	0
3	E	27	0	12	6	0
3	G	27	0	12	4	0
3	I	27	0	12	4	0
3	K	27	0	12	4	0
3	M	27	0	12	4	0
3	O	27	0	12	4	0
3	Q	27	0	12	4	0
3	S	27	0	12	4	0
3	U	27	0	12	4	0
3	W	27	0	12	4	0
3	Y	27	0	12	4	0
3	a	27	0	12	0	0
3	c	27	0	12	0	0
3	e	27	0	12	0	0
All	All	126512	0	96016	17758	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 80.

The worst 5 of 17758 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:410:LEU:HB3	1:U:426:TYR:CE1	1.29	1.68
1:E:410:LEU:HB3	1:E:426:TYR:CE1	1.29	1.67
1:C:410:LEU:HB3	1:C:426:TYR:CE1	1.29	1.67
1:W:410:LEU:HB3	1:W:426:TYR:CE1	1.29	1.66
1:W:183:LEU:HD22	1:W:186:CYS:SG	1.35	1.66



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	A	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	21	67
1	C	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	21	67
1	E	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	21	67
1	G	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	21	67
1	I	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	21	67
1	K	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	21	67
1	M	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	21	67
1	O	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	21	67
1	Q	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	21	67
1	S	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	21	67
1	U	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	21	67
1	W	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	21	67
1	Y	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	21	67
1	a	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	21	67
1	c	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	21	67
1	e	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	21	67
2	B	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	19	65
2	D	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	19	65
2	F	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	19	65
2	H	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	19	65
2	J	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	19	65
2	L	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	19	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	19	65
2	P	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	19	65
2	R	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	19	65
2	T	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	19	65
2	V	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	19	65
2	X	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	19	65
2	Z	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	19	65
2	b	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	19	65
2	d	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	19	65
2	f	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	19	65
All	All	10096/24832 (41%)	8704 (86%)	1296 (13%)	96 (1%)	24	65

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	VAL
1	A	346	CYS
1	C	316	VAL
1	C	346	CYS
1	E	316	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	501/551 (91%)	361 (72%)	140 (28%)	0	4
1	C	501/551 (91%)	361 (72%)	140 (28%)	0	4
1	E	501/551 (91%)	361 (72%)	140 (28%)	0	4
1	G	501/551 (91%)	361 (72%)	140 (28%)	0	4
1	I	501/551 (91%)	361 (72%)	140 (28%)	0	4
1	K	501/551 (91%)	361 (72%)	140 (28%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	501/551 (91%)	361 (72%)	140 (28%)	0	4
1	O	501/551 (91%)	361 (72%)	140 (28%)	0	4
1	Q	501/551 (91%)	361 (72%)	140 (28%)	0	4
1	S	501/551 (91%)	361 (72%)	140 (28%)	0	4
1	U	501/551 (91%)	361 (72%)	140 (28%)	0	4
1	W	501/551 (91%)	361 (72%)	140 (28%)	0	4
1	Y	501/551 (91%)	361 (72%)	140 (28%)	0	4
1	a	501/551 (91%)	361 (72%)	140 (28%)	0	4
1	c	501/551 (91%)	361 (72%)	140 (28%)	0	4
1	e	501/551 (91%)	361 (72%)	140 (28%)	0	4
2	B	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	D	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	F	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	H	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	J	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	L	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	N	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	P	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	R	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	T	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	V	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	X	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	Z	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	b	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	d	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	f	94/404 (23%)	63 (67%)	31 (33%)	0	2
All	All	9520/15280 (62%)	6784 (71%)	2736 (29%)	2	4

5 of 2736 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	162	LEU
2	R	81	GLN

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Mol	Chain	Res	Type
1	c	539	VAL
1	O	242	LEU
1	Q	78	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 331 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	257	ASN
1	S	96	GLN
1	c	520	GLN
1	O	403	ASN
1	Q	216	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ADP	A	2000	-	24,29,29	0.93	1 (4%)	23,45,45	1.66	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ADP	C	2000	-	24,29,29	0.93	1 (4%)	23,45,45	1.65	3 (13%)
3	ADP	E	2000	-	24,29,29	0.93	1 (4%)	23,45,45	1.64	3 (13%)
3	ADP	G	2000	-	24,29,29	0.93	1 (4%)	23,45,45	1.65	3 (13%)
3	ADP	I	2000	-	24,29,29	0.93	1 (4%)	23,45,45	1.64	3 (13%)
3	ADP	K	2000	-	24,29,29	0.93	1 (4%)	23,45,45	1.65	3 (13%)
3	ADP	M	2000	-	24,29,29	0.93	1 (4%)	23,45,45	1.64	3 (13%)
3	ADP	O	2000	-	24,29,29	0.93	1 (4%)	23,45,45	1.65	3 (13%)
3	ADP	Q	2000	-	24,29,29	0.93	1 (4%)	23,45,45	1.64	3 (13%)
3	ADP	S	2000	-	24,29,29	0.93	1 (4%)	23,45,45	1.66	3 (13%)
3	ADP	U	2000	-	24,29,29	0.93	1 (4%)	23,45,45	1.66	3 (13%)
3	ADP	W	2000	-	24,29,29	0.93	1 (4%)	23,45,45	1.66	3 (13%)
3	ADP	Y	2000	-	24,29,29	0.93	1 (4%)	23,45,45	1.66	3 (13%)
3	ADP	a	2000	-	24,29,29	0.93	1 (4%)	23,45,45	1.66	3 (13%)
3	ADP	c	2000	-	24,29,29	0.93	1 (4%)	23,45,45	1.66	3 (13%)
3	ADP	e	2000	-	24,29,29	0.93	1 (4%)	23,45,45	1.66	3 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	2000	-	-	0/12/32/32	0/3/3/3
3	ADP	C	2000	-	-	0/12/32/32	0/3/3/3
3	ADP	E	2000	-	-	0/12/32/32	0/3/3/3
3	ADP	G	2000	-	-	0/12/32/32	0/3/3/3
3	ADP	I	2000	-	-	0/12/32/32	0/3/3/3
3	ADP	K	2000	-	-	0/12/32/32	0/3/3/3
3	ADP	M	2000	-	-	0/12/32/32	0/3/3/3
3	ADP	O	2000	-	-	0/12/32/32	0/3/3/3
3	ADP	Q	2000	-	-	0/12/32/32	0/3/3/3
3	ADP	S	2000	-	-	0/12/32/32	0/3/3/3
3	ADP	U	2000	-	-	0/12/32/32	0/3/3/3
3	ADP	W	2000	-	-	0/12/32/32	0/3/3/3
3	ADP	Y	2000	-	-	0/12/32/32	0/3/3/3
3	ADP	a	2000	-	-	0/12/32/32	0/3/3/3
3	ADP	c	2000	-	-	0/12/32/32	0/3/3/3
3	ADP	e	2000	-	-	0/12/32/32	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2000	ADP	C5-C4	2.97	1.47	1.40
3	A	2000	ADP	C5-C4	2.97	1.47	1.40
3	M	2000	ADP	C5-C4	2.97	1.47	1.40
3	c	2000	ADP	C5-C4	2.97	1.47	1.40
3	I	2000	ADP	C5-C4	2.97	1.47	1.40

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2000	ADP	N3-C2-N1	-5.62	124.46	128.87
3	O	2000	ADP	N3-C2-N1	-5.62	124.46	128.87
3	K	2000	ADP	N3-C2-N1	-5.62	124.46	128.87
3	W	2000	ADP	N3-C2-N1	-5.62	124.46	128.87
3	S	2000	ADP	N3-C2-N1	-5.62	124.46	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2000	ADP	4	0
3	C	2000	ADP	6	0
3	E	2000	ADP	6	0
3	G	2000	ADP	4	0
3	I	2000	ADP	4	0
3	K	2000	ADP	4	0
3	M	2000	ADP	4	0
3	O	2000	ADP	4	0
3	Q	2000	ADP	4	0
3	S	2000	ADP	4	0
3	U	2000	ADP	4	0
3	W	2000	ADP	4	0
3	Y	2000	ADP	4	0

## 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.