



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 15, 2017 – 08:41 PM EST

PDB ID : 5JUL
EMDB ID: : EMD-8177
Title : Near atomic structure of the Dark apoptosome
Authors : Cheng, T.C.; Akey, I.V.; Yuan, S.; Yu, Z.; Ludtke, S.J.; Akey, C.W.
Deposited on : 2016-05-10
Resolution : 4.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
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) : rb-20028442

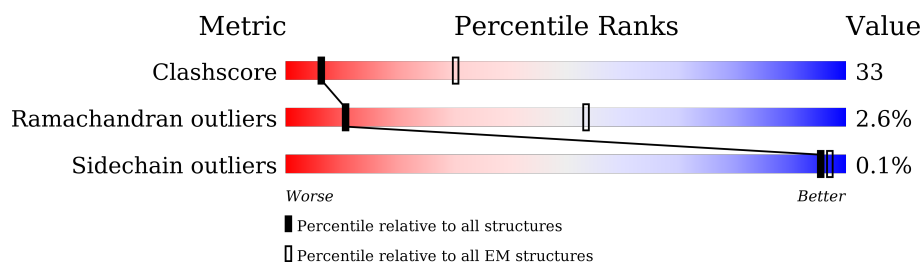
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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.




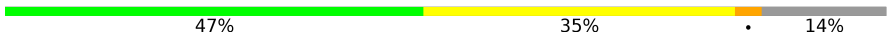
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 ≥ 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	1440	48% 35% 14%
1	B	1440	47% 36% 14%
1	C	1440	47% 36% 14%
1	D	1440	46% 36% 14%
1	E	1440	48% 35% 14%
1	F	1440	47% 36% 14%
1	G	1440	47% 35% 14%
1	H	1440	47% 35% 14%
1	I	1440	47% 36% 14%

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Mol	Chain	Length	Quality of chain
1	J	1440	
1	K	1440	
1	L	1440	
1	M	1440	
1	N	1440	
1	O	1440	
1	P	1440	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 161200 atoms, of which 0 are hydrogens and 0 are deuteriums.

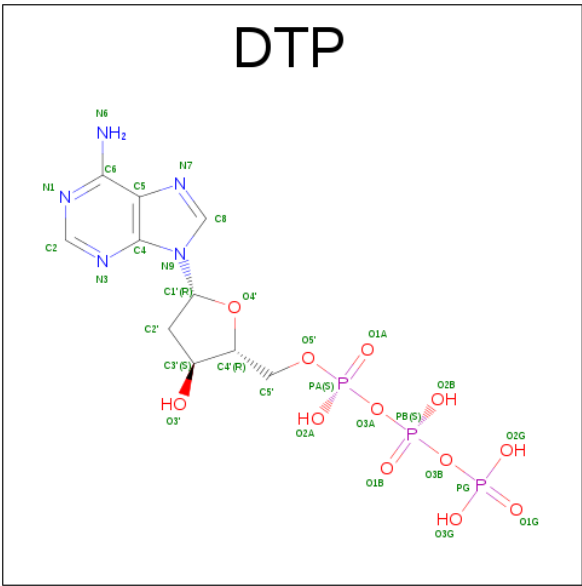
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Apaf-1 related killer DARK.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1233	Total	C	N	O	P	S	0	0
			10045	6434	1698	1860	1	52		
1	B	1233	Total	C	N	O	P	S	0	0
			10045	6434	1698	1860	1	52		
1	C	1233	Total	C	N	O	P	S	0	0
			10045	6434	1698	1860	1	52		
1	D	1233	Total	C	N	O	P	S	0	0
			10045	6434	1698	1860	1	52		
1	E	1233	Total	C	N	O	P	S	0	0
			10045	6434	1698	1860	1	52		
1	F	1233	Total	C	N	O	P	S	0	0
			10045	6434	1698	1860	1	52		
1	G	1233	Total	C	N	O	P	S	0	0
			10045	6434	1698	1860	1	52		
1	H	1233	Total	C	N	O	P	S	0	0
			10045	6434	1698	1860	1	52		
1	I	1233	Total	C	N	O	P	S	0	0
			10045	6434	1698	1860	1	52		
1	J	1233	Total	C	N	O	P	S	0	0
			10045	6434	1698	1860	1	52		
1	K	1233	Total	C	N	O	P	S	0	0
			10045	6434	1698	1860	1	52		
1	L	1233	Total	C	N	O	P	S	0	0
			10045	6434	1698	1860	1	52		
1	M	1233	Total	C	N	O	P	S	0	0
			10045	6434	1698	1860	1	52		
1	N	1233	Total	C	N	O	P	S	0	0
			10045	6434	1698	1860	1	52		
1	O	1233	Total	C	N	O	P	S	0	0
			10045	6434	1698	1860	1	52		
1	P	1233	Total	C	N	O	P	S	0	0
			10045	6434	1698	1860	1	52		

- Molecule 2 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (for-

mula: C₁₀H₁₆N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	B	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	C	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	D	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	E	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	F	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	G	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	H	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	I	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	J	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	K	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	L	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	M	1	Total	C	N	O	P	0
			30	10	5	12	3	

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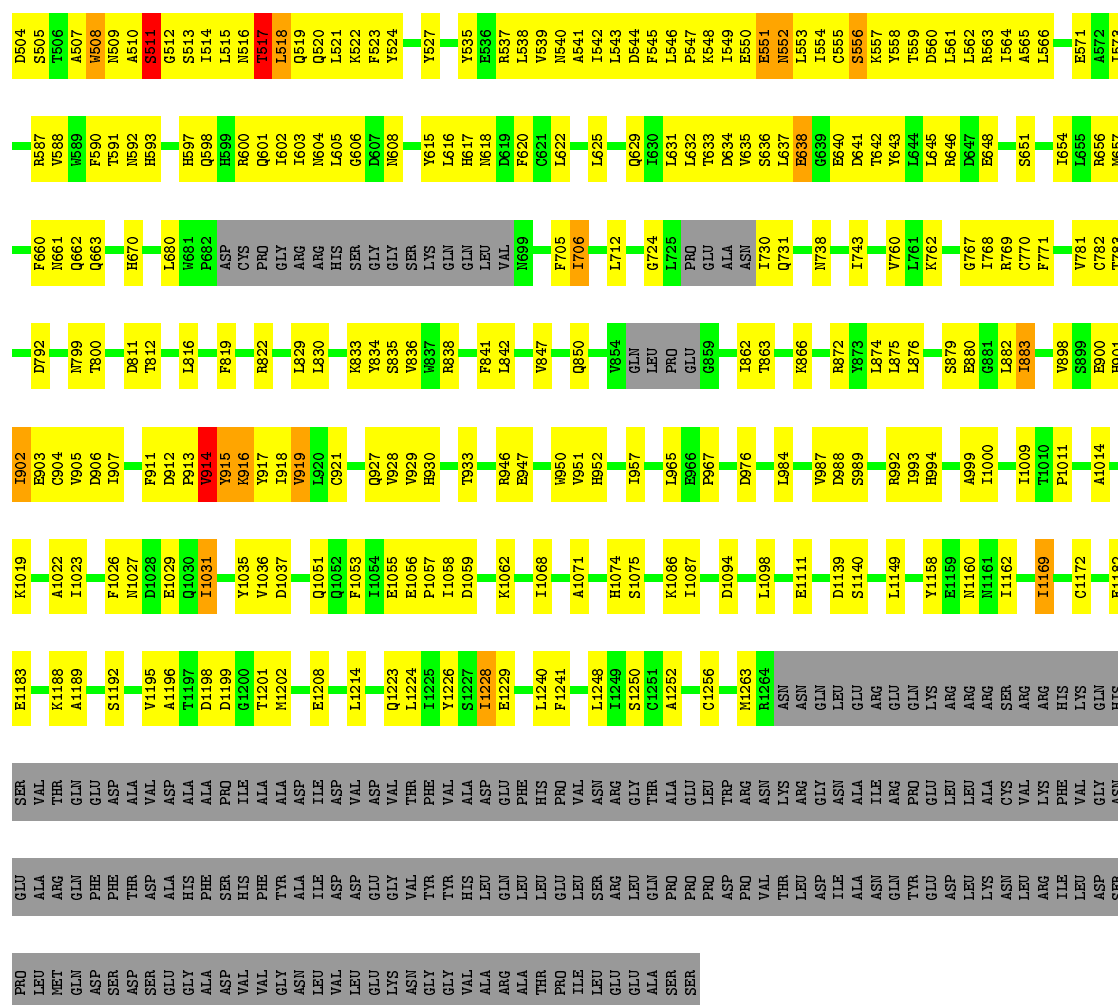
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Mol	Chain	Residues	Atoms					AltConf
2	N	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	O	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	P	1	Total	C	N	O	P	0
			30	10	5	12	3	

- Molecule 1: Apaf-1 related killer DARK

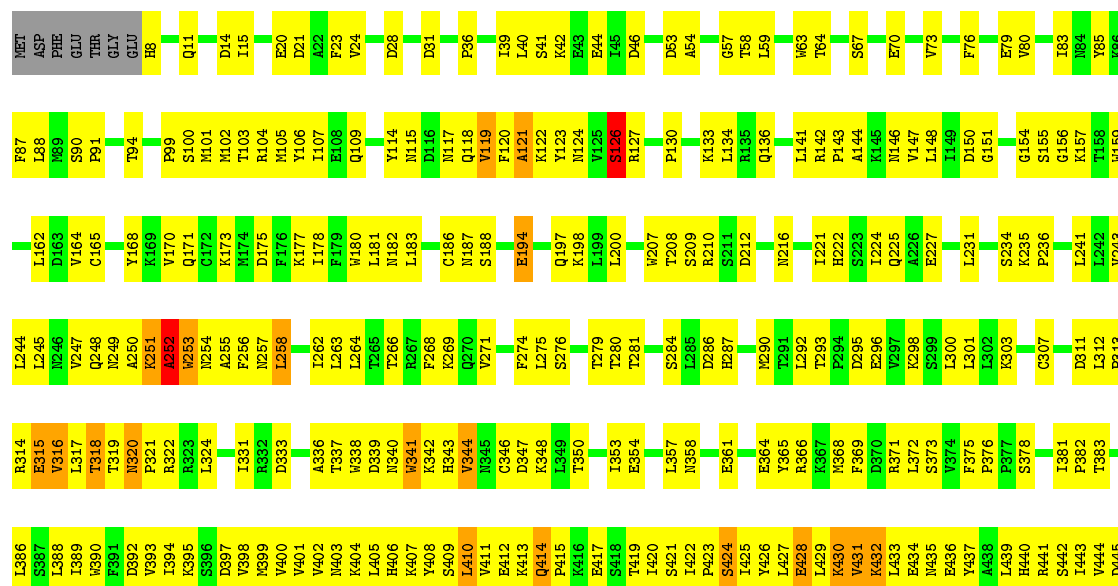






- Molecule 1: Apaf-1 related killer DARK

Chain G:  47% 35% 0% 14%

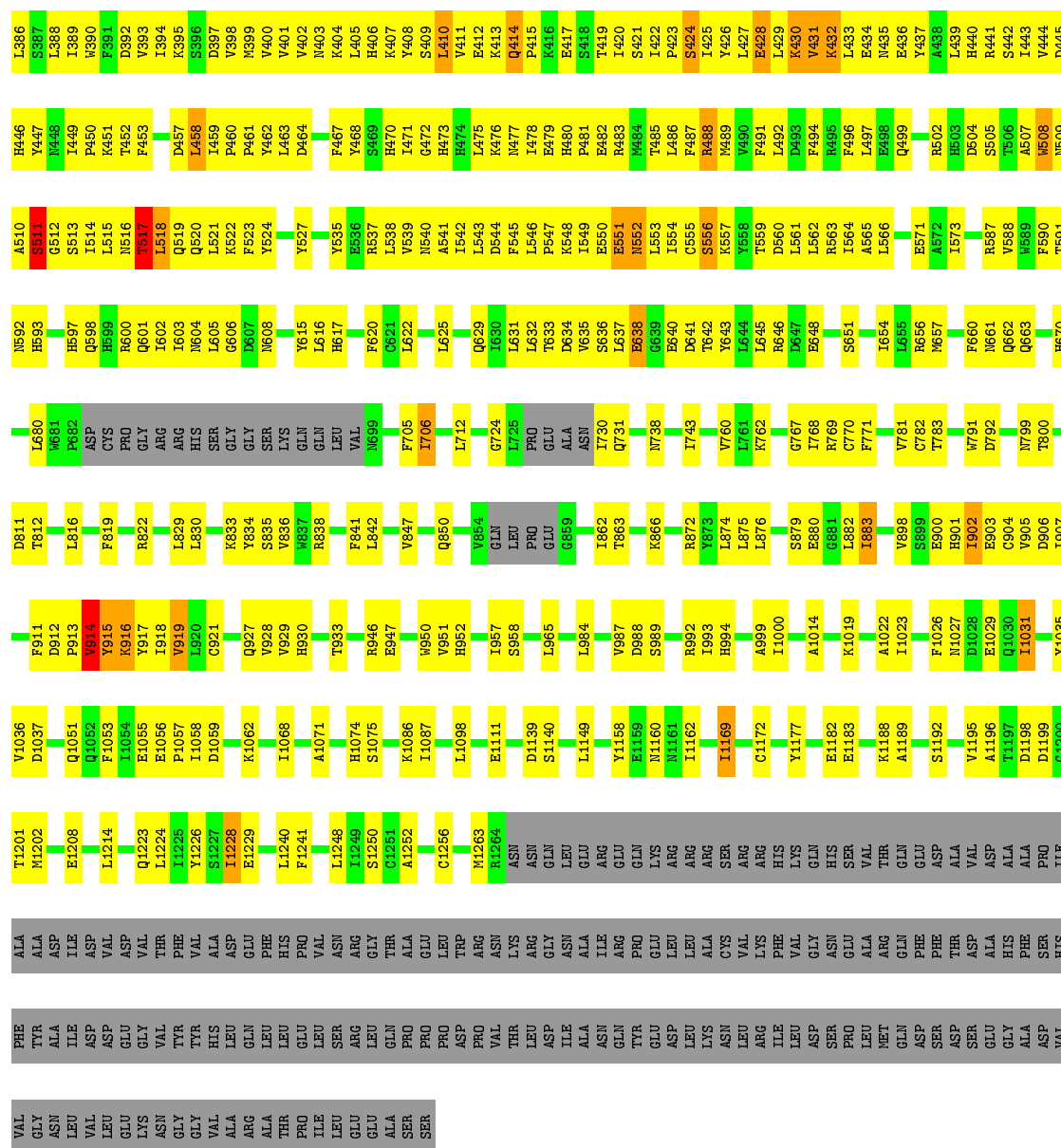


H446	A510	Q663	C904	D1028	A1196	ALA	PHE	ALA	PHE	ALA
Y447	S511	H799	V905	E1029	T1201	PRO	SER	ASP	SER	ASP
Y448	G512	T800	V906	Q1030	M1202	ILE	HIS	VAL	HIS	VAL
I449	S513	H592	I907	I1031		ALA	THR	ALA	THR	ALA
P450	I514	H593				GLY	TTR	ASP	TTR	GLY
K451	I515	H597	F911	Y1035	E1208	ILE	ILE	ILE	ILE	LEU
T452	N516	H598	D912	V1036	L1214	ASP	ASP	VAL	ASP	VAL
F453	T517	H599	F913	D1037		VAL	ASP	VAL	ASP	VAL
	L518	CYS	Y914	Q1051	Q1223	ASP	ASP	ASP	ASP	ASP
D457	Q519	PRO	Y915	Q1052	L1224	GLY	GLY	GLY	GLY	GLY
L458	Q520	GLY	X916	F1053	I1225	VAL	VAL	VAL	VAL	VAL
I459	L521	ARG	Y917	F1054	I1226	THR	THR	THR	THR	THR
P460	K522	ARG	I918	I1054	S1227	VAL	TTR	VAL	TTR	VAL
P461	F523	HIS	Y919	E1055	I1228	ALA	HIS	ALA	HIS	ALA
Y462	Y524	SER	C921	E1056	O1057	ASP	LEU	ASP	LEU	ASP
L463		GLY		P1057	I1058	GLY	GLN	GLY	GLN	GLY
D464	Y527	GLY	Q927	D1059	L1240	PHE	LEU	PHE	LEU	PHE
		SER	V928		F1241	HIS	LEU	HIS	LEU	HIS
F467	Y535	LYS	V929	K1062	L1247	PRO	GLY	PRO	GLY	PRO
Y468	S536	GLN	H930	I1068	I1249	VAL	LEU	VAL	LEU	VAL
S469	R537	LEU	V931	I1069	I1250	ASN	SER	ASN	SER	ASN
H470	L538	VAL	H932		C1251	ARG	THR	ARG	THR	ARG
I471	V539	VAL	T933	A1071	A1252	ALA	ALA	ALA	ALA	ALA
G472	N540	N699	R946	H1074		GLY	GLY	GLY	GLY	GLY
H473	A541	F705	E947	S1075	C1256	ALA	PRO	ALA	PRO	ALA
H474	I542	I706		I1086		GLY	PRO	GLY	PRO	GLY
L475	L543	L712	N950	K1086	M1263	LEU	ASP	LEU	ASP	LEU
L476	D544	L717	V951	I1087	I1264	ASN	VAL	ASN	VAL	ASN
K477	F545	Q629	H952	D1094	ASN	LYS	THR	LYS	THR	LYS
I478	L546	L630			ASN	ARG	LEU	ARG	LEU	ARG
P479	P547	L631	T957	L1098	GLY	GLY	ASP	GLY	ASP	GLY
H480	K548	L632	L965	L1099	LEU	ILE	ILE	ILE	ILE	ILE
P481	E549	L633	H965	E1111	GLY	ALA	ALA	ALA	ALA	ALA
E482	E550	L634	R984	E1112	ARG	ILE	ASN	ILE	ASN	ILE
R483	N552	GLU		L1149	GLY	ARG	GLN	ARG	GLN	ARG
H485	L553	ALA	V987	L1159	LYS	PRO	TTR	PRO	TTR	PRO
L486	I554	ASN	D988	E1160	GLY	GLY	ASP	GLY	ASP	GLY
F487	C555	I730	S989	N1161	ARG	LEU	ASP	LEU	ASP	LEU
R488	S556	Q731		N1162	ARG	VAL	VAL	VAL	VAL	VAL
K489	K557	N738	R992	I1169	GLY	PHE	PHE	PHE	PHE	PHE
Y490	Y558	T642	I993	G1172	LYS	GLY	GLY	GLY	GLY	GLY
F491	T559	T643	H994		ASN	ASN	ASN	ASN	ASN	ASN
L492	D560	Y643	L995	Y1177	VAL	GLY	PRO	GLY	PRO	GLY
D493	L561	L644	I996	E1182	VAL	ALA	LEU	VAL	LEU	VAL
F494	R563	R645		E1183	THR	THR	THR	THR	THR	THR
F495	I564	R646		K1188	GLN	GLN	GLN	GLN	GLN	GLN
F496	I564	R647		A1189	GLY	ASP	ASP	ASP	ASP	ASP
L497	A565	E648		S1192	ALA	ALA	THR	ALA	THR	ALA
F498	L566			V1195	VAL	ASP	ASP	VAL	ASP	VAL
Q499		S651	A1014		ALA	HIS	HIS	ALA	HIS	ALA
	E571		K1019	E1182	VAL	GLY	GLY	VAL	GLY	VAL
R502	A572	R769	I1020	E1183	THR	THR	THR	THR	THR	THR
H503	I573	C770	N1021	K1188	GLN	GLN	GLN	GLN	GLN	GLN
D504	I573	F771	H998	A1189	GLY	ASP	ASP	ASP	ASP	ASP
S505	F584	R656	I1022	S899	ASP	PHE	PHE	PHE	PHE	PHE
T506	D585	R657	I1023	E900	ALA	ALA	THR	ALA	THR	ALA
A507	D586	F660	F1026	R901	VAL	ASP	ASP	VAL	ASP	VAL
R508	R587	N661	N1027	I902	ASP	ALA	ALA	ASP	ALA	ASP
Y509	V588	Q662		E903		HIS	HIS		HIS	

• Molecule 1: Apaf-1 related killer DARK

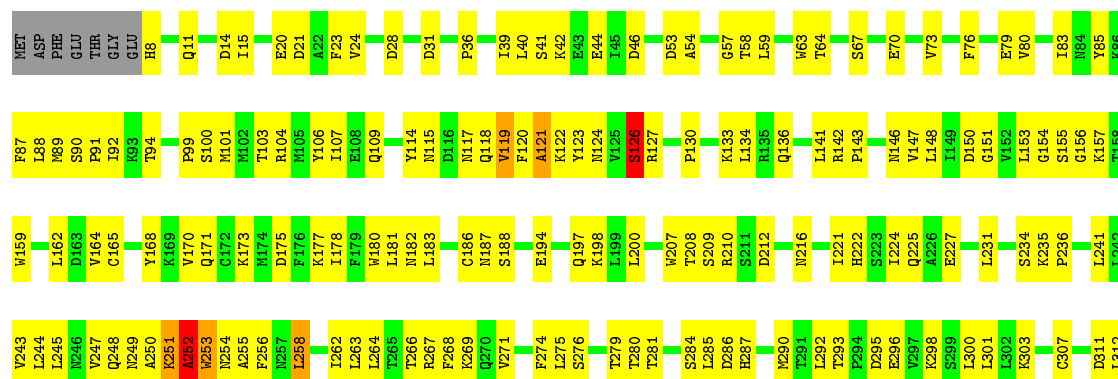
Chain H:  47% 35% 14%

Y247	R314	K86	T158	V247	R314	K86	T158	V247	R314	K86
Q248	E315	F87	W159	Q248	E315	F87	W159	Q248	E315	F87
N249	V316	L88	L162	N249	V316	L88	L162	N249	V316	L88
A250	L317	M89	D163	A250	L317	M89	D163	A250	L317	M89
K251	T318	S90	D164	K251	T318	S90	D164	K251	T318	S90
A252	T319	P91	V164	A252	T319	P91	V164	A252	T319	P91
K253	N320	I92	C165	K253	N320	I92	C165	K253	N320	I92
N254	P321	R93		N254	P321	R93		N254	P321	R93
A255	R322	T94	Y168	A255	R322	T94	Y168	A255	R322	T94
F256	L323	P99	K169	F256	L323	P99	K169	F256	L323	P99
L258	L324	S100	Y170	L258	L324	S100	Y170	L258	L324	S100
		Q101	Q171			Q101	Q171			Q101
I262	I331	M102	K172	I262	I331	M102	K172	I262	I331	M102
L263	R332	T103	M174	L263	R332	T103	M174	L263	R332	T103
L264	D333	R104	F175	L264	D333	R104	F175	L264	D333	R104
T265		M105	F176	T265		M105	F176	T265		M105
T266	A336	Y106	K177	T266	A336	Y106	K177	T266	A336	Y106
R267	T337	I107	L178	R267	T337	I107	L178	R267	T337	I107
F268	K338	E108	F179	F268	K338	E108	F179	F268	K338	E108
K269	D339	Q109		K269	D339	Q109		K269	D339	Q109
Q270	N340	L113	W180	Q270	N340	L113	W180	Q270	N340	L113
V271	K341	N182	N182	V271	K341	N182	N182	V271	K341	N182
	H342	L183			H342	L183			H342	L183
V344	R343	Y114		V344	R343	Y114		V344	R343	Y114
N345	V344	N115		N345	V344	N115		N345	V344	N115
C346	N345	D116	C186	C346	N345	D116	C186	C346	N345	D116
D347	N347	N117	N187	D347	N347	N117	N187	D347	N347	N117
K348	C347	Q118	S188	K348	C347	Q118	S188	K348	C347	Q118
L349	K348	V119	L40	L349	K348	V119	L40	L349	K348	V119
T350	T350	F120	E194	T350	T350	F120	E194	T350	T350	F120
		K42	K42			K42	K42			K42
H282	H282	K122	Q197	H282	H282	K122	Q197	H282	H282	K122
L283	L283	Y123	K198	L283	L283	Y123	K198	L283	L283	Y123
S284	S284	M124	E44	S284	S284	M124	E44	S284	S284	M124
D286	D286	V125	T45	D286	D286	V125	T45	D286	D286	V125
H287	H287	S126	D46	H287	H287	S126	D46	H287	H287	S126
		R127	D53			R127	D53			R127
		A54	A54			A54	A54			A54
		G57	G57			G57	G57			G57
		T58	T58			T58	T58			T58
		L59	L59			L59	L59			L59
		K63	K63			K63	K63			K63
		T64	T64			T64	T64			T64
		S67	S67			S67	S67			S67
		E70	E70			E70	E70			E70
		V73	V73			V73	V73			V73
		F76	F76			F76	F76			F76
		D150	D150			D150	D150			D150
		G151	G151			G151	G151			G151
		V80	V80			V80	V80			V80
		L241	L241			L241	L241			L241
		V243	V243			V243	V243			V243
		L244	L244			L244	L244			L244
		K157	K157			K157	K157			K157



• Molecule 1: Apaf-1 related killer DARK

Chain I: 47% 36% 14%

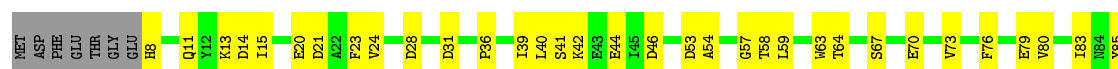


P313	L386	D445	N509	T591	H670	D611	P911	D1028	S1192	ASP	ALA	ALA	GLU
R314	L387	H446	A510	H592	H671	T512	D912	E1029	V1195	ALA	PHE	HIS	GLY
E315	S387	Y447	S511	H593	L660	T513	P913	Q1030	A1196	PRQ	ASP	ASP	ASP
V316	L388	N448	S512	H597	W681	L316	P914	I1031	A1197	ALA	ALA	ALA	ALA
L317	L389	P450	S513	Q598	W682	L317	T915	Y1035	T1201	ALA	PHE	VAL	VAL
W390	W390	P451	I514	Q599	W683	L318	R916	Y1036	M1202	ALA	THR	THR	GLY
T319	P391	K451	L515	H600	ASP	P819	Y917	D1037	M1203	ALA	ALA	ALA	ASN
N320	D392	F452	T517	H601	CYS	L229	V919	Q1051	E1208	ASP	ALA	ALA	ASN
P321	V393	F453	Q519	Q601	PRQ	L230	V920	Q1052	E1209	ASP	ALA	ALA	LEU
R322	K394	L395	Q520	L602	GLY	L231	V921	F1053	L1214	ASP	VAL	ASP	VAL
L324	S396	D458	Q521	L603	ARG	K333	C921	F1054	L1215	ASP	VAL	ASP	VAL
L331	D397	L458	Q522	L604	HIS	W834	Q927	E1055	Q1223	ASP	VAL	GLY	LYS
R332	V398	L459	K522	L605	SER	S835	V928	E1056	L1224	THR	THR	ASN	ASN
D333	M399	P461	F523	G606	GLY	W836	V929	P1057	I1225	PHE	THR	GLY	GLY
L336	Y400	Y462	Y524	N608	GLY	W837	H930	I1058	Y1226	VAL	VAL	VAL	VAL
L337	V401	L463	Y527	L622	SER	R838	T933	D1059	S1227	ALA	ALA	ALA	VAL
A336	V402	D464	L463	L623	LYS	P841	V934	D1060	E1228	ASP	ALA	ALA	ARG
T337	N403	F467	Y535	L616	GLN	L242	R946	K1062	E1229	GLY	GLY	GLY	ALA
N338	K404	Y468	E536	H617	GLN	L243	R947	K1063	L1240	PHE	THR	LEU	ALA
D339	L405	F469	R537	H618	LEU	V847	E947	I1068	F1241	HIS	THR	LEU	THR
N340	H406	H470	L538	D619	VAL	V848	N950	K1069	L1242	PRQ	PRQ	GLY	PRQ
W341	K407	H471	W539	F620	N699	V849	V951	A1071	L1243	VAL	VAL	LEU	PRQ
K342	Y408	L471	W540	G621	F705	Q850	H952	H1074	L1244	ARG	ARG	LEU	PRQ
K343	S409	G472	A541	L622	I706	W854	H953	S1075	S1250	GLY	GLY	GLY	GLY
T344	L410	H473	I542	L623	L712	L625	V957	S1076	C1256	THR	THR	ALA	SER
N345	V411	H474	L543	L624	LEU	GLU	R958	K1086	Q1257	ASP	ASP	ALA	SER
C346	E412	K476	D544	L625	L713	GLU	V959	I1087	G1258	TRP	TRP	ALA	SER
D347	K413	N477	F545	L626	G724	GLU	L965	K1088	C1259	ARG	ARG	ALA	ASP
K348	Q414	L478	F546	L627	I725	GLU	R966	K1089	G1260	ASN	ASN	ALA	PRQ
L349	P415	E479	P547	L628	P706	GLU	P967	D1094	M1263	LEU	LEU	ALA	PRQ
T350	E417	H480	K548	L629	I726	GLU	D976	L1098	R1264	ASN	ASN	ALA	PRQ
L353	S418	H481	I549	L630	ALA	T863	R977	L1099	S1140	LEU	LEU	ALA	PRQ
E354	T419	E482	E550	L631	ASN	T864	D978	E1111	L1149	GLY	GLY	ALA	PRQ
L357	I420	R483	N551	L632	I730	K366	R979	E1112	Y1158	ASP	ASP	ALA	PRQ
N358	S421	L485	L553	L633	Q731	R872	D980	D1139	E1159	LEU	LEU	ALA	PRQ
E361	I422	F487	C555	L634	N738	L374	S989	S1141	M1160	ALA	ALA	ALA	PRQ
E364	I425	R488	S556	L635	I743	L375	R992	L1149	I1161	VAL	VAL	ALA	PRQ
Y365	Y426	N489	K557	L636	V760	L376	R993	Y1159	I1162	ARG	ARG	ALA	PRQ
R366	L427	Y490	Y558	L637	L761	S879	H994	E1160	E1163	LEU	LEU	ALA	PRQ
K367	L429	E493	T559	L638	K762	E880	A999	M1161	E1164	LEU	LEU	ALA	PRQ
N368	K430	F494	D493	L639	G767	G881	I1000	I1162	I1165	ALA	ALA	ALA	PRQ
F369	V431	F495	R563	L640	I768	L882	I1001	I1163	I1166	VAL	VAL	ALA	PRQ
D370	K432	R496	R564	L641	R769	I883	I1002	I1164	I1167	ARG	ARG	ALA	PRQ
R371	L433	L497	A565	L642	C770	V898	I1003	I1165	I1168	THR	THR	ALA	PRQ
L372	E434	E498	L566	L643	F771	S899	I1004	I1166	I1169	GLY	GLY	ALA	PRQ
S373	N435	E499	L567	L644	V781	E900	A1014	I1167	I1170	ASP	ASP	ALA	PRQ
V374	E436	Q499	E571	L645	V782	R901	K1019	Y1177	Y1178	GLY	GLY	ALA	PRQ
F375	A438	R502	A572	L646	R783	L885	K1020	E1182	E1183	VAL	VAL	ALA	PRQ
P376	L439	H503	I573	L647	D792	E903	I1021	E1184	E1185	THR	THR	ALA	PRQ
P377	H440	D504	L574	L648	D793	C904	I1022	E1186	E1187	GLN	GLN	ALA	PRQ
S378	R441	S505	R587	L649	D794	V905	I1023	E1188	E1189	PHE	PHE	ALA	PRQ
L381	S442	T506	W588	L650	D795	R906	I1024	K1188	A1189	THR	THR	ALA	PRQ
P382	I443	A507	W589	L651	D796	T907	F1026	K1189	A1190	ASP	ASP	ALA	PRQ
T383	V444	N508	F590	L652	D797	T908	I1027	K1190	A1191	VAL	VAL	ALA	PRQ

• Molecule 1: Apaf-1 related killer DARK

Chain J: 48% 35% 14%

MET	S90	C165	W207	Q11	S90	P91	Y168	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P99	P9
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- Molecule 1: Apaf-1 related killer DARK



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• Molecule 1: Apaf-1 related killer DARK

Chain O: 

PRO	Y1035	I907	W799	Q663	H589	A507	I443	P382	P313	I246	K157	F87	MET
ILE	V1036	F911	T800	I1E	F590	M508	V444	T383	R314	V247	I158	L88	ASP
M1201	D1037	F912	D811	H670	T591	M509	D445	M159	E315	Q248	W159	M89	PHE
E1208	Q1051	P913	T812	L680	H593	S511	H446	L386	V316	N249	L162	P91	THR
L1214	Q1052	Y914	L816	M681	H597	G512	H448	L388	L317	A250	D163	I92	GLY
Q1223	F1053	K916	F819	ASP	Q598	S513	T449	W390	T319	M253	V164	R93	GLU
L1224	E1055	Y917	F819	CYS	H599	L515	K451	D391	P321	N254	K165	T94	H8
I1225	P1057	P1057	L829	GLY	R600	N516	T452	D392	R322	A255	Y168	Q11	
Y1226	I1058	L920	L830	GLY	Q601	T517	F453	V393	R323	F256	K169	Q98	
D1059	G921	VAL	L830	ARG	I602	L518	F453	I394	L324	N257	V170	P99	D14
E1128	S1227	ARG	L833	ARG	I603	Q519	D457	K395	I324	L258	Q171	S100	I15
E1229	K1062	ALA	H833	HIS	N604	Q520	L458	S396	I331		C172	M101	
GLU	Y928	ASP	F841	SER	L605	L521	L459	D397	R332	L262	K173	M102	E20
PHE	L1068	GLY	S835	GLY	G606	K522	P460	M399	D333	L263	M174	T103	D21
F1241	A1071	SER	H836	GLY	V837	F523	P461	V399	N340	L264	D175	M104	A22
L1247	S1074	LYS	H838	SER	N608	Y524	Y462	V400	A336	T265	F176	M105	F23
L1248	H1075	GLN		GLN	Y615	Y527	L463	V401	T337	T266	K177	Y106	V24
I1249	S1076	LEU	F841	GLN	H617		D464	V402	W338	R267	F179	E108	D28
C1251	K1086	VAL	H842	VAL	F620	S537	F467	K407	D339	T268	M180	Q109	D31
A1252	I1087	ALA	H847	H699	G621	L538	S469	S409	N340	K269	L181	M182	P36
C1256	L1098	LEU	Q850	F705	L622	M540	K472	Y408	R344	F274	I117	Y114	
M1263	E1111	TRP	H854	I706	L625	A541	H473	L410	C346	S276	M187	M115	L39
H1264	S958	ARG	GLN	L712	Q629	L542	H474	V411	D347		S188	Q118	S41
ASN	D1139	LYS	LEU	F724	L630	L543	L475	E412	K348	T279	E194	Y119	K42
ARG	S1140	ASN	PRO	L725	L631	F545	M477	K413	L349	T280	F120	M121	E43
GLN	L965	GLY	GLU	L726	L632	L546	L478	Q414	T350	T281	K121	E44	E44
ASN	L984	LEU	H859	GLU	T633	P547	E479	K416	P415	E282	Q197	K122	D45
ALA	L1149	ALA	L862	ALA	K634	K548	H480	S284	K198	L283	Y123	M124	D46
ILE	Y1158	ARG	T863	ASN	V635	L549	P481	S418	E354	S284	W207	Y125	D53
ARG	E1159	D988	H863	I730	S636	E550	E482	T419	S355	L285	T208	S126	A54
GLU	M1161	S989	K866	Q731	L637	M552	H483	S421	K356	H287	S209	R127	
LEU	L1162	LYS	H872	N738	E639	L553	H484	I422	L357		R210	Y127	
LEU	L1169	ARG	H873	I743	E640	C555	T485	P423	N358	M290	S211	P130	G57
ALA	S1172	SER	L874		D641	C555	F487	M423		T291	D212	L141	T58
CYS	C1172	VAL	L875	F760	T642	S556	R488	I425	E361	L292	M216	K133	L59
PHE	Y1177	LYS	L876	L761	L644	M558	M489	Y426	E364	T293	L134	L134	M63
VAL	E1177	ARG	H879	K762	L645	T559	F491	L427	V365	D295	I221	Q136	T64
GLY	E1182	HIS	H881	I767	R646	D560	L492	E428	R366	E296	H221		S67
GLN	E1183	GLN	L882	G767	E647	L561	L493	K430	K368	T297	Q225	L141	E70
GLU	K1188	VAL	H883	F769	E648	L562	F494	V431	F369	S299	A226	P143	
THR	A1189	THR	H898	F771	S651	L563	F496	K432	R371	L300	E227	K146	V73
GLN	S1192	GLN	E900	I781	L654	L564	L497	L433	D370	L301	S224	M147	F76
PHE	V1195	ASP	H901	T782	R656	L564	F496	E434	R371	L302	K234	L147	
THR	T1197	ALA	H902	F783	M657	A565	L497	M435	S373	L303	K235	L148	F76
ALA	H1198	ASP	Q904	W791	F660	L566	F498	E436	V374	Y304	P236	L149	
ALA	D1198	ALA	V905	D792	H661	E571	Q499	I437	F375	L305	L241	M149	E79
THR	P1200	THR	D906	D792	H662	ASP			P376	D306		G151	V80

SER	HIS	PHE	TYR	ALA	ILE	ASP	GLY	GLU	VAL	TYR	TYR	HIS	LEU	GLN	SER	ARG	LEU	GLN	LEU	GLU	LEU	LEU	LEU	LYS	ASN	LEU	ARG	ILE	LEU	ASP	LYS	ASN	GLN	TYR	GLU	GLU	ASP	LEU	LEU	SER	SER	ASP	SER	GLU	GLY
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ASP VAL VAL GLY ASN LEU VAL LEU GLU LYS ASN GLY GLY VAL ALA ARG ALA THR PRO ILE LEU GLU GLU ALA SER SER

- Molecule 1: Apaf-1 related killer DARK

Chain P:  47% 35% 1% 14%

MET	ASP	PHE	GLU	THR	GLY	GLU	H8	Q11	D14	I16	E20	A22	F23	V24	D28	D31	P36	I39	L40	S41	K42	E43	E44	I46	D46	D63	A54	G57	T58	L59	M63	T64	S67	E70	V73	F76	E79	V80	I83	M84	Y86
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F87	L88	P89	S90	P91		T94		P99	S100	M101	M102	T103	R104	M105	Y106	L107	E108	Q109		Y114	N115	D116	M117	Q118	V119	F120	A121	K122	T123	M124	V125	S126	R127		P130	K133	L134	R135	Q136		L141	R142	P143		N146	L147	L148	I149	D150	M151	G151	V152	L153	S154	G155	G156	K157	L158
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L162 D163 V164 C165 V168 L169 V170 Q171 G172 K173 M174 D175 F176 K177 L178 F179 M180 L181 M182 L183 C186 M187 S188 E189 Q197 L200 L207 T208 S209 R210 S211 S212 D212 N216 L221 H222 S223 L224 Q225 Q226 E227 L231 S234 K236 P236 L241 L242 V243

L245	L246	L247	L248	L249	L250	L251	L252	L253	L254	L255	L256	L257	L258	L259	L260	L261	L262	L263	L264	L265	L266	L267	L268	L269	L270	L271	L272	L273	L274	L275	L276	L277	L278	L279	L280	L281	L282	L283	L284	L285	L286	L287	L288	L289	L290	L291	L292	L293	L294	L295	L296	L297	L298	L299	L300	L301	L302	L303	L304	L305	L306	L307	L308	L309	L310	L311	L312	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
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Country	2017	2018	2019	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030	2031	2032	2033	2034	2035	2036	2037	2038	2039	2040	2041	2042	2043	2044	2045	2046	2047	2048	2049	2050																																																																																								
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[illegible]

Category	Germany	France	Italy	Spain	Others
1. Country of origin	45%	35%	15%	5%	0%
2. Country of residence	95%	5%	0%	0%	0%
3. Country of birth	95%	5%	0%	0%	0%
4. Country of citizenship	95%	5%	0%	0%	0%
5. Country of current employment	95%	5%	0%	0%	0%
6. Country of previous employment	95%	5%	0%	0%	0%
7. Country of previous residence	95%	5%	0%	0%	0%
8. Country of previous birth	95%	5%	0%	0%	0%
9. Country of previous citizenship	95%	5%	0%	0%	0%
10. Country of previous employment	95%	5%	0%	0%	0%

[illegible]

ASP	ALA	ALA	HIS	GLU
ALA	PHE	HIS	ASP	GLY
PRO	ILE	PHE	VAL	ALA
ALA	TYR	ALA	VAL	ASP
ASP	ILE	ASN	GLY	ASN
ILE	ASP	VAL	LEU	VAL
ASP	ASP	LEU	VAL	LEU
VAL	ASP	GLY	LYS	GLY
ASP	VAL	ASN	ASN	ASN
VAL	THR	VAL	GLY	THR
PHE	VAL	TYR	GLY	GLY
ALA	ALA	HIS	VAL	ALA
ASP	GLU	LEU	ALA	ARG
GLU	GLY	GLN	ARG	ALA
THR	VAL	LEU	LEU	ALA
PHE	TYR	LEU	THR	ALA
ALA	TYR	GLU	PRO	ALA
ASP	GLY	LEU	PRO	GLU
VAL	ASN	ILE	ASP	LEU
ASP	ARG	LEU	PRO	TRP
VAL	GLY	GLN	ASN	ARG
THR	THR	PRO	VAL	ASN
ALA	ALA	PRO	THR	LYS
GLU	ILE	LEU	LEU	ARG
LEU	ASN	ASP	ILE	GLY
LEU	ALA	ILE	ALA	ASN
ALA	ILE	ASN	ASN	ALA
ARG	ARG	GLN	GLN	ILE
PRO	PRO	TYR	TYR	PRO
GLU	GLU	GLU	GLU	GLU
LEU	LEU	ASP	ASP	LEU
LEU	LYS	LEU	LEU	LEU
ALA	LYS	ASN	ASN	ALA
CYS	ASN	LEU	LEU	CYS
VAL	ARG	LEU	LEU	VAL
LYS	ILE	ILE	ILE	LYS
PHE	LEU	ASP	ASP	PHE
VAL	VAL	LEU	LEU	VAL
GLY	GLY	THR	THR	GLY
GLU	GLU	ALA	ALA	GLU
ALA	ALA	ARG	ARG	ALA
THR	THR	GLN	GLN	THR
ASP	ASP	PHE	PHE	ASP
THR	THR	ASP	ASP	THR
ASP	ASP	SER	SER	ASP

GLU	GLY	ALA	ASP	VAL	VAL	GLY	ASN	VAL	LEU	GLU	LYS	ASN	GLY	GLY	VAL	ALA	ARG	ALA	THR	PRO	ILE	LEU	GLU	GLU	ALA	SER	SER
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	17769	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	B	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	C	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	D	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	E	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	F	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	G	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	H	0.51	6/10231 (0.1%)	0.62	10/13873 (0.1%)
1	I	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	J	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	K	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	L	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	M	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	N	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	O	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	P	0.51	6/10231 (0.1%)	0.62	10/13873 (0.1%)
All	All	0.51	96/163696 (0.1%)	0.62	146/221968 (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	15
1	B	0	15
1	C	0	15
1	D	0	15
1	E	0	15
1	F	0	15
1	G	0	15

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	15
1	I	0	15
1	J	0	15
1	K	0	15
1	L	0	15
1	M	0	15
1	N	0	15
1	O	0	15
1	P	0	15
All	All	0	240

The worst 5 of 96 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	250	ALA	CA-CB	-10.19	1.31	1.52
1	J	250	ALA	CA-CB	-10.19	1.31	1.52
1	F	250	ALA	CA-CB	-10.18	1.31	1.52
1	L	250	ALA	CA-CB	-10.17	1.31	1.52
1	B	250	ALA	CA-CB	-10.16	1.31	1.52

The worst 5 of 146 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	559	THR	O-C-N	-7.67	110.42	122.70
1	L	559	THR	O-C-N	-7.66	110.44	122.70
1	N	559	THR	O-C-N	-7.66	110.44	122.70
1	J	559	THR	O-C-N	-7.65	110.46	122.70
1	D	559	THR	O-C-N	-7.65	110.46	122.70

There are no chirality outliers.

5 of 240 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	ASN	Peptide
1	A	123	TYR	Peptide
1	A	126	SER	Peptide
1	A	143	PRO	Peptide
1	A	8	HIS	Peptide

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	10045	0	10046	666	0
1	B	10045	0	10046	684	0
1	C	10045	0	10046	679	0
1	D	10045	0	10046	692	0
1	E	10045	0	10046	670	0
1	F	10045	0	10046	692	0
1	G	10045	0	10046	683	0
1	H	10045	0	10046	661	0
1	I	10045	0	10046	671	0
1	J	10045	0	10046	666	0
1	K	10045	0	10046	694	0
1	L	10045	0	10046	686	0
1	M	10045	0	10045	674	0
1	N	10045	0	10046	662	0
1	O	10045	0	10046	666	0
1	P	10045	0	10046	672	0
2	A	30	0	9	6	0
2	B	30	0	9	7	0
2	C	30	0	9	6	0
2	D	30	0	9	6	0
2	E	30	0	9	6	0
2	F	30	0	9	6	0
2	G	30	0	9	6	0
2	H	30	0	9	6	0
2	I	30	0	9	6	0
2	J	30	0	9	6	0
2	K	30	0	9	6	0
2	L	30	0	9	6	0
2	M	30	0	9	6	0
2	N	30	0	9	6	0
2	O	30	0	9	6	0
2	P	30	0	9	6	0
All	All	161200	0	160879	10606	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 33.

The worst 5 of 10606 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:I:875:LEU:HD11	1:I:911:PHE:CE2	1.25	1.72
1:E:875:LEU:HD11	1:E:911:PHE:CE2	1.25	1.72
1:J:875:LEU:HD11	1:J:911:PHE:CE2	1.25	1.71
1:F:875:LEU:HD11	1:F:911:PHE:CE2	1.25	1.71
1:C:875:LEU:HD11	1:C:911:PHE:CE2	1.25	1.71

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	7	47
1	B	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	7	47
1	C	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	7	47
1	D	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	7	47
1	E	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	7	47
1	F	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	7	47
1	G	1224/1440 (85%)	989 (81%)	202 (16%)	33 (3%)	6	47
1	H	1224/1440 (85%)	988 (81%)	204 (17%)	32 (3%)	7	47
1	I	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	7	47
1	J	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	7	47
1	K	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	7	47
1	L	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	7	47
1	M	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	7	47
1	N	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	7	47
1	O	1224/1440 (85%)	988 (81%)	203 (17%)	33 (3%)	6	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	7	47
All	All	19584/23040 (85%)	15822 (81%)	3248 (17%)	514 (3%)	11	47

5 of 514 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	ALA
1	A	315	GLU
1	A	517	THR
1	A	638	GLU
1	A	760	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	1138/1315 (86%)	1137 (100%)	1 (0%)	95	97
1	B	1138/1315 (86%)	1137 (100%)	1 (0%)	95	97
1	C	1138/1315 (86%)	1137 (100%)	1 (0%)	95	97
1	D	1138/1315 (86%)	1137 (100%)	1 (0%)	95	97
1	E	1138/1315 (86%)	1137 (100%)	1 (0%)	95	97
1	F	1138/1315 (86%)	1137 (100%)	1 (0%)	95	97
1	G	1138/1315 (86%)	1137 (100%)	1 (0%)	95	97
1	H	1138/1315 (86%)	1137 (100%)	1 (0%)	95	97
1	I	1138/1315 (86%)	1137 (100%)	1 (0%)	95	97
1	J	1138/1315 (86%)	1137 (100%)	1 (0%)	95	97
1	K	1138/1315 (86%)	1137 (100%)	1 (0%)	95	97
1	L	1138/1315 (86%)	1137 (100%)	1 (0%)	95	97
1	M	1138/1315 (86%)	1137 (100%)	1 (0%)	95	97
1	N	1138/1315 (86%)	1137 (100%)	1 (0%)	95	97
1	O	1138/1315 (86%)	1137 (100%)	1 (0%)	95	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	1138/1315 (86%)	1137 (100%)	1 (0%)	95	97
All	All	18208/21040 (86%)	18192 (100%)	16 (0%)	95	97

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	914	VAL
1	I	914	VAL
1	M	914	VAL
1	G	914	VAL
1	N	914	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 462 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	222	HIS
1	I	1027	ASN
1	O	850	GLN
1	H	477	ASN
1	I	171	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

16 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	APK	A	251	1	28,33,33	3.09	10 (35%)	27,47,47	3.57	5 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	APK	B	251	1	28,33,33	3.08	10 (35%)	27,47,47	3.57	5 (18%)
1	APK	C	251	1	28,33,33	3.08	10 (35%)	27,47,47	3.56	5 (18%)
1	APK	D	251	1	28,33,33	3.09	10 (35%)	27,47,47	3.57	5 (18%)
1	APK	E	251	1	28,33,33	3.08	10 (35%)	27,47,47	3.56	5 (18%)
1	APK	F	251	1	28,33,33	3.08	10 (35%)	27,47,47	3.57	5 (18%)
1	APK	G	251	1	28,33,33	3.08	10 (35%)	27,47,47	3.57	5 (18%)
1	APK	H	251	1	28,33,33	3.09	10 (35%)	27,47,47	3.56	5 (18%)
1	APK	I	251	1	28,33,33	3.08	10 (35%)	27,47,47	3.56	5 (18%)
1	APK	J	251	1	28,33,33	3.08	10 (35%)	27,47,47	3.57	5 (18%)
1	APK	K	251	1	28,33,33	3.09	10 (35%)	27,47,47	3.56	5 (18%)
1	APK	L	251	1	28,33,33	3.09	10 (35%)	27,47,47	3.56	5 (18%)
1	APK	M	251	1	28,33,33	3.08	11 (39%)	27,47,47	3.56	5 (18%)
1	APK	N	251	1	28,33,33	3.08	11 (39%)	27,47,47	3.56	5 (18%)
1	APK	O	251	1	28,33,33	3.08	10 (35%)	27,47,47	3.57	5 (18%)
1	APK	P	251	1	28,33,33	3.08	10 (35%)	27,47,47	3.57	5 (18%)

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
1	APK	A	251	1	-	0/14/37/37	0/3/3/3
1	APK	B	251	1	-	0/14/37/37	0/3/3/3
1	APK	C	251	1	-	0/14/37/37	0/3/3/3
1	APK	D	251	1	-	0/14/37/37	0/3/3/3
1	APK	E	251	1	-	0/14/37/37	0/3/3/3
1	APK	F	251	1	-	0/14/37/37	0/3/3/3
1	APK	G	251	1	-	0/14/37/37	0/3/3/3
1	APK	H	251	1	-	0/14/37/37	0/3/3/3
1	APK	I	251	1	-	0/14/37/37	0/3/3/3
1	APK	J	251	1	-	0/14/37/37	0/3/3/3
1	APK	K	251	1	-	0/14/37/37	0/3/3/3
1	APK	L	251	1	-	0/14/37/37	0/3/3/3
1	APK	M	251	1	-	0/14/37/37	0/3/3/3
1	APK	N	251	1	-	0/14/37/37	0/3/3/3
1	APK	O	251	1	-	0/14/37/37	0/3/3/3
1	APK	P	251	1	-	0/14/37/37	0/3/3/3

The worst 5 of 162 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	251	APK	C2'-C3'	-8.28	1.31	1.53
1	B	251	APK	C2'-C3'	-8.28	1.31	1.53
1	K	251	APK	C2'-C3'	-8.27	1.31	1.53
1	N	251	APK	C2'-C3'	-8.26	1.31	1.53
1	G	251	APK	C2'-C3'	-8.26	1.31	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	251	APK	N3-C2-N1	-10.71	120.46	128.87
1	D	251	APK	N3-C2-N1	-10.70	120.47	128.87
1	E	251	APK	N3-C2-N1	-10.70	120.47	128.87
1	F	251	APK	N3-C2-N1	-10.69	120.47	128.87
1	P	251	APK	N3-C2-N1	-10.69	120.48	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 99 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	251	APK	6	0
1	B	251	APK	6	0
1	C	251	APK	7	0
1	D	251	APK	7	0
1	E	251	APK	6	0
1	F	251	APK	6	0
1	G	251	APK	6	0
1	H	251	APK	6	0
1	I	251	APK	6	0
1	J	251	APK	6	0
1	K	251	APK	7	0
1	L	251	APK	7	0
1	M	251	APK	6	0
1	N	251	APK	6	0
1	O	251	APK	5	0
1	P	251	APK	6	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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$
2	DTP	A	1501	-	25,32,32	3.36	6 (24%)	26,50,50	2.73	6 (23%)
2	DTP	B	1501	-	25,32,32	3.37	6 (24%)	26,50,50	2.72	6 (23%)
2	DTP	C	1501	-	25,32,32	3.37	6 (24%)	26,50,50	2.72	6 (23%)
2	DTP	D	1501	-	25,32,32	3.37	6 (24%)	26,50,50	2.73	6 (23%)
2	DTP	E	1501	-	25,32,32	3.36	6 (24%)	26,50,50	2.73	6 (23%)
2	DTP	F	1501	-	25,32,32	3.36	6 (24%)	26,50,50	2.72	6 (23%)
2	DTP	G	1501	-	25,32,32	3.37	6 (24%)	26,50,50	2.72	6 (23%)
2	DTP	H	1501	-	25,32,32	3.36	6 (24%)	26,50,50	2.73	6 (23%)
2	DTP	I	1501	-	25,32,32	3.36	6 (24%)	26,50,50	2.69	5 (19%)
2	DTP	J	1501	-	25,32,32	3.36	6 (24%)	26,50,50	2.70	5 (19%)
2	DTP	K	1501	-	25,32,32	3.36	6 (24%)	26,50,50	2.69	5 (19%)
2	DTP	L	1501	-	25,32,32	3.36	6 (24%)	26,50,50	2.70	5 (19%)
2	DTP	M	1501	-	25,32,32	3.36	6 (24%)	26,50,50	2.70	5 (19%)
2	DTP	N	1501	-	25,32,32	3.36	6 (24%)	26,50,50	2.69	5 (19%)
2	DTP	O	1501	-	25,32,32	3.36	6 (24%)	26,50,50	2.69	5 (19%)
2	DTP	P	1501	-	25,32,32	3.36	6 (24%)	26,50,50	2.70	5 (19%)

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
2	DTP	A	1501	-	-	0/18/34/34	0/3/3/3
2	DTP	B	1501	-	-	0/18/34/34	0/3/3/3
2	DTP	C	1501	-	-	0/18/34/34	0/3/3/3
2	DTP	D	1501	-	-	0/18/34/34	0/3/3/3
2	DTP	E	1501	-	-	0/18/34/34	0/3/3/3
2	DTP	F	1501	-	-	0/18/34/34	0/3/3/3
2	DTP	G	1501	-	-	0/18/34/34	0/3/3/3
2	DTP	H	1501	-	-	0/18/34/34	0/3/3/3
2	DTP	I	1501	-	-	0/18/34/34	0/3/3/3
2	DTP	J	1501	-	-	0/18/34/34	0/3/3/3
2	DTP	K	1501	-	-	0/18/34/34	0/3/3/3
2	DTP	L	1501	-	-	0/18/34/34	0/3/3/3
2	DTP	M	1501	-	-	0/18/34/34	0/3/3/3
2	DTP	N	1501	-	-	0/18/34/34	0/3/3/3
2	DTP	O	1501	-	-	0/18/34/34	0/3/3/3
2	DTP	P	1501	-	-	0/18/34/34	0/3/3/3

The worst 5 of 96 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1501	DTP	C2'-C3'	-12.07	1.20	1.52
2	D	1501	DTP	C2'-C3'	-12.07	1.20	1.52
2	M	1501	DTP	C2'-C3'	-12.07	1.20	1.52
2	G	1501	DTP	C2'-C3'	-12.06	1.20	1.52
2	F	1501	DTP	C2'-C3'	-12.06	1.20	1.52

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	1501	DTP	N3-C2-N1	-9.94	121.06	128.87
2	L	1501	DTP	N3-C2-N1	-9.93	121.07	128.87
2	H	1501	DTP	N3-C2-N1	-9.92	121.08	128.87
2	M	1501	DTP	N3-C2-N1	-9.92	121.08	128.87
2	E	1501	DTP	N3-C2-N1	-9.92	121.08	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 97 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1501	DTP	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1501	DTP	7	0
2	C	1501	DTP	6	0
2	D	1501	DTP	6	0
2	E	1501	DTP	6	0
2	F	1501	DTP	6	0
2	G	1501	DTP	6	0
2	H	1501	DTP	6	0
2	I	1501	DTP	6	0
2	J	1501	DTP	6	0
2	K	1501	DTP	6	0
2	L	1501	DTP	6	0
2	M	1501	DTP	6	0
2	N	1501	DTP	6	0
2	O	1501	DTP	6	0
2	P	1501	DTP	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.