



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:26 PM BST

PDB ID : 4V4L
EMDB ID: : EMD-5235
Title : Structure of the Drosophila apoptosome
Authors : Yuan, S.; Topf, M.; Akey, C.W.; Ludtke, S.J.
Deposited on : 2010-10-04
Resolution : 6.90 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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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

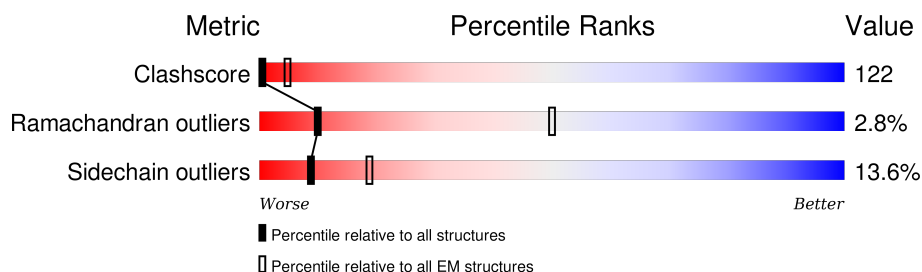
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.90 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	1221	52% 38% 8% .
1	B	1221	52% 38% 8% .
1	C	1221	52% 38% 8% .
1	D	1221	52% 38% 8% .
1	E	1221	52% 38% 8% .
1	F	1221	53% 38% 8% .
1	G	1221	52% 38% 8% .
1	H	1221	52% 38% 8% .
1	I	1221	52% 38% 8% .

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Mol	Chain	Length	Quality of chain
1	J	1221	 52% 38% 8%
1	K	1221	 52% 38% 8%
1	L	1221	 52% 38% 8%
1	M	1221	 52% 38% 8%
1	N	1221	 52% 38% 8%
1	O	1221	 52% 38% 8%
1	P	1221	 53% 38% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DTP	A	1402	-	-	X	-
3	DTP	B	1402	-	-	X	-
3	DTP	C	1402	-	-	X	-
3	DTP	D	1402	-	-	X	-
3	DTP	E	1402	-	-	X	-
3	DTP	F	1402	-	-	X	-
3	DTP	G	1402	-	-	X	-
3	DTP	H	1402	-	-	X	-
3	DTP	I	1402	-	-	X	-
3	DTP	J	1402	-	-	X	-
3	DTP	K	1402	-	-	X	-
3	DTP	L	1402	-	-	X	-
3	DTP	M	1402	-	-	X	-
3	DTP	N	1402	-	-	X	-
3	DTP	O	1402	-	-	X	-
3	DTP	P	1402	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 128176 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	1215	Total 7980	C 4994	N 1446	O 1514	S 26	0	0
1	B	1215	Total 7980	C 4994	N 1446	O 1514	S 26	0	0
1	C	1215	Total 7980	C 4994	N 1446	O 1514	S 26	0	0
1	D	1215	Total 7980	C 4994	N 1446	O 1514	S 26	0	0
1	E	1215	Total 7980	C 4994	N 1446	O 1514	S 26	0	0
1	F	1215	Total 7980	C 4994	N 1446	O 1514	S 26	0	0
1	G	1215	Total 7980	C 4994	N 1446	O 1514	S 26	0	0
1	H	1215	Total 7980	C 4994	N 1446	O 1514	S 26	0	0
1	I	1215	Total 7980	C 4994	N 1446	O 1514	S 26	0	0
1	J	1215	Total 7980	C 4994	N 1446	O 1514	S 26	0	0
1	K	1215	Total 7980	C 4994	N 1446	O 1514	S 26	0	0
1	L	1215	Total 7980	C 4994	N 1446	O 1514	S 26	0	0
1	M	1215	Total 7980	C 4994	N 1446	O 1514	S 26	0	0
1	N	1215	Total 7980	C 4994	N 1446	O 1514	S 26	0	0
1	O	1215	Total 7980	C 4994	N 1446	O 1514	S 26	0	0
1	P	1215	Total 7980	C 4994	N 1446	O 1514	S 26	0	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q7KLI1
A	-4	HIS	-	EXPRESSION TAG	UNP Q7KLI1
A	-3	HIS	-	EXPRESSION TAG	UNP Q7KLI1
A	-2	HIS	-	EXPRESSION TAG	UNP Q7KLI1
A	-1	HIS	-	EXPRESSION TAG	UNP Q7KLI1
A	0	HIS	-	EXPRESSION TAG	UNP Q7KLI1
B	-5	HIS	-	EXPRESSION TAG	UNP Q7KLI1
B	-4	HIS	-	EXPRESSION TAG	UNP Q7KLI1
B	-3	HIS	-	EXPRESSION TAG	UNP Q7KLI1
B	-2	HIS	-	EXPRESSION TAG	UNP Q7KLI1
B	-1	HIS	-	EXPRESSION TAG	UNP Q7KLI1
B	0	HIS	-	EXPRESSION TAG	UNP Q7KLI1
C	-5	HIS	-	EXPRESSION TAG	UNP Q7KLI1
C	-4	HIS	-	EXPRESSION TAG	UNP Q7KLI1
C	-3	HIS	-	EXPRESSION TAG	UNP Q7KLI1
C	-2	HIS	-	EXPRESSION TAG	UNP Q7KLI1
C	-1	HIS	-	EXPRESSION TAG	UNP Q7KLI1
C	0	HIS	-	EXPRESSION TAG	UNP Q7KLI1
D	-5	HIS	-	EXPRESSION TAG	UNP Q7KLI1
D	-4	HIS	-	EXPRESSION TAG	UNP Q7KLI1
D	-3	HIS	-	EXPRESSION TAG	UNP Q7KLI1
D	-2	HIS	-	EXPRESSION TAG	UNP Q7KLI1
D	-1	HIS	-	EXPRESSION TAG	UNP Q7KLI1
D	0	HIS	-	EXPRESSION TAG	UNP Q7KLI1
E	-5	HIS	-	EXPRESSION TAG	UNP Q7KLI1
E	-4	HIS	-	EXPRESSION TAG	UNP Q7KLI1
E	-3	HIS	-	EXPRESSION TAG	UNP Q7KLI1
E	-2	HIS	-	EXPRESSION TAG	UNP Q7KLI1
E	-1	HIS	-	EXPRESSION TAG	UNP Q7KLI1
E	0	HIS	-	EXPRESSION TAG	UNP Q7KLI1
F	-5	HIS	-	EXPRESSION TAG	UNP Q7KLI1
F	-4	HIS	-	EXPRESSION TAG	UNP Q7KLI1
F	-3	HIS	-	EXPRESSION TAG	UNP Q7KLI1
F	-2	HIS	-	EXPRESSION TAG	UNP Q7KLI1
F	-1	HIS	-	EXPRESSION TAG	UNP Q7KLI1
F	0	HIS	-	EXPRESSION TAG	UNP Q7KLI1
G	-5	HIS	-	EXPRESSION TAG	UNP Q7KLI1
G	-4	HIS	-	EXPRESSION TAG	UNP Q7KLI1
G	-3	HIS	-	EXPRESSION TAG	UNP Q7KLI1
G	-2	HIS	-	EXPRESSION TAG	UNP Q7KLI1
G	-1	HIS	-	EXPRESSION TAG	UNP Q7KLI1
G	0	HIS	-	EXPRESSION TAG	UNP Q7KLI1
H	-5	HIS	-	EXPRESSION TAG	UNP Q7KLI1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-4	HIS	-	EXPRESSION TAG	UNP Q7KLI1
H	-3	HIS	-	EXPRESSION TAG	UNP Q7KLI1
H	-2	HIS	-	EXPRESSION TAG	UNP Q7KLI1
H	-1	HIS	-	EXPRESSION TAG	UNP Q7KLI1
H	0	HIS	-	EXPRESSION TAG	UNP Q7KLI1
I	-5	HIS	-	EXPRESSION TAG	UNP Q7KLI1
I	-4	HIS	-	EXPRESSION TAG	UNP Q7KLI1
I	-3	HIS	-	EXPRESSION TAG	UNP Q7KLI1
I	-2	HIS	-	EXPRESSION TAG	UNP Q7KLI1
I	-1	HIS	-	EXPRESSION TAG	UNP Q7KLI1
I	0	HIS	-	EXPRESSION TAG	UNP Q7KLI1
J	-5	HIS	-	EXPRESSION TAG	UNP Q7KLI1
J	-4	HIS	-	EXPRESSION TAG	UNP Q7KLI1
J	-3	HIS	-	EXPRESSION TAG	UNP Q7KLI1
J	-2	HIS	-	EXPRESSION TAG	UNP Q7KLI1
J	-1	HIS	-	EXPRESSION TAG	UNP Q7KLI1
J	0	HIS	-	EXPRESSION TAG	UNP Q7KLI1
K	-5	HIS	-	EXPRESSION TAG	UNP Q7KLI1
K	-4	HIS	-	EXPRESSION TAG	UNP Q7KLI1
K	-3	HIS	-	EXPRESSION TAG	UNP Q7KLI1
K	-2	HIS	-	EXPRESSION TAG	UNP Q7KLI1
K	-1	HIS	-	EXPRESSION TAG	UNP Q7KLI1
K	0	HIS	-	EXPRESSION TAG	UNP Q7KLI1
L	-5	HIS	-	EXPRESSION TAG	UNP Q7KLI1
L	-4	HIS	-	EXPRESSION TAG	UNP Q7KLI1
L	-3	HIS	-	EXPRESSION TAG	UNP Q7KLI1
L	-2	HIS	-	EXPRESSION TAG	UNP Q7KLI1
L	-1	HIS	-	EXPRESSION TAG	UNP Q7KLI1
L	0	HIS	-	EXPRESSION TAG	UNP Q7KLI1
M	-5	HIS	-	EXPRESSION TAG	UNP Q7KLI1
M	-4	HIS	-	EXPRESSION TAG	UNP Q7KLI1
M	-3	HIS	-	EXPRESSION TAG	UNP Q7KLI1
M	-2	HIS	-	EXPRESSION TAG	UNP Q7KLI1
M	-1	HIS	-	EXPRESSION TAG	UNP Q7KLI1
M	0	HIS	-	EXPRESSION TAG	UNP Q7KLI1
N	-5	HIS	-	EXPRESSION TAG	UNP Q7KLI1
N	-4	HIS	-	EXPRESSION TAG	UNP Q7KLI1
N	-3	HIS	-	EXPRESSION TAG	UNP Q7KLI1
N	-2	HIS	-	EXPRESSION TAG	UNP Q7KLI1
N	-1	HIS	-	EXPRESSION TAG	UNP Q7KLI1
N	0	HIS	-	EXPRESSION TAG	UNP Q7KLI1
O	-5	HIS	-	EXPRESSION TAG	UNP Q7KLI1

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-4	HIS	-	EXPRESSION TAG	UNP Q7KLI1
O	-3	HIS	-	EXPRESSION TAG	UNP Q7KLI1
O	-2	HIS	-	EXPRESSION TAG	UNP Q7KLI1
O	-1	HIS	-	EXPRESSION TAG	UNP Q7KLI1
O	0	HIS	-	EXPRESSION TAG	UNP Q7KLI1
P	-5	HIS	-	EXPRESSION TAG	UNP Q7KLI1
P	-4	HIS	-	EXPRESSION TAG	UNP Q7KLI1
P	-3	HIS	-	EXPRESSION TAG	UNP Q7KLI1
P	-2	HIS	-	EXPRESSION TAG	UNP Q7KLI1
P	-1	HIS	-	EXPRESSION TAG	UNP Q7KLI1
P	0	HIS	-	EXPRESSION TAG	UNP Q7KLI1

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

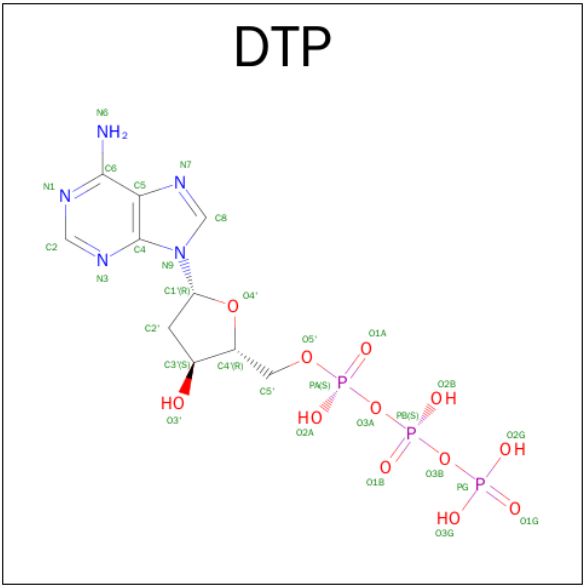
Mol	Chain	Residues	Atoms	AltConf
2	P	1	Total Mg 1 1	0
2	G	1	Total Mg 1 1	0
2	J	1	Total Mg 1 1	0
2	D	1	Total Mg 1 1	0
2	K	1	Total Mg 1 1	0
2	E	1	Total Mg 1 1	0
2	H	1	Total Mg 1 1	0
2	B	1	Total Mg 1 1	0
2	I	1	Total Mg 1 1	0
2	C	1	Total Mg 1 1	0
2	A	1	Total Mg 1 1	0
2	N	1	Total Mg 1 1	0
2	O	1	Total Mg 1 1	0
2	L	1	Total Mg 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
2	F	1	Total	Mg	0
			1	1	
2	M	1	Total	Mg	0
			1	1	

- Molecule 3 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃).



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

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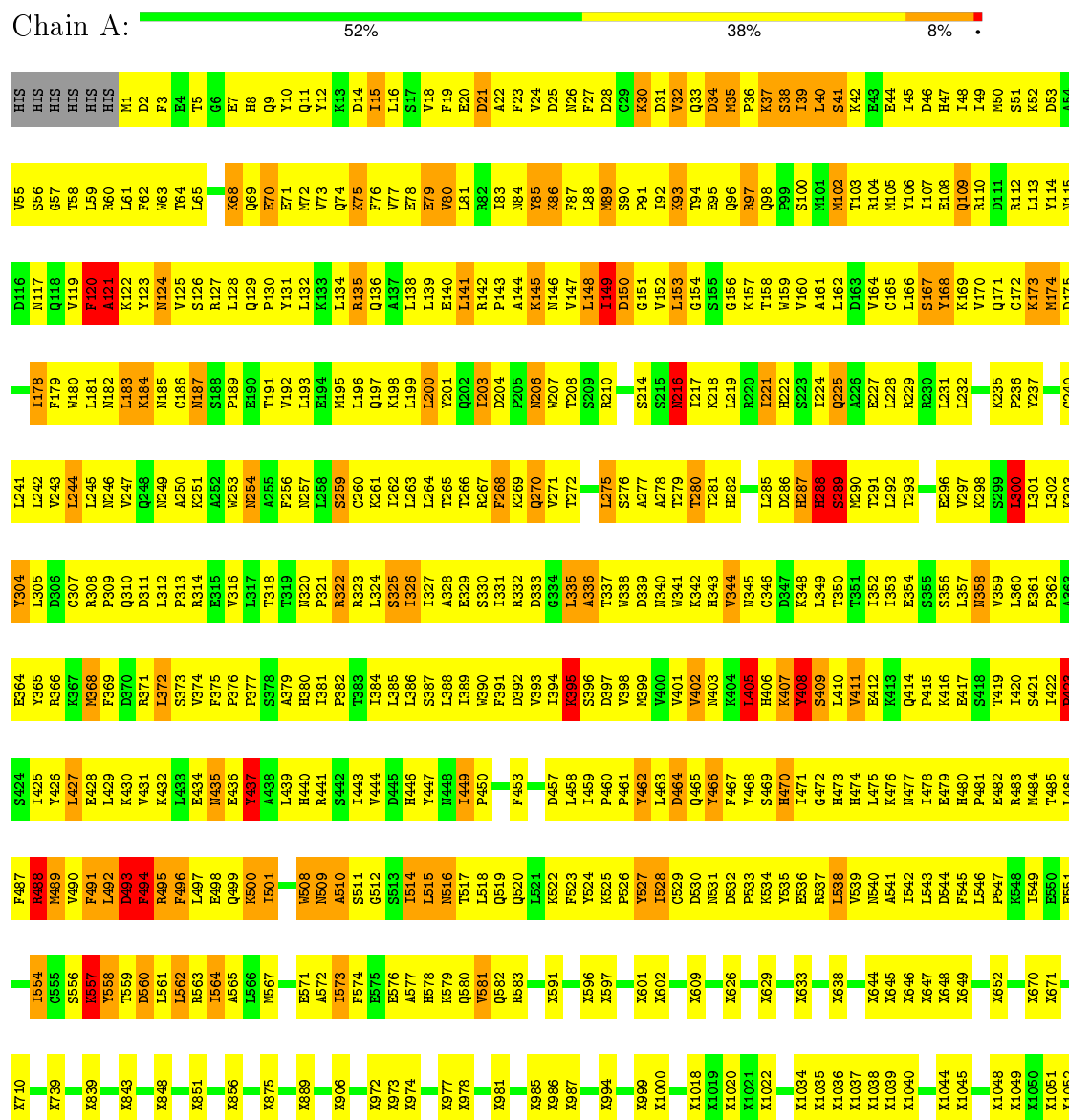
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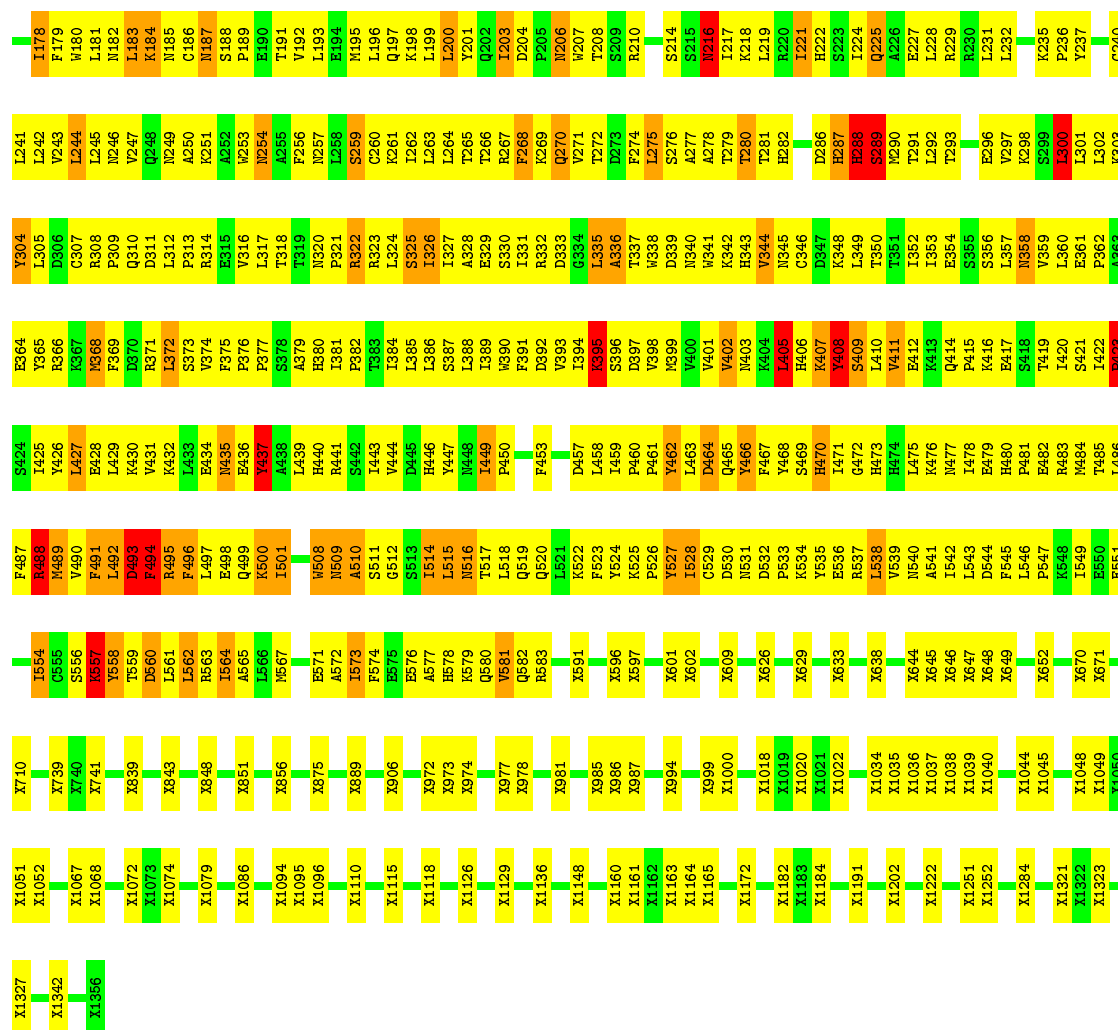
Mol	Chain	Residues	Atoms					AltConf
3	J	1	Total	C	N	O	P	0
			30	10	5	12	3	
3	K	1	Total	C	N	O	P	0
			30	10	5	12	3	
3	L	1	Total	C	N	O	P	0
			30	10	5	12	3	
3	M	1	Total	C	N	O	P	0
			30	10	5	12	3	
3	N	1	Total	C	N	O	P	0
			30	10	5	12	3	
3	O	1	Total	C	N	O	P	0
			30	10	5	12	3	
3	P	1	Total	C	N	O	P	0
			30	10	5	12	3	

3 Residue-property plots

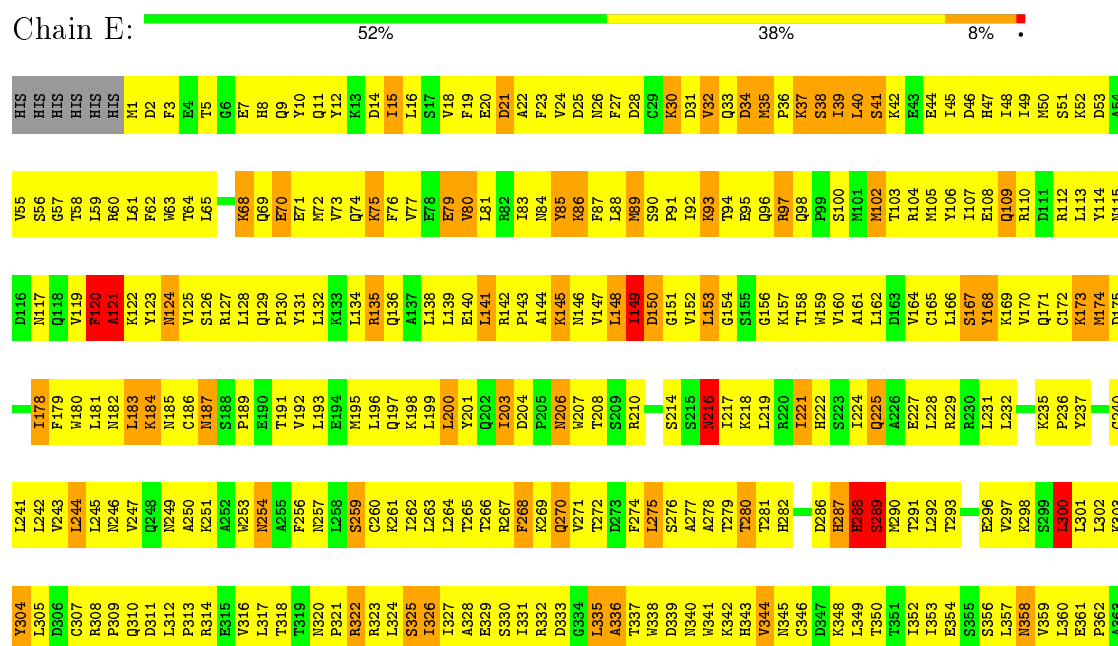
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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.

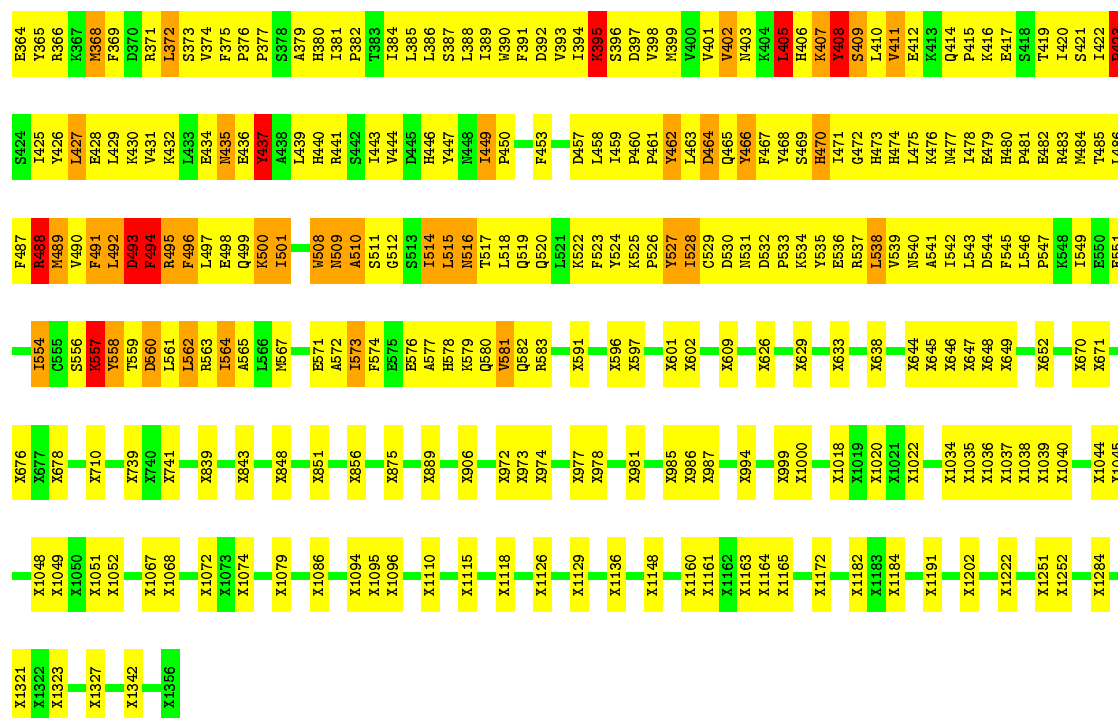
- Molecule 1: Apaf-1 related killer DARK





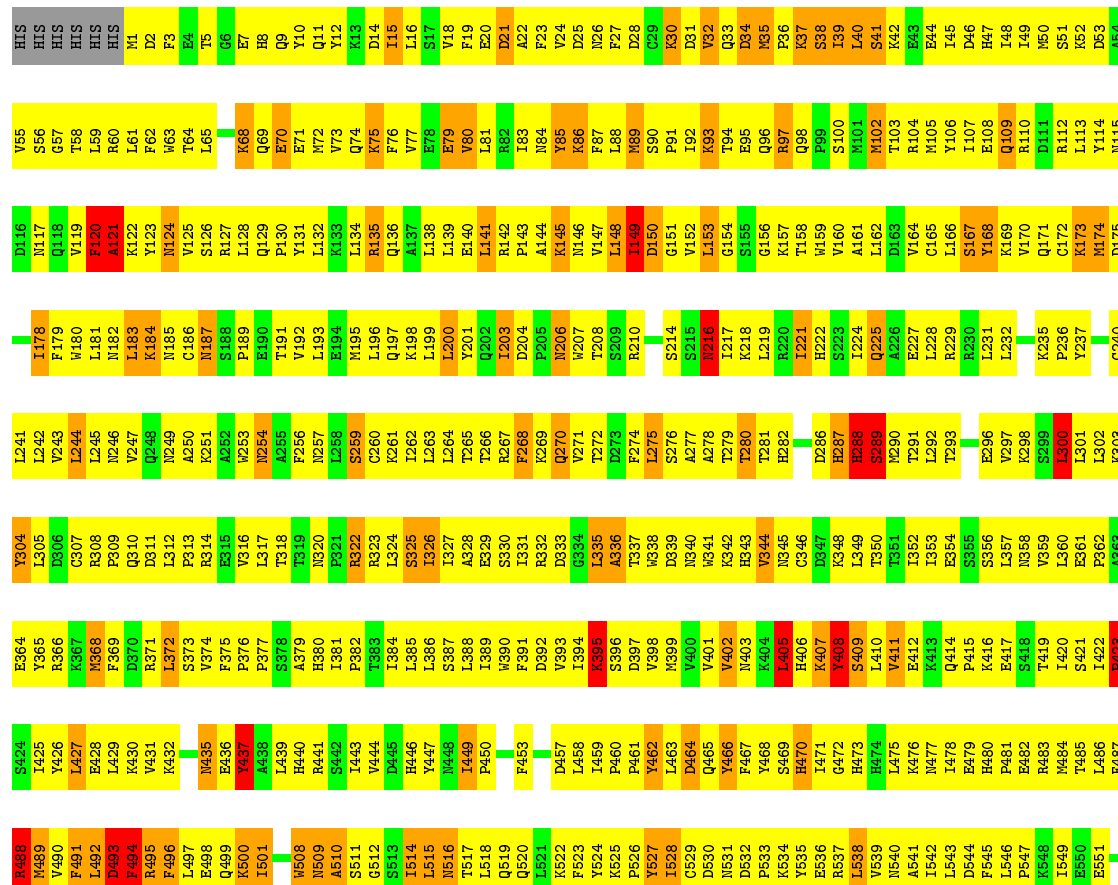
• Molecule 1: Apaf-1 related killer DARK





- Molecule 1: Apaf-1 related killer DARK

Chain F: 53% 38% 8%



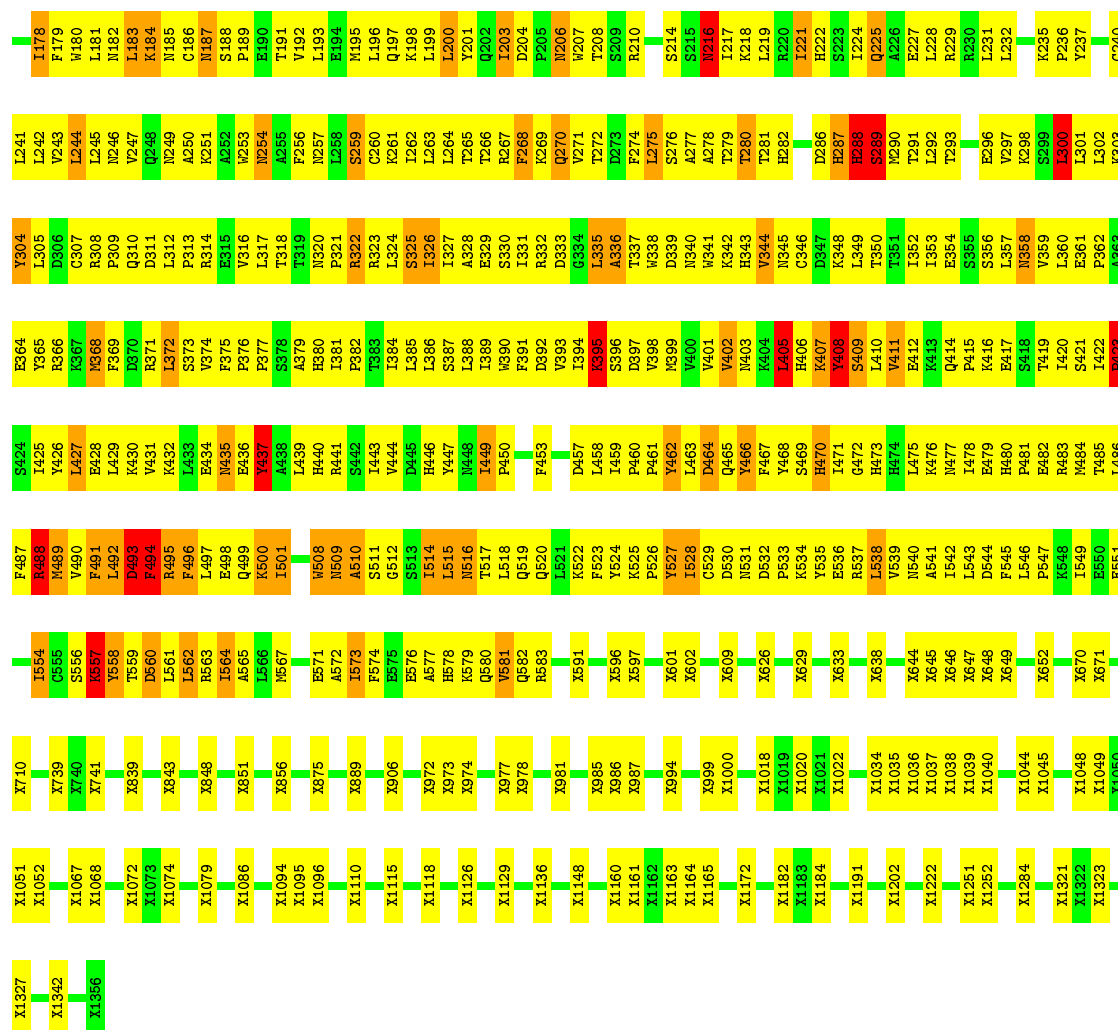


X1321	X1048	X676	F487	S424	E364	Y304	L241	D116	V55	HIS
X1322	X1049	X677	R488	L425	R365	L305	L242	M117	S56	HIS
X1323	X1050	X678	N489	Y426	R366	D306	V243	Q118	G57	HIS
X1327	X1051	X710	V490	L427	K367	C307	L244	V119	T58	HIS
X1342	X1052	X711	F491	E428	M368	R308	L245	F120	L59	HIS
X1356	X1067	X739	L492	L429	P369	P309	N246	A121	R60	HIS
	X1068	X740	D493	K430	D370	Q310	Q247	K122	L61	M1
	X1069	X741	F494	V431	R371	D311	Q248	Y123	F62	D2
	X1072	X839	R495	K432	L372	L312	A250	L124	W63	F3
	X1073	X843	F496	L433	S373	P313	R250	V125	W63	F4
	X1074	X844	L497	E434	V374	K251	K251	S126	T64	E4
	X1079	X848	E498	M435	P375	R315	A252	R127	L65	T5
			E499	R436	P376	E316	E253	L128		G6
			K500	Y437	P377	L317	A254	Q129	K68	E7
			M567	A438	S378	T318	E255	P130	Q69	H8
				L439	A379	T319	F256	Y131	E71	Y10
	X1086	X851	H508	H440	H380	N320	N257	L132	M72	Y11
	X1094	X856	N509	R441	L381	P321	L258	K133	M72	Y12
	X1095	X875	A510	S442	P382	R322	S259	L134	Q74	K13
	X1096		F574	L443	T383	R323	C260	R135	K75	D14
			E575	V444	L384	L324	K261	Q136	F76	I15
	X1110	X889	E576	D445	L385	S325	K262	A137	V77	L16
			A577	H446	L386	L326	L263	L138	E78	S17
	X1115	X906	L514	Y447	S387	L327	L264	L139	E79	V18
	X1118		L515	H448	L388	A328	T265	E140	V80	F19
	X1126	X973	K579	T449	L389	E329	T266	L141	L81	E20
		X974	Q580	P450	W390	S330	R267	R142	R82	D21
	X1129	X977	V581	F453	F391	L331	F268	P143	I83	A22
	X1136	X978	E591		D392	R332	K269	A144	N84	F23
		X981	X596		V393	D333	Q270	K145	Y85	V24
	X1148	X985	X597		L394	G334	T271	N146	K86	D25
		X986	X598		R395	L335	D273	L148	F87	N26
	X1160	X987	X601		S396	A336	T272	S209	L88	F27
	X1161		X602		D397	T337	F274	R210	M89	D28
	X1162	X994	X626		V398	D338	L275	D150	S90	C29
	X1164		X629		M399	D339	S276	G151	P91	K30
	X1165	X999	X633		V400	N340	A277	V152	I92	D31
		X1000	X638		H406	D346	D286	L153	K93	V32
	X1172	X1018	X644		K407	C347	H287	G154	T94	Q33
		X1019	X645		Y408	K348	R230	S155	E95	D34
	X1182	X1020	X646		S409	L349	L224	K218	Q96	K35
	X1183	X1021	H473		L410	T350	Q225	L219	R97	P36
	X1184	X1022	H474		V411	T351	M290	K157	Q98	K37
			H475		E412	L352	T291	T158	P99	S38
	X1191	X1034	X647		K413	L353	L293	V159	S100	I39
		X1035	X648		R413	E354	T293	A161	M101	L40
	X1202	X1036	X649		Q414	L354	L296	L162	M102	S41
		X1037	X652		V402	H473	S238	D163	T103	E43
	X1222	X1038	X657		N404	T351	M290	E227	R104	R43
		X1039	X670		L405	L352	T291	L228	M105	E44
	X1251	X1040	X671		H406	L353	L293	R229	Y106	I45
			X676		K407	E354	L296	L167	I107	D46
	X1284	X1044	X677		Y408	L355	L297	K168	E108	H47
			X678		S418	L356	V297	L169	Q109	I48
			X679		E417	L357	L298	V170	R110	I49
			X680		N418	L358	S299	Q171	D111	M50
			X681		T419	V359	L301	C172	R112	S51
			X682		L420	L360	Y237	K173	L113	K52
			X683		S421	E361	L302	M174	Y114	D53
			X684		L422	P362	L302	D175	N115	E54
			X685		R423	L363	L302			
			X686		E423	L363	L302			

• Molecule 1: Apaf-1 related killer DARK

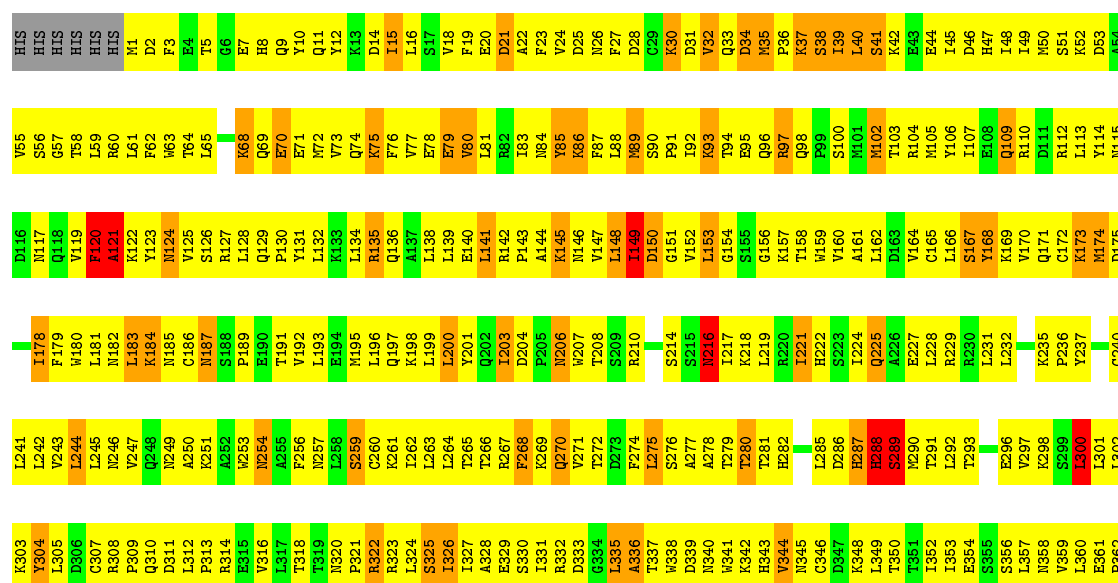
Chain J:  52% 38% 8%

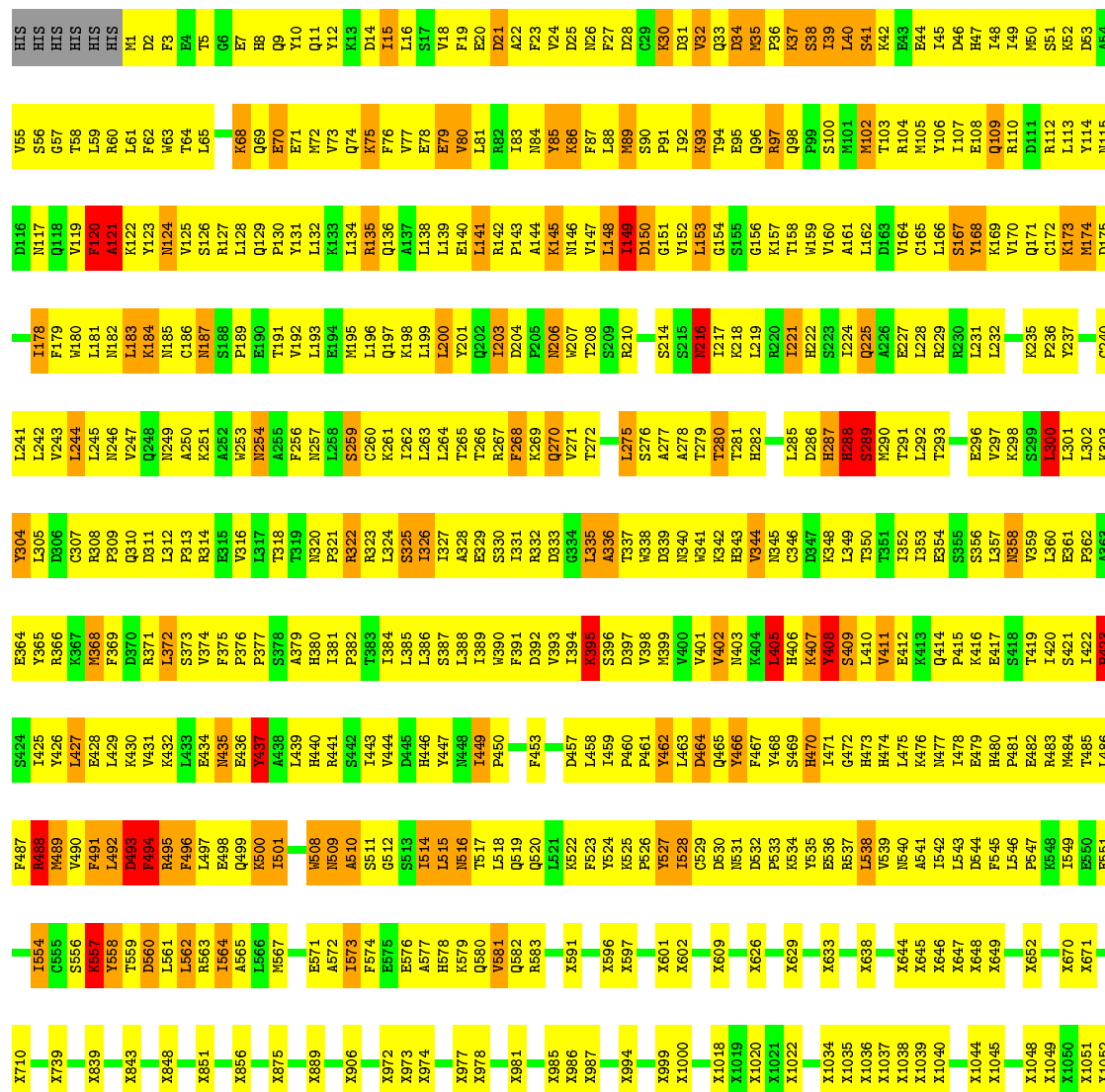
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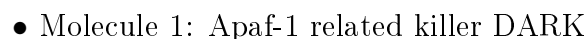


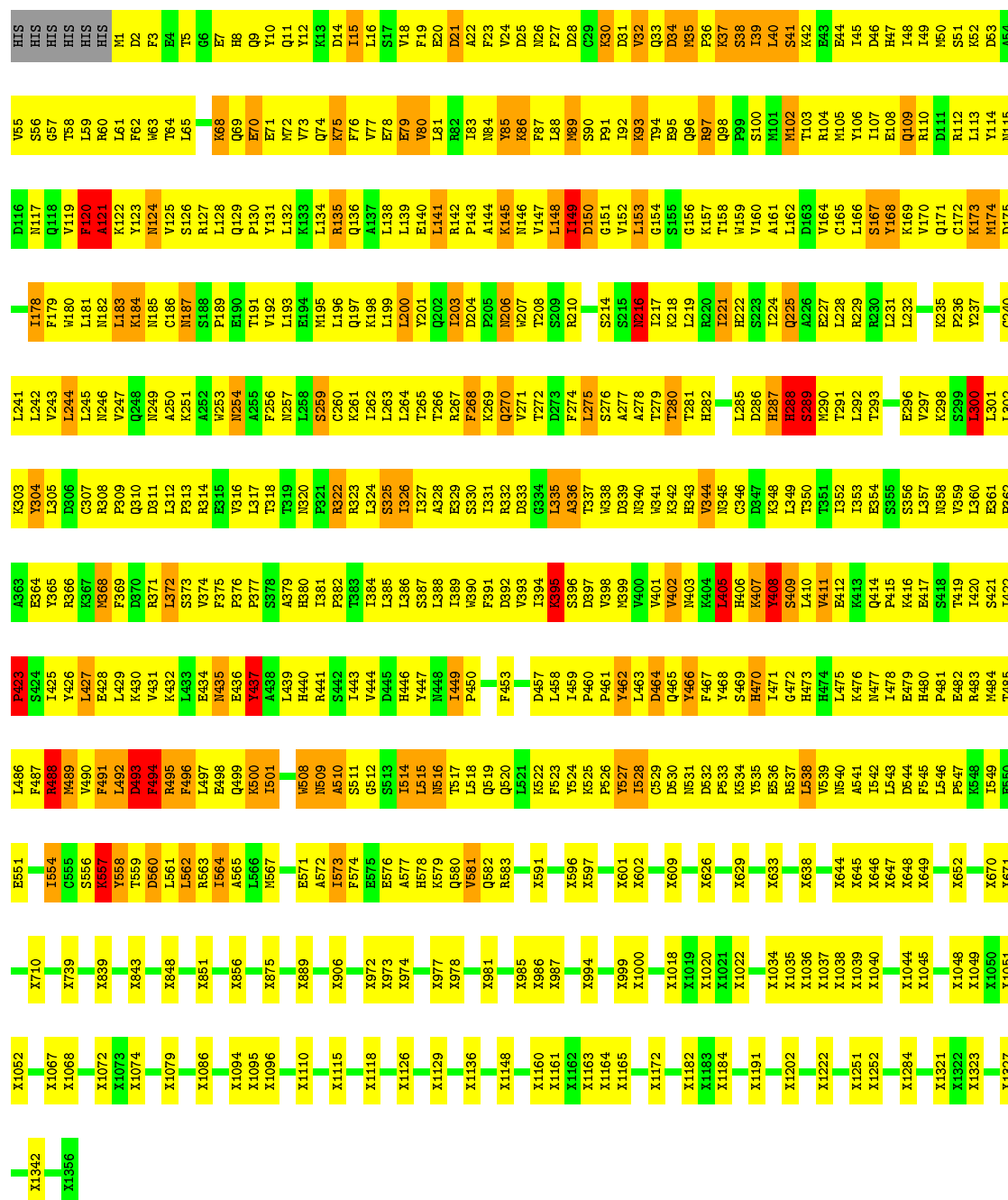
• Molecule 1: Apaf-1 related killer DARK

Chain K: 52% 38% 8%







Chain O: 

X1067	X1068	X739	I554	R488	S424	E364	Y304	L241	I178	D116
X1072	X1073	X839	C555	M489	I425	T365	L305	L242	I179	M117
X1074	X1075	X843	S556	V490	Y427	R367	D306	L243	M180	Q118
X1079	X1086	X848	Y558	F491	E428	X368	C307	L244	L181	V119
X1094	X1095	X851	T559	L492	L429	F369	R308	L245	M182	A120
X1096	X1110	X856	D560	D493	K430	D370	P309	L246	L183	A121
X1115	X1118	X906	L561	R494	V431	R371	Q310	Q247	K184	K122
X1126	X1129	X972	L562	R495	N435	L372	D311	L249	M185	Y123
X1136	X1161	X973	R563	F496	E436	S373	L312	L250	M186	M124
X1162	X1163	X974	L564	L497	Y437	V374	P313	K251	C186	S126
X1164	X1165	X977	A565	Q499	A438	F375	R314	K252	M187	L127
X1172	X1191	X978	L566	R500	P377	P376	R315	K253	S188	R128
X1191	X1202	X981	M567	I501	S378	F377	L317	K254	P189	Q129
X1222	X1251	X985	E571	M508	L439	S379	T318	A255	T191	P130
X1252	X1284	X986	A572	N509	H440	A379	T319	F256	V192	P131
X1321	X1322	X987	I573	A510	R441	H380	T318	N257	L193	L132
X1323	X1342	X994	F574	S511	A442	I381	P321	L258	E190	Y131
X1327	X1356	X995	E575	G512	V444	T382	R322	S259	E191	Q129
X1356	X1051	X996	S576	S513	D445	I384	R323	C260	E192	P130
X1052	X1052	X997	A577	L514	H446	L385	L324	L261	E193	L133
X1052	X1052	X998	H578	L515	Y447	L386	S325	L262	E194	L134
X1052	X1052	X999	K579	N516	N448	S387	I327	L264	E195	L135
X1052	X1052	X1000	Q580	L517	I449	L388	T327	T265	E196	L136
X1052	X1052	X1001	P581	L518	P450	T389	A328	T266	E197	L137
X1052	X1052	X1002	Q582	Q519	F453	R390	S330	R267	E198	L138
X1052	X1052	X1003	R583	Q520	F453	F391	I331	R268	E199	L139
X1052	X1052	X1004	X591	L521	D457	R392	R332	F269	E200	L140
X1052	X1052	X1005	X592	P523	L458	R393	R333	Q270	E201	L141
X1052	X1052	X1006	X593	Y524	I459	L394	G334	V271	E202	L142
X1052	X1052	X1007	X594	P525	P460	R395	L335	T272	E203	L143
X1052	X1052	X1008	X595	P526	P461	R396	A336	D273	E204	L144
X1052	X1052	X1009	X596	Y527	Y462	V398	T337	L275	E205	L145
X1052	X1052	X1010	X601	I528	L463	R399	R338	S276	E206	L146
X1052	X1052	X1011	X602	C529	D464	V400	N340	A277	E207	L147
X1052	X1052	X1012	X609	D530	Q465	V401	R341	A278	E208	L148
X1052	X1052	X1013	X610	N531	Y466	Y402	K342	T279	E209	L149
X1052	X1052	X1014	X626	D532	F467	R403	R343	T280	E210	L150
X1052	X1052	X1015	X629	P533	Y468	R404	V344	T281	E211	L151
X1052	X1052	X1016	X633	K534	S469	L405	N345	H282	E212	L152
X1052	X1052	X1017	X638	Y535	H470	R406	C346	D286	E213	L153
X1052	X1052	X1018	X638	E536	I471	R407	D347	H287	E214	L154
X1052	X1052	X1019	X638	R537	G472	Y408	K348	H288	E215	L155
X1052	X1052	X1020	X638	L538	H473	S409	L349	S289	E216	L156
X1052	X1052	X1021	X644	V539	R474	L410	T350	Q285	E217	L157
X1052	X1052	X1022	X645	N540	L475	V411	T351	K290	E218	L158
X1052	X1052	X1023	X646	A541	K476	B412	I352	T291	E219	L159
X1052	X1052	X1024	X647	L542	N477	V413	I353	L292	E220	L160
X1052	X1052	X1025	X648	L543	I478	Q414	E354	T293	E221	L161
X1052	X1052	X1026	X649	D544	E479	R415	S355	E296	E222	L162
X1052	X1052	X1027	X652	F545	H480	R416	L356	L231	E223	L163
X1052	X1052	X1028	X652	L546	P481	B417	L357	L232	E224	L164
X1052	X1052	X1029	X652	Y547	P482	S418	N358	K298	Q225	L165
X1052	X1052	X1030	X670	R483	T419	T419	V359	S299	Q226	L166
X1052	X1052	X1031	X671	M484	I420	S421	L360	L300	E227	L167
X1052	X1052	X1032	X671	T485	S421	E421	L361	L301	E228	L168
X1052	X1052	X1033	X671	L486	L486	L486	P362	L302	E229	L169
X1052	X1052	X1034	X671	E551	F487	P487	A363	L303	E230	L170
X1052	X1052	X1035	X671	E551	F487	P487	A363	L303	E231	L171
X1052	X1052	X1036	X671	E551	F487	P487	A363	L303	E232	L172
X1052	X1052	X1037	X671	E551	F487	P487	A363	L303	E233	L173
X1052	X1052	X1038	X671	E551	F487	P487	A363	L303	E234	L174
X1052	X1052	X1039	X671	E551	F487	P487	A363	L303	E235	L175
X1052	X1052	X1040	X671	E551	F487	P487	A363	L303	E236	L176
X1052	X1052	X1041	X671	E551	F487	P487	A363	L303	E237	L177
X1052	X1052	X1042	X671	E551	F487	P487	A363	L303	E238	L178
X1052	X1052	X1043	X671	E551	F487	P487	A363	L303	E239	L179
X1052	X1052	X1044	X671	E551	F487	P487	A363	L303	E240	L180
X1052	X1052	X1045	X671	E551	F487	P487	A363	L303	E241	L181
X1052	X1052	X1046	X671	E551	F487	P487	A363	L303	E242	L182
X1052	X1052	X1047	X671	E551	F487	P487	A363	L303	E243	L183
X1052	X1052	X1048	X671	E551	F487	P487	A363	L303	E244	L184
X1052	X1052	X1049	X671	E551	F487	P487	A363	L303	E245	L185
X1052	X1052	X1050	X671	E551	F487	P487	A363	L303	E246	L186
X1052	X1052	X1051	X671	E551	F487	P487	A363	L303	E247	L187
X1052	X1052	X1052	X671	E551	F487	P487	A363	L303	E248	L188
X1052	X1052	X1053	X671	E551	F487	P487	A363	L303	E249	L189
X1052	X1052	X1054	X671	E551	F487	P487	A363	L303	E250	L190
X1052	X1052	X1055	X671	E551	F487	P487	A363	L303	E251	L191
X1052	X1052	X1056	X671	E551	F487	P487	A363	L303	E252	L192
X1052	X1052	X1057	X671	E551	F487	P487	A363	L303	E253	L193
X1052	X1052	X1058	X671	E551	F487	P487	A363	L303	E254	L194
X1052	X1052	X1059	X671	E551	F487	P487	A363	L303	E255	L195
X1052	X1052	X1060	X671	E551	F487	P487	A363	L303	E256	L196
X1052	X1052	X1061	X671	E551	F487	P487	A363	L303	E257	L197
X1052	X1052	X1062	X671	E551	F487	P487	A363	L303	E258	L198
X1052	X1052	X1063	X671	E551	F487	P487	A363	L303	E259	L199
X1052	X1052	X1064	X671	E551	F487	P487	A363	L303	E260	L200
X1052	X1052	X1065	X671	E551	F487	P487	A363	L303	E261	L201
X1052	X1052	X1066	X671	E551	F487	P487	A363	L303	E262	L202
X1052	X1052	X1067	X671	E551	F487	P487	A363	L303	E263	L203
X1052	X1052	X1068	X671	E551	F487	P487	A363	L303	E264	L204
X1052	X1052	X1069	X671	E551	F487	P487	A363	L303	E265	L205
X1052	X1052	X1070	X671	E551	F487	P487	A363	L303	E266	L206
X1052	X1052	X1071	X671	E551	F487	P487	A363	L303	E267	L207
X1052	X1052	X1072	X671	E551	F487	P487	A363	L303	E268	L208
X1052	X1052	X1073	X671	E551	F487	P487	A363	L303	E269	L209
X1052	X1052	X1074	X671	E551	F487	P487	A363	L303	E270	L210
X1052	X1052	X1075	X671	E551	F487	P487	A363	L303	E271	L211
X1052	X1052	X1076	X671	E551	F487	P487	A363	L303	E272	L212
X1052	X1052	X1077	X671	E551	F487	P487	A363	L303	E273	L213
X1052	X1052	X1078	X671	E551	F487	P487	A363	L303	E274	L214
X1052	X1052	X1079	X671	E551	F487	P487	A363	L303	E275	L215
X1052	X1052	X1080	X671	E551	F487	P487	A363	L303	E276	L216
X1052	X1052	X1081	X671	E551	F487	P487	A363	L303	E277	L217
X1052	X1052	X1082	X671	E551	F487	P487	A363	L303	E278	L218
X1052	X1052	X1083	X671	E551	F487	P487	A363	L303	E279	L219
X1052	X1052	X1084	X671	E551	F487	P487	A363	L303	E280	L220
X1052	X1052	X1085	X671	E551	F487	P487	A363	L303	E281	L221
X1052	X1052	X1086	X671	E551	F487	P487	A363	L303	E282	L222
X1052	X1052	X1087	X671	E551	F487	P487	A363	L303	E283	L223
X1052	X1052	X1088	X671	E551	F487	P487	A363	L303	E284	L224
X1052	X1052	X1089	X671	E551	F487	P487	A363	L303	E285	L225
X1052	X1052	X1090	X671	E551	F487	P487	A363	L303	E286	L226
X1052	X1052	X1091	X671	E551	F487	P487	A363	L303	E287	L227
X1052	X1052	X1092	X671	E551	F487	P487	A363	L303	E288	L228
X1052	X1052	X1093	X671	E551	F487	P487	A363	L303	E289	L229
X1052	X1052	X1094	X671	E551	F487	P487	A363	L303	E290	L230
X1052	X1052	X1095	X671	E551	F487	P487	A363	L303	E291	L231
X1052	X1052	X1096	X671	E551	F487	P487	A363	L303	E292	L232
X1052	X1052	X1097	X671	E551	F487	P487	A363	L303	E293	L233
X1052	X1052	X1098	X671	E551	F487	P487	A363	L303	E294	L234
X1052	X1052	X1099	X671	E551	F487	P487	A363	L303	E295	L235
X1052	X1052	X1100	X671	E551	F487	P487	A363	L303	E296	L236
X1052	X1052	X1101	X671	E551	F487	P487	A363	L303	E297	L237
X1052	X1052	X1102	X671	E551	F487	P487	A363	L303	E298	L238
X1052	X1052	X1103	X671	E551	F487	P487	A363	L303	E299	L239
X1052	X1052	X1104	X671	E551	F487	P487	A363	L303	E300	L240
X1052	X1052	X1105	X671	E551	F487	P487	A363	L303	E301	L241
X1052	X1052	X1106	X671	E551	F487	P487	A363	L303	E302	

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D	Depositor
Number of images	48271	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	each CCD frame	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	160	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	50000	Depositor
Image detector	TVIPS 4kx4k CCD camera	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	1.03	7/4928 (0.1%)	1.79	71/6672 (1.1%)
1	B	1.03	7/4928 (0.1%)	1.79	71/6672 (1.1%)
1	C	1.03	7/4928 (0.1%)	1.79	71/6672 (1.1%)
1	D	1.03	7/4928 (0.1%)	1.79	71/6672 (1.1%)
1	E	1.03	7/4928 (0.1%)	1.79	71/6672 (1.1%)
1	F	1.03	7/4928 (0.1%)	1.79	71/6672 (1.1%)
1	G	1.03	7/4928 (0.1%)	1.79	71/6672 (1.1%)
1	H	1.03	7/4928 (0.1%)	1.79	71/6672 (1.1%)
1	I	1.03	7/4928 (0.1%)	1.79	71/6672 (1.1%)
1	J	1.03	7/4928 (0.1%)	1.79	71/6672 (1.1%)
1	K	1.03	7/4928 (0.1%)	1.79	71/6672 (1.1%)
1	L	1.03	7/4928 (0.1%)	1.79	71/6672 (1.1%)
1	M	1.03	7/4928 (0.1%)	1.79	71/6672 (1.1%)
1	N	1.03	7/4928 (0.1%)	1.79	71/6672 (1.1%)
1	O	1.03	7/4928 (0.1%)	1.79	71/6672 (1.1%)
1	P	1.03	7/4928 (0.1%)	1.79	71/6672 (1.1%)
All	All	1.03	112/78848 (0.1%)	1.79	1136/106752 (1.1%)

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	5
1	B	0	5
1	C	0	5
1	D	0	5
1	E	0	5
1	F	0	5
1	G	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	5
1	I	0	5
1	J	0	5
1	K	0	5
1	L	0	5
1	M	0	5
1	N	0	5
1	O	0	5
1	P	0	5
All	All	0	80

The worst 5 of 112 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	494	PHE	CB-CG	-7.98	1.37	1.51
1	D	494	PHE	CB-CG	-7.98	1.37	1.51
1	F	494	PHE	CB-CG	-7.98	1.37	1.51
1	H	494	PHE	CB-CG	-7.98	1.37	1.51
1	J	494	PHE	CB-CG	-7.98	1.37	1.51

The worst 5 of 1136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	408	TYR	CB-CG-CD1	-44.15	94.51	121.00
1	D	408	TYR	CB-CG-CD1	-44.15	94.51	121.00
1	F	408	TYR	CB-CG-CD1	-44.15	94.51	121.00
1	H	408	TYR	CB-CG-CD1	-44.15	94.51	121.00
1	J	408	TYR	CB-CG-CD1	-44.15	94.51	121.00

There are no chirality outliers.

5 of 80 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1136	UNK	Peptide
1	A	268	PHE	Mainchain
1	A	407	LYS	Peptide
1	A	408	TYR	Peptide
1	A	488	ARG	Sidechain

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	7980	0	5616	1735	0
1	B	7980	0	5616	1741	0
1	C	7980	0	5616	1746	0
1	D	7980	0	5616	1740	0
1	E	7980	0	5616	1727	0
1	F	7980	0	5616	1727	0
1	G	7980	0	5616	1737	0
1	H	7980	0	5616	1743	0
1	I	7980	0	5616	1726	0
1	J	7980	0	5616	1743	0
1	K	7980	0	5616	1738	0
1	L	7980	0	5616	1740	0
1	M	7980	0	5616	1735	0
1	N	7980	0	5616	1743	0
1	O	7980	0	5616	1739	0
1	P	7980	0	5616	1730	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	30	0	12	16	0
3	B	30	0	12	15	0
3	C	30	0	12	17	0
3	D	30	0	12	17	0
3	E	30	0	12	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	30	0	12	15	0
3	G	30	0	12	15	0
3	H	30	0	12	16	0
3	I	30	0	12	16	0
3	J	30	0	12	17	0
3	K	30	0	12	17	0
3	L	30	0	12	15	0
3	M	30	0	12	16	0
3	N	30	0	12	17	0
3	O	30	0	12	16	0
3	P	30	0	12	15	0
All	All	128176	0	90048	26556	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 122.

The worst 5 of 26556 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:M:114:TYR:CE1	1:N:280:THR:HG21	1.21	1.73
1:A:114:TYR:CE1	1:H:280:THR:HG21	1.21	1.72
1:G:280:THR:HG21	1:H:114:TYR:CE1	1.21	1.72
1:N:114:TYR:CE1	1:O:280:THR:HG21	1.21	1.71
1:O:114:TYR:CD1	1:P:280:THR:HG23	1.19	1.70

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	581/1221 (48%)	529 (91%)	36 (6%)	16 (3%)	6 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	581/1221 (48%)	529 (91%)	36 (6%)	16 (3%)	6	44
1	C	581/1221 (48%)	529 (91%)	36 (6%)	16 (3%)	6	44
1	D	581/1221 (48%)	529 (91%)	36 (6%)	16 (3%)	6	44
1	E	581/1221 (48%)	529 (91%)	36 (6%)	16 (3%)	6	44
1	F	581/1221 (48%)	529 (91%)	36 (6%)	16 (3%)	6	44
1	G	581/1221 (48%)	529 (91%)	36 (6%)	16 (3%)	6	44
1	H	581/1221 (48%)	529 (91%)	36 (6%)	16 (3%)	6	44
1	I	581/1221 (48%)	529 (91%)	36 (6%)	16 (3%)	6	44
1	J	581/1221 (48%)	529 (91%)	36 (6%)	16 (3%)	6	44
1	K	581/1221 (48%)	529 (91%)	36 (6%)	16 (3%)	6	44
1	L	581/1221 (48%)	529 (91%)	36 (6%)	16 (3%)	6	44
1	M	581/1221 (48%)	529 (91%)	36 (6%)	16 (3%)	6	44
1	N	581/1221 (48%)	529 (91%)	36 (6%)	16 (3%)	6	44
1	O	581/1221 (48%)	529 (91%)	36 (6%)	16 (3%)	6	44
1	P	581/1221 (48%)	529 (91%)	36 (6%)	16 (3%)	6	44
All	All	9296/19536 (48%)	8464 (91%)	576 (6%)	256 (3%)	10	44

5 of 256 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	41	SER
1	A	121	ALA
1	A	206	ASN
1	A	289	SER

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	551/557 (99%)	476 (86%)	75 (14%)	5	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	551/557 (99%)	476 (86%)	75 (14%)	5	27
1	C	551/557 (99%)	476 (86%)	75 (14%)	5	27
1	D	551/557 (99%)	476 (86%)	75 (14%)	5	27
1	E	551/557 (99%)	476 (86%)	75 (14%)	5	27
1	F	551/557 (99%)	476 (86%)	75 (14%)	5	27
1	G	551/557 (99%)	476 (86%)	75 (14%)	5	27
1	H	551/557 (99%)	476 (86%)	75 (14%)	5	27
1	I	551/557 (99%)	476 (86%)	75 (14%)	5	27
1	J	551/557 (99%)	476 (86%)	75 (14%)	5	27
1	K	551/557 (99%)	476 (86%)	75 (14%)	5	27
1	L	551/557 (99%)	476 (86%)	75 (14%)	5	27
1	M	551/557 (99%)	476 (86%)	75 (14%)	5	27
1	N	551/557 (99%)	476 (86%)	75 (14%)	5	27
1	O	551/557 (99%)	476 (86%)	75 (14%)	5	27
1	P	551/557 (99%)	476 (86%)	75 (14%)	5	27
All	All	8816/8912 (99%)	7616 (86%)	1200 (14%)	9	27

5 of 1200 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	120	PHE
1	I	562	LEU
1	O	494	PHE
1	H	203	ILE
1	I	79	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 365 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	216	ASN
1	I	531	ASN
1	O	474	HIS
1	H	282	HIS
1	I	124	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 for Mogul analysis.

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	DTP	A	1402	2	25,32,32	1.79	5 (20%)	26,50,50	1.57	7 (26%)
3	DTP	B	1402	2	25,32,32	1.79	5 (20%)	26,50,50	1.57	7 (26%)
3	DTP	C	1402	2	25,32,32	1.79	5 (20%)	26,50,50	1.57	7 (26%)
3	DTP	D	1402	2	25,32,32	1.79	5 (20%)	26,50,50	1.57	7 (26%)
3	DTP	E	1402	2	25,32,32	1.79	5 (20%)	26,50,50	1.57	7 (26%)
3	DTP	F	1402	2	25,32,32	1.79	5 (20%)	26,50,50	1.57	7 (26%)
3	DTP	G	1402	2	25,32,32	1.79	5 (20%)	26,50,50	1.57	7 (26%)
3	DTP	H	1402	2	25,32,32	1.79	5 (20%)	26,50,50	1.57	7 (26%)
3	DTP	I	1402	2	25,32,32	1.79	5 (20%)	26,50,50	1.57	7 (26%)
3	DTP	J	1402	2	25,32,32	1.79	5 (20%)	26,50,50	1.57	7 (26%)
3	DTP	K	1402	2	25,32,32	1.79	5 (20%)	26,50,50	1.57	7 (26%)
3	DTP	L	1402	2	25,32,32	1.79	5 (20%)	26,50,50	1.57	7 (26%)
3	DTP	M	1402	2	25,32,32	1.79	5 (20%)	26,50,50	1.57	7 (26%)
3	DTP	N	1402	2	25,32,32	1.79	5 (20%)	26,50,50	1.57	7 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DTP	O	1402	2	25,32,32	1.79	5 (20%)	26,50,50	1.57	7 (26%)
3	DTP	P	1402	2	25,32,32	1.79	5 (20%)	26,50,50	1.57	7 (26%)

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	DTP	A	1402	2	-	0/18/34/34	0/3/3/3
3	DTP	B	1402	2	-	0/18/34/34	0/3/3/3
3	DTP	C	1402	2	-	0/18/34/34	0/3/3/3
3	DTP	D	1402	2	-	0/18/34/34	0/3/3/3
3	DTP	E	1402	2	-	0/18/34/34	0/3/3/3
3	DTP	F	1402	2	-	0/18/34/34	0/3/3/3
3	DTP	G	1402	2	-	0/18/34/34	0/3/3/3
3	DTP	H	1402	2	-	0/18/34/34	0/3/3/3
3	DTP	I	1402	2	-	0/18/34/34	0/3/3/3
3	DTP	J	1402	2	-	0/18/34/34	0/3/3/3
3	DTP	K	1402	2	-	0/18/34/34	0/3/3/3
3	DTP	L	1402	2	-	0/18/34/34	0/3/3/3
3	DTP	M	1402	2	-	0/18/34/34	0/3/3/3
3	DTP	N	1402	2	-	0/18/34/34	0/3/3/3
3	DTP	O	1402	2	-	0/18/34/34	0/3/3/3
3	DTP	P	1402	2	-	0/18/34/34	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1402	DTP	C2-N1	2.01	1.37	1.33
3	D	1402	DTP	C2-N1	2.01	1.37	1.33
3	B	1402	DTP	C2-N1	2.01	1.37	1.33
3	F	1402	DTP	C2-N1	2.01	1.37	1.33
3	N	1402	DTP	C2-N1	2.01	1.37	1.33

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1402	DTP	C2'-C3'-C4'	-3.04	96.60	102.77
3	K	1402	DTP	C2'-C3'-C4'	-3.04	96.60	102.77
3	E	1402	DTP	C2'-C3'-C4'	-3.04	96.60	102.77
3	A	1402	DTP	C2'-C3'-C4'	-3.04	96.60	102.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	1402	DTP	C2'-C3'-C4'	-3.04	96.60	102.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 256 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1402	DTP	16	0
3	B	1402	DTP	15	0
3	C	1402	DTP	17	0
3	D	1402	DTP	17	0
3	E	1402	DTP	16	0
3	F	1402	DTP	15	0
3	G	1402	DTP	15	0
3	H	1402	DTP	16	0
3	I	1402	DTP	16	0
3	J	1402	DTP	17	0
3	K	1402	DTP	17	0
3	L	1402	DTP	15	0
3	M	1402	DTP	16	0
3	N	1402	DTP	17	0
3	O	1402	DTP	16	0
3	P	1402	DTP	15	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	P	9
1	G	9
1	J	9
1	D	9
1	K	9

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Mol	Chain	Number of breaks
1	E	9
1	H	9
1	B	9
1	I	9
1	C	9
1	A	9
1	N	9
1	O	9
1	L	9
1	F	9
1	M	9

The worst 5 of 144 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	583:ARG	C	587:UNK	N	29.89
1	B	583:ARG	C	587:UNK	N	29.89
1	C	583:ARG	C	587:UNK	N	29.89
1	D	583:ARG	C	587:UNK	N	29.89
1	E	583:ARG	C	587:UNK	N	29.89