



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 10, 2017 – 12:35 PM EST

PDB ID : 3JBT
EMDB ID: : EMD-6480
Title : Atomic structure of the Apaf-1 apoptosome
Authors : Zhou, M.; Li, Y.; Hu, Q.; Bai, X.; Huang, W.; Yan, C.; Scheres, S.H.W.; Shi, Y.
Deposited on : 2015-10-15
Resolution : 3.80 Å(reported)
Based on PDB ID : 3J2T, 4RSZ

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.

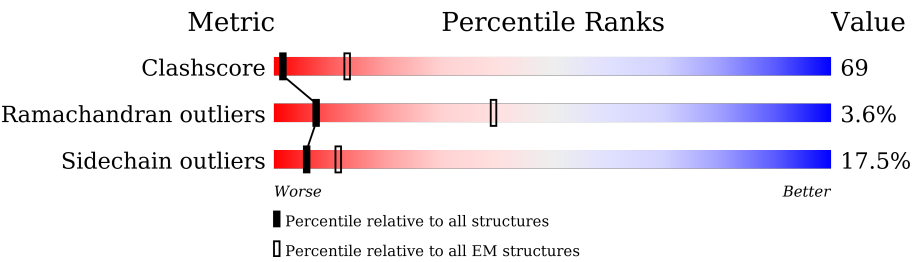
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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








Metric	Whole archive (#Entries)	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	1260	<div><div>32%</div><div>45%</div><div>13%</div><div>•</div><div>9%</div></div>
1	C	1260	<div><div>31%</div><div>45%</div><div>13%</div><div>•</div><div>9%</div></div>
1	E	1260	<div><div>32%</div><div>45%</div><div>13%</div><div>•</div><div>9%</div></div>
1	G	1260	<div><div>32%</div><div>45%</div><div>13%</div><div>•</div><div>9%</div></div>
1	I	1260	<div><div>32%</div><div>45%</div><div>13%</div><div>•</div><div>9%</div></div>
1	K	1260	<div><div>32%</div><div>45%</div><div>13%</div><div>•</div><div>9%</div></div>
1	M	1260	<div><div>32%</div><div>45%</div><div>13%</div><div>•</div><div>9%</div></div>
2	B	105	<div><div>82%</div><div>15%</div><div>••</div></div>
2	D	105	<div><div>82%</div><div>15%</div><div>••</div></div>

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Mol	Chain	Length	Quality of chain
2	F	105	 82%15%..
2	H	105	 82%15%..
2	J	105	 83%14%..
2	L	105	 82%15%..
2	N	105	 82%16%..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 70252 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 Apoptotic protease-activating factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	C	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	E	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	G	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	I	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	K	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	M	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1249	LEU	-	EXPRESSION TAG	UNP O14727
A	1250	GLU	-	EXPRESSION TAG	UNP O14727
A	1251	HIS	-	EXPRESSION TAG	UNP O14727
A	1252	HIS	-	EXPRESSION TAG	UNP O14727
A	1253	HIS	-	EXPRESSION TAG	UNP O14727
A	1254	HIS	-	EXPRESSION TAG	UNP O14727
A	1255	HIS	-	EXPRESSION TAG	UNP O14727
A	1256	HIS	-	EXPRESSION TAG	UNP O14727
A	1257	HIS	-	EXPRESSION TAG	UNP O14727
A	1258	HIS	-	EXPRESSION TAG	UNP O14727
A	1259	HIS	-	EXPRESSION TAG	UNP O14727
A	1260	HIS	-	EXPRESSION TAG	UNP O14727
C	1249	LEU	-	EXPRESSION TAG	UNP O14727
C	1250	GLU	-	EXPRESSION TAG	UNP O14727
C	1251	HIS	-	EXPRESSION TAG	UNP O14727
C	1252	HIS	-	EXPRESSION TAG	UNP O14727

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1253	HIS	-	EXPRESSION TAG	UNP O14727
C	1254	HIS	-	EXPRESSION TAG	UNP O14727
C	1255	HIS	-	EXPRESSION TAG	UNP O14727
C	1256	HIS	-	EXPRESSION TAG	UNP O14727
C	1257	HIS	-	EXPRESSION TAG	UNP O14727
C	1258	HIS	-	EXPRESSION TAG	UNP O14727
C	1259	HIS	-	EXPRESSION TAG	UNP O14727
C	1260	HIS	-	EXPRESSION TAG	UNP O14727
E	1249	LEU	-	EXPRESSION TAG	UNP O14727
E	1250	GLU	-	EXPRESSION TAG	UNP O14727
E	1251	HIS	-	EXPRESSION TAG	UNP O14727
E	1252	HIS	-	EXPRESSION TAG	UNP O14727
E	1253	HIS	-	EXPRESSION TAG	UNP O14727
E	1254	HIS	-	EXPRESSION TAG	UNP O14727
E	1255	HIS	-	EXPRESSION TAG	UNP O14727
E	1256	HIS	-	EXPRESSION TAG	UNP O14727
E	1257	HIS	-	EXPRESSION TAG	UNP O14727
E	1258	HIS	-	EXPRESSION TAG	UNP O14727
E	1259	HIS	-	EXPRESSION TAG	UNP O14727
E	1260	HIS	-	EXPRESSION TAG	UNP O14727
G	1249	LEU	-	EXPRESSION TAG	UNP O14727
G	1250	GLU	-	EXPRESSION TAG	UNP O14727
G	1251	HIS	-	EXPRESSION TAG	UNP O14727
G	1252	HIS	-	EXPRESSION TAG	UNP O14727
G	1253	HIS	-	EXPRESSION TAG	UNP O14727
G	1254	HIS	-	EXPRESSION TAG	UNP O14727
G	1255	HIS	-	EXPRESSION TAG	UNP O14727
G	1256	HIS	-	EXPRESSION TAG	UNP O14727
G	1257	HIS	-	EXPRESSION TAG	UNP O14727
G	1258	HIS	-	EXPRESSION TAG	UNP O14727
G	1259	HIS	-	EXPRESSION TAG	UNP O14727
G	1260	HIS	-	EXPRESSION TAG	UNP O14727
I	1249	LEU	-	EXPRESSION TAG	UNP O14727
I	1250	GLU	-	EXPRESSION TAG	UNP O14727
I	1251	HIS	-	EXPRESSION TAG	UNP O14727
I	1252	HIS	-	EXPRESSION TAG	UNP O14727
I	1253	HIS	-	EXPRESSION TAG	UNP O14727
I	1254	HIS	-	EXPRESSION TAG	UNP O14727
I	1255	HIS	-	EXPRESSION TAG	UNP O14727
I	1256	HIS	-	EXPRESSION TAG	UNP O14727
I	1257	HIS	-	EXPRESSION TAG	UNP O14727
I	1258	HIS	-	EXPRESSION TAG	UNP O14727

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Chain	Residue	Modelled	Actual	Comment	Reference
I	1259	HIS	-	EXPRESSION TAG	UNP O14727
I	1260	HIS	-	EXPRESSION TAG	UNP O14727
K	1249	LEU	-	EXPRESSION TAG	UNP O14727
K	1250	GLU	-	EXPRESSION TAG	UNP O14727
K	1251	HIS	-	EXPRESSION TAG	UNP O14727
K	1252	HIS	-	EXPRESSION TAG	UNP O14727
K	1253	HIS	-	EXPRESSION TAG	UNP O14727
K	1254	HIS	-	EXPRESSION TAG	UNP O14727
K	1255	HIS	-	EXPRESSION TAG	UNP O14727
K	1256	HIS	-	EXPRESSION TAG	UNP O14727
K	1257	HIS	-	EXPRESSION TAG	UNP O14727
K	1258	HIS	-	EXPRESSION TAG	UNP O14727
K	1259	HIS	-	EXPRESSION TAG	UNP O14727
K	1260	HIS	-	EXPRESSION TAG	UNP O14727
M	1249	LEU	-	EXPRESSION TAG	UNP O14727
M	1250	GLU	-	EXPRESSION TAG	UNP O14727
M	1251	HIS	-	EXPRESSION TAG	UNP O14727
M	1252	HIS	-	EXPRESSION TAG	UNP O14727
M	1253	HIS	-	EXPRESSION TAG	UNP O14727
M	1254	HIS	-	EXPRESSION TAG	UNP O14727
M	1255	HIS	-	EXPRESSION TAG	UNP O14727
M	1256	HIS	-	EXPRESSION TAG	UNP O14727
M	1257	HIS	-	EXPRESSION TAG	UNP O14727
M	1258	HIS	-	EXPRESSION TAG	UNP O14727
M	1259	HIS	-	EXPRESSION TAG	UNP O14727
M	1260	HIS	-	EXPRESSION TAG	UNP O14727

- Molecule 2 is a protein called Cytochrome c.

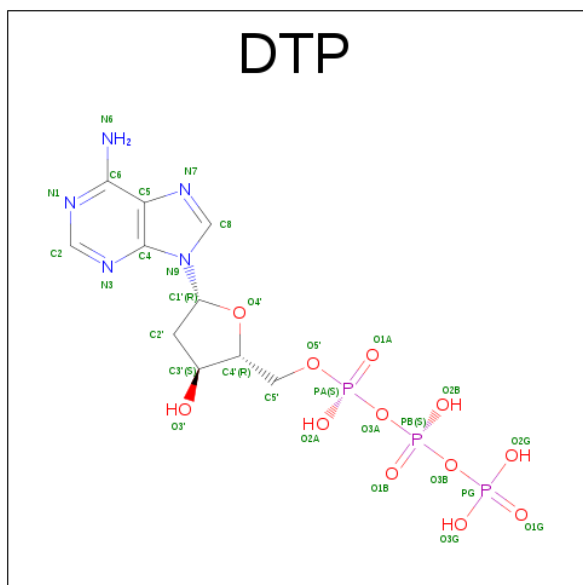
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	104	Total 823	C 524	N 144	O 151	S 4	0	0
2	D	104	Total 823	C 524	N 144	O 151	S 4	0	0
2	F	104	Total 823	C 524	N 144	O 151	S 4	0	0
2	H	104	Total 823	C 524	N 144	O 151	S 4	0	0
2	J	104	Total 823	C 524	N 144	O 151	S 4	0	0
2	L	104	Total 823	C 524	N 144	O 151	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	104	Total	C	N	O	S	0	0
			823	524	144	151	4		

- Molecule 3 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
3	A	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	E	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	I	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	M	1	Total	C	N	O	P	0
			30	10	5	12	3	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

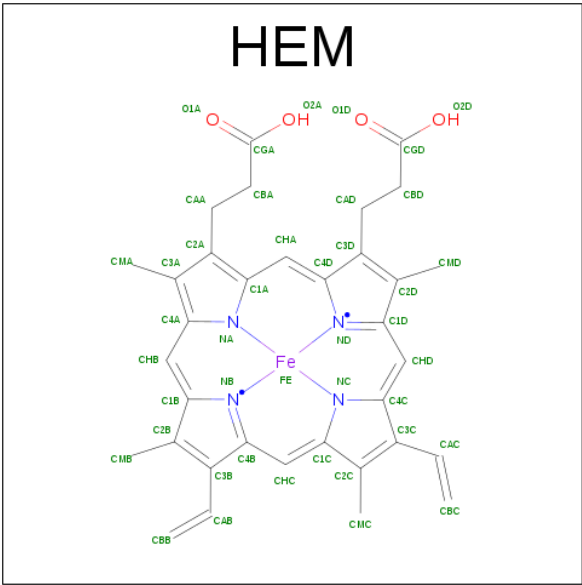
Mol	Chain	Residues	Atoms		AltConf
4	G	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
4	K	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	
4	I	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	A	1	Total	Mg	0
			1	1	
4	M	1	Total	Mg	0
			1	1	

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	H	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	J	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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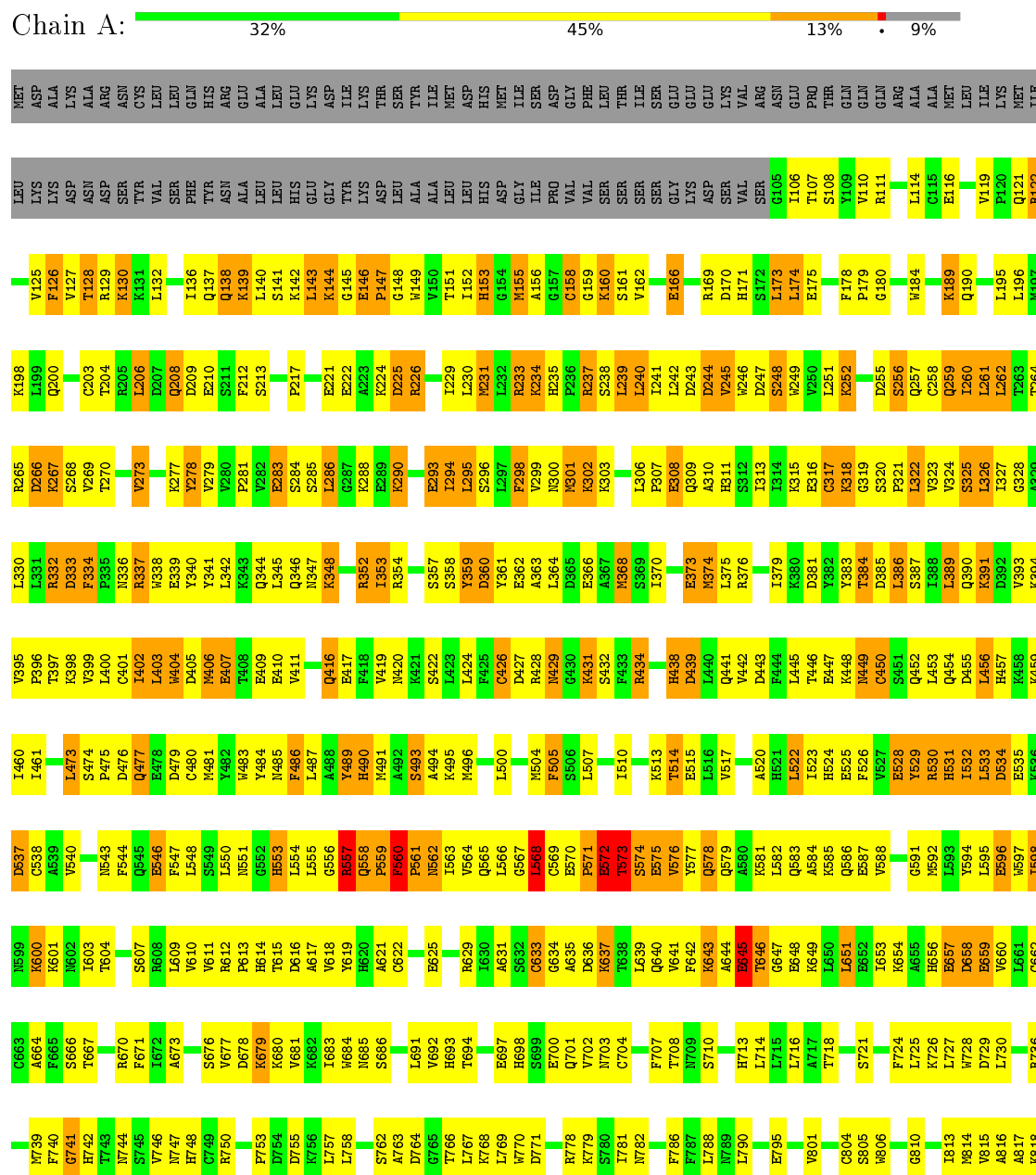
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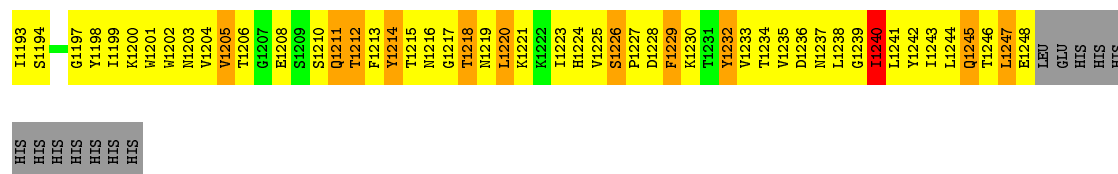
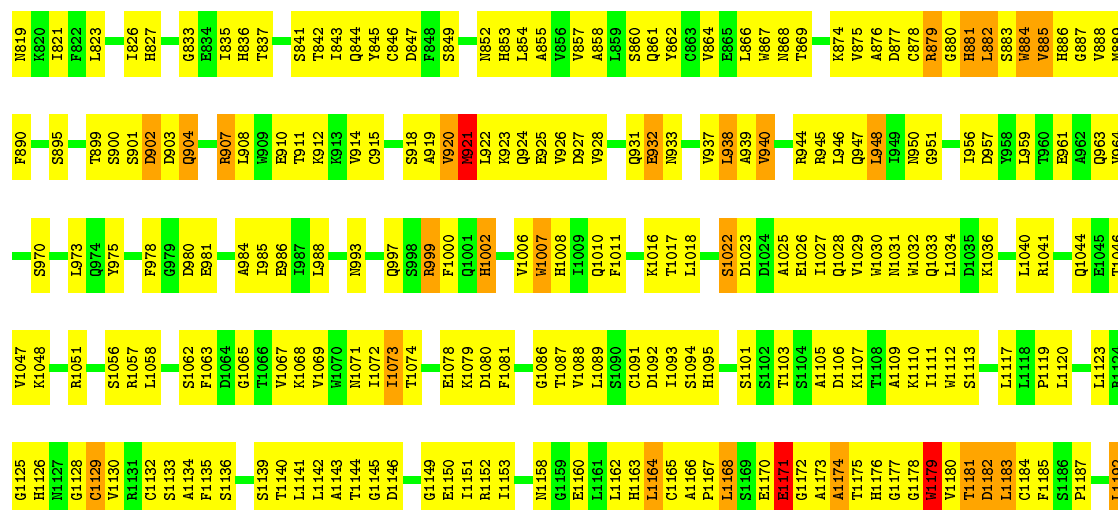
Mol	Chain	Residues	Atoms					AltConf
5	L	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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.

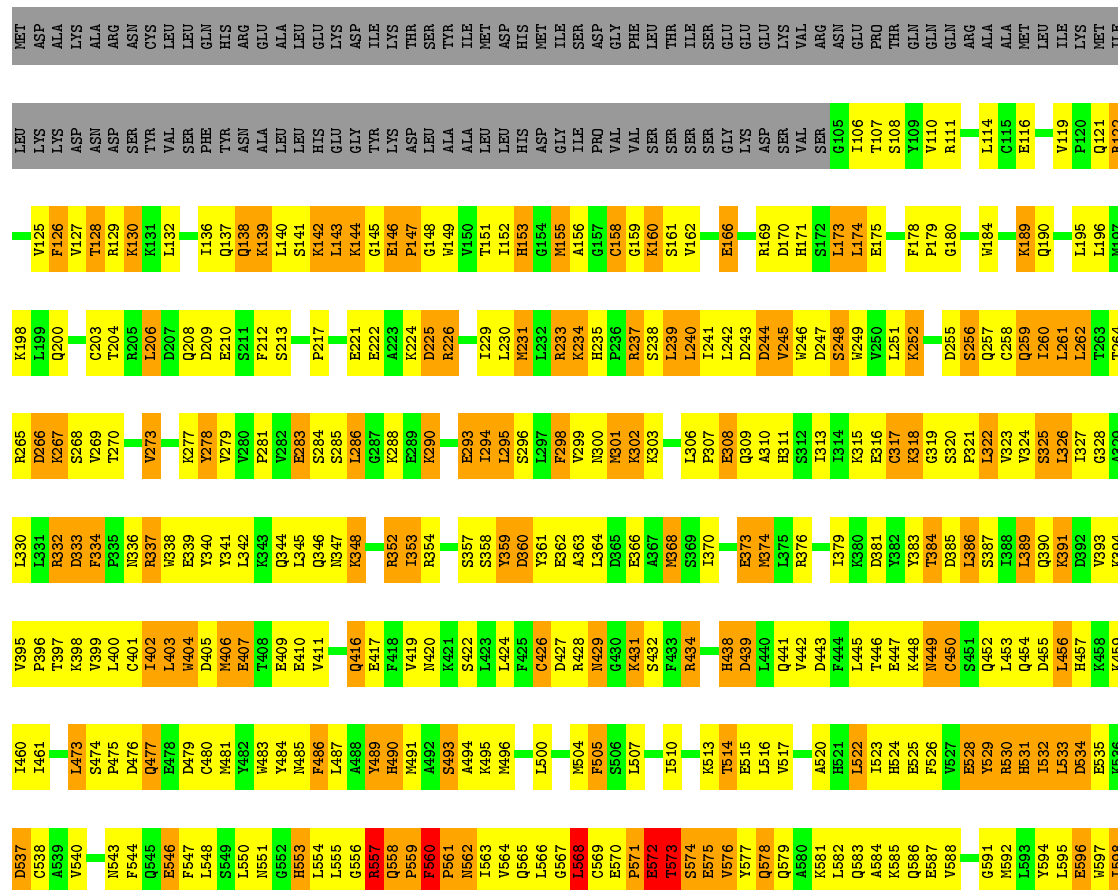
- Molecule 1: Apoptotic protease-activating factor 1

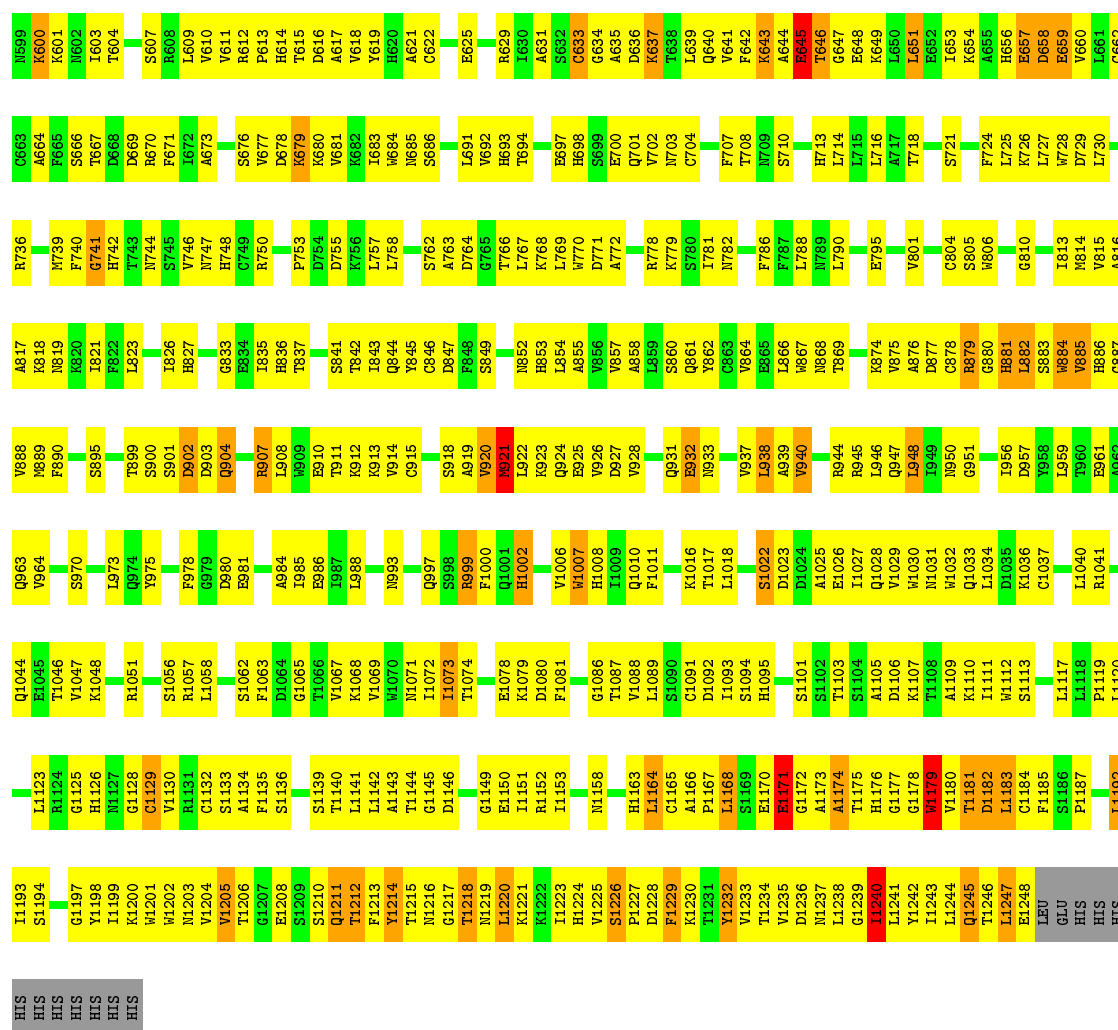




- Molecule 1: Apoptotic protease-activating factor 1

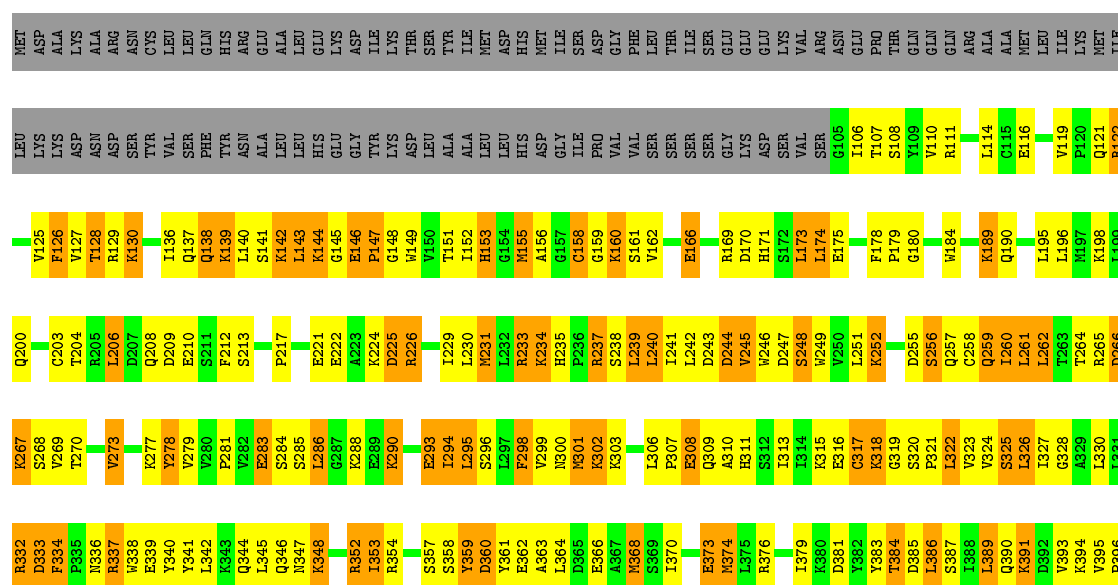
Chain C: 31% 45% 13% 9%

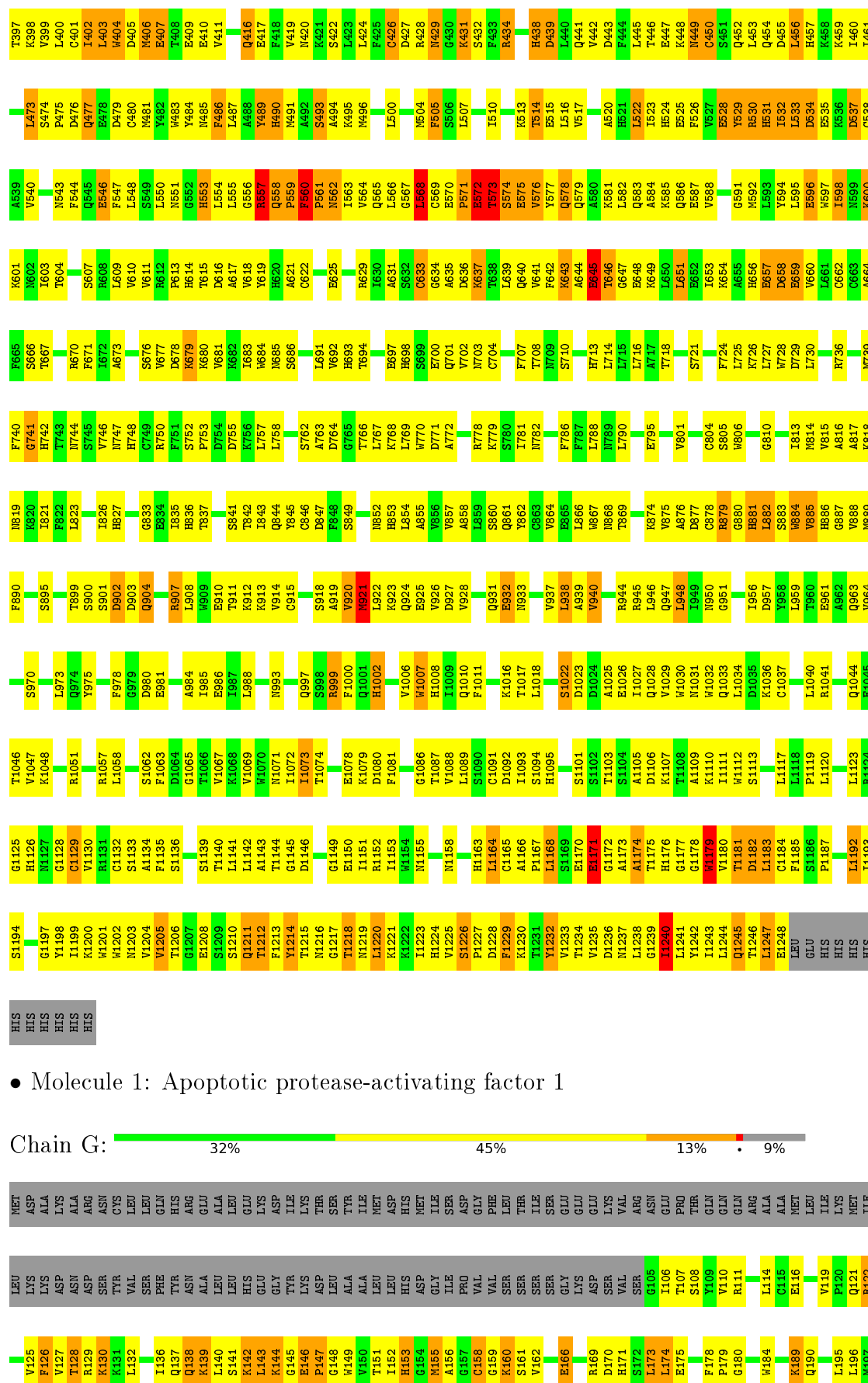




• Molecule 1: Apoptotic protease-activating factor 1

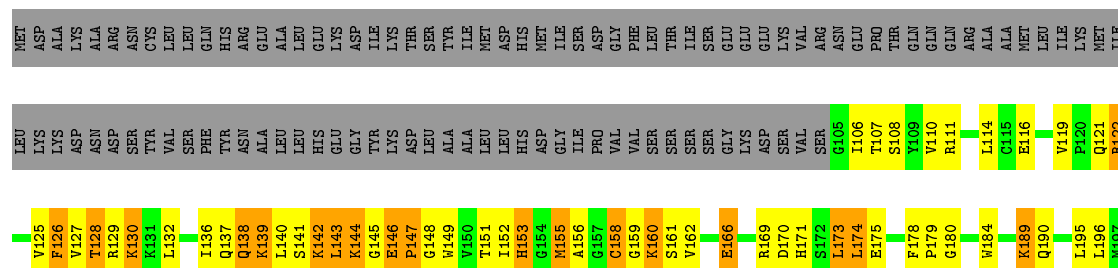
Chain E: 32% 45% 13% 9%





- Molecule 1: Apoptotic protease-activating factor 1

Chain G: 32% 45% 13% • 9%



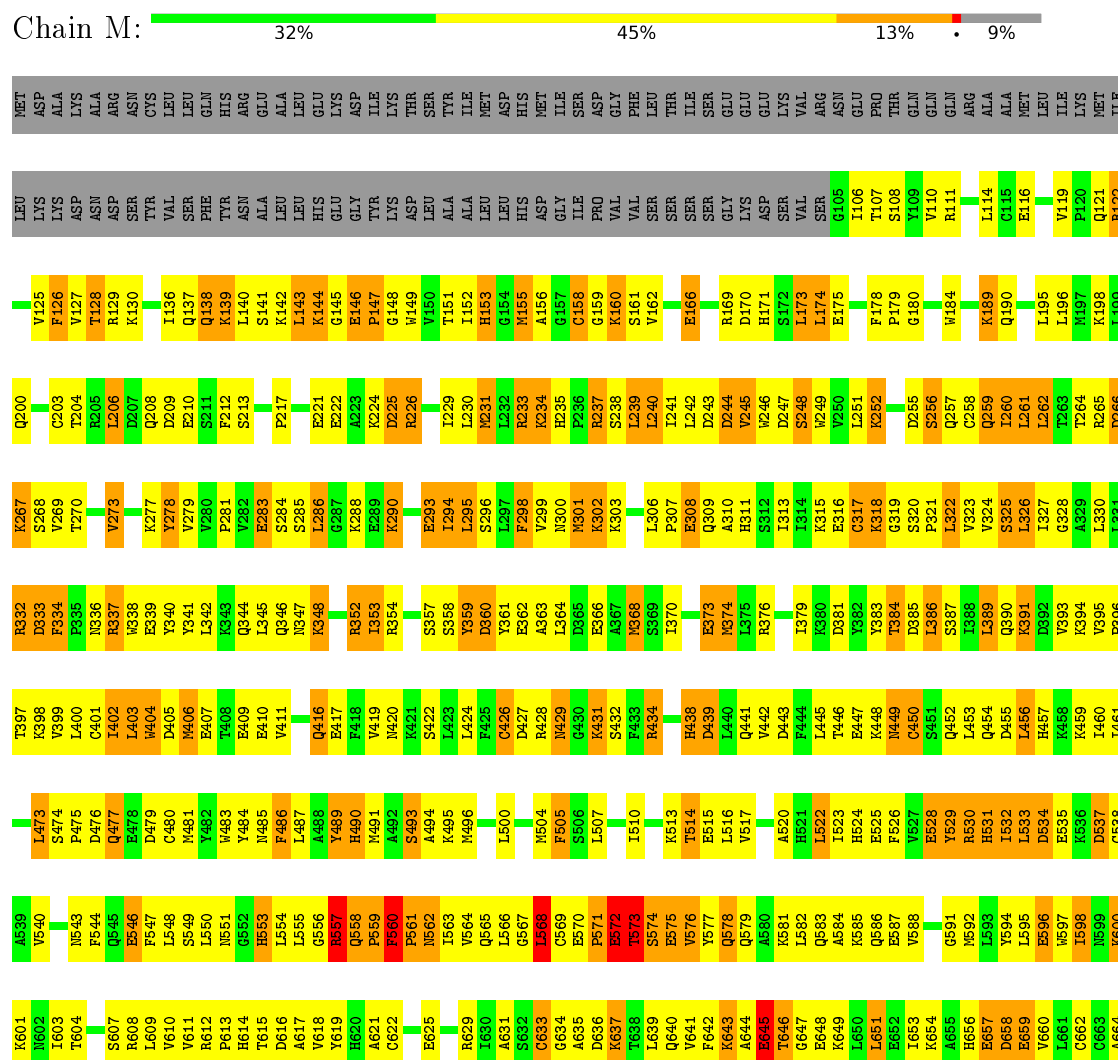
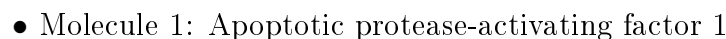
HIS	L1182	L1123	E1045	Q963	V888	A817	A664	R600	C538	L460	V395	L330	R265	K198
HIS	L1193	R1124	T1046	V964	M889	K818	F685	R601	A539	L461	P396	L331	D266	L199
HIS	S1194	G1125	K1048	S970	F890	M819	S666	R602	V540	R332	T397	R332	R267	Q200
HIS		N1127			S895	R820	D668	T604	N543	L473	L400	F334	S268	C203
HIS	G1197	G1128	R1051	L973	T899	F822	D669	S607	F544	D476	L401	P335	V269	T204
HIS	Y1198	G1129	S1056	Q974	S900	L823	R670	R608	Q545	Q477	L402	R336	V273	R205
HIS	K1200	R1130	R1057	Y975	S901	T826	F671	L609	E546	D478	L403	R337		L206
HIS	W1202	C1132	L1058	F978	D902	R827	L672	V610	F547	D479	W404	F338	K277	Q208
HIS	N1203	S1133	S1062	G979	D903	H827	A673	V611	L548	C480	Y405	F340	Y278	D209
HIS	A1134	F1135	F1063	D980	Q904	G833	S676	R612	L550	Y483	M406	F341	V279	E210
HIS	F1135	S1136	D1064	E981	R907	R835	R677	R613	G552	Y484	E408	L342	V280	S211
							D678	R614	R553	Q478	E409	K343	P281	F212
							F679	T615	R553	Q479	E410	Q344	V282	F213
							K680	R616	R553	Q480	E411	L345	E283	
							F681	A621	R553	L487	Q346	Q347	S284	
							G682	V618	G556	L488	N347	L347	S285	
							F683	V619	R557	Y489	Q416	K348	L286	E221
							R684	R620	Q558	H490	E417	R352	G287	A222
							S686	C622	P559	A492	V419	R353	E289	K224
									P561	S493	N420	R354	K290	D225
									R562	A494	K421		L286	R226
							L691	E625	L563	K495	S422	S357	E293	
							R692	R629	V564	N496	L453	S358	L294	T229
							T694	R630	Q565	L500	L424	F359	L295	L230
							F695	A631	L566	F425	R426	P361	S296	W231
							R697	S632	G567	N504	D427	F362	L297	L232
							R698	G633	L568	F505	R428	A363	V299	R233
							S699	G634	C569	F506	M429	L364	R304	K234
							E700	A635	E570	S506	G430	D365	N301	H235
							Q701	D636	E571	L507	K432	E366	F236	F237
							W702	R637	E572	S431	R432	A367	S238	R237
							T703	T638	E573	L510	F433	K368	K303	E239
							C704	L639	S574	K513	R434	S369	L306	L240
							R707	Q640	E575	T514	H438	L370	P307	T241
							T708	V641	V576	T515	L445	E373	E308	L242
							S709	F642	Y577	L516	D439	K374	Q309	D243
							S710	R643	Q578	V517	L443	L375	A310	D244
							H713	A644	A580	A520	Q441	R376	H311	V245
							L714	T646	L581	H521	D443	E312	S312	D247
							L715	Q647	L582	L522	F444	I379	I313	D248
							A716	R649	Q583	L523	L445	K380	I314	S246
							T717	L650	A584	H524	T446	D381	K315	W249
							T718	L651	Q586	E525	E447	F382	E316	V250
							S721	R652	E587	F526	K448	Y383	C317	L251
								L653	V588	V527	M449	F384	K318	K252
							F724	R654	G591	E528	C450	D385	G319	D255
							L725	A655	M592	V529	S451	L386	S321	S256
							K726	R657	M592	H530	Q452	L322	P321	Q257
							L727	E587	L593	H531	L453	F323	V323	C258
							R728	D658	Y594	F532	Q454	F389	V324	Q259
							D729	R659	L595	L533	D455	Q390	S325	T260
							L730	V660	E596	D534	L456	K391	L326	L261
								L661	M597	E535	H457	D392	I327	L262
								C662	V597	E536	K458	F393	G328	T263
							R736	C663	M599	D537	K459	K394	A329	T264

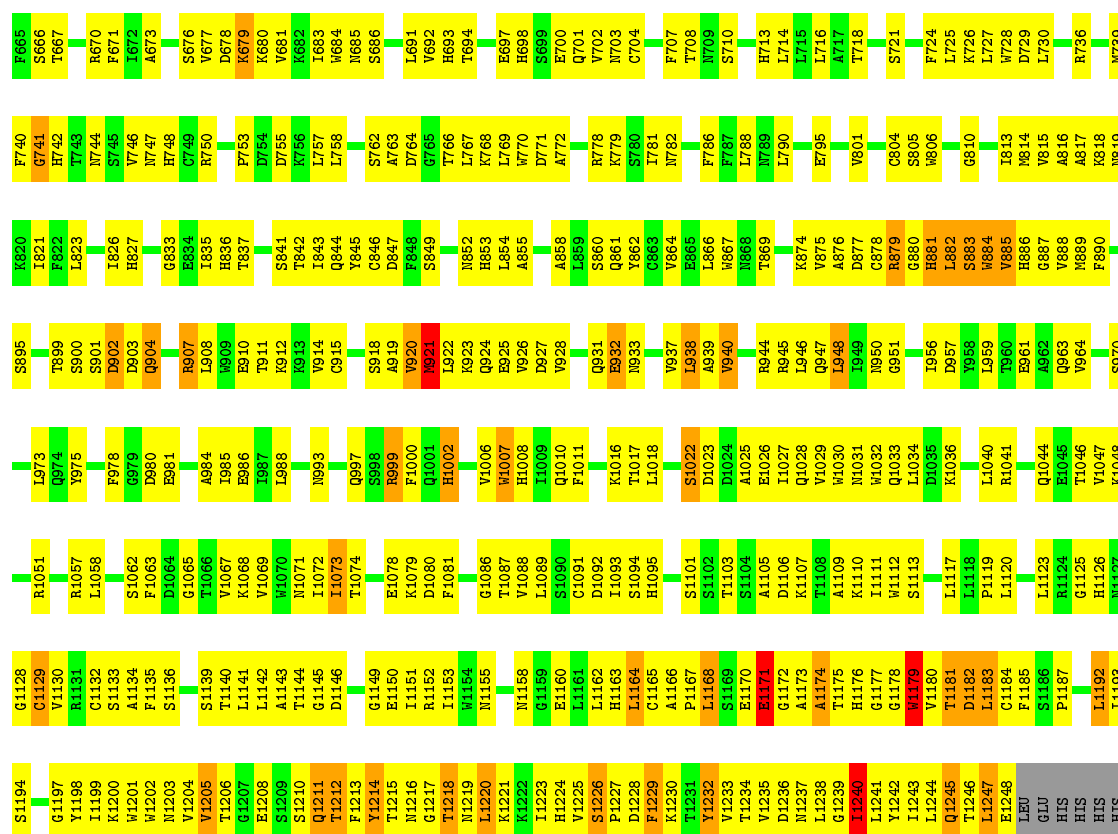
• Molecule 1: Apoptotic protease-activating factor 1

Frequency	Percentage
Daily	32%
Often	45%
Sometimes	13%
Rarely	9%
Never	1%



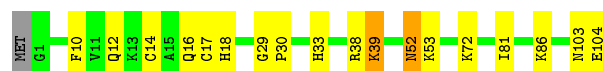






- Molecule 2: Cytochrome c

Chain B: 82% 15% ..



- Molecule 2: Cytochrome c

Chain D: 82% 15% ..




- Molecule 2: Cytochrome c

Chain F: 82% 15% ..




- Molecule 2: Cytochrome c

Chain H:  82% 15% ..




- Molecule 2: Cytochrome c

Chain J:  83% 14% ..




- Molecule 2: Cytochrome c

Chain L:  82% 15% ..



- Molecule 2: Cytochrome c

Chain N:  82% 16% ..



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	134919	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 (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: HEM, 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	0.30	0/9337	0.51	2/12636 (0.0%)
1	C	0.30	0/9337	0.51	2/12636 (0.0%)
1	E	0.30	0/9337	0.51	2/12636 (0.0%)
1	G	0.30	0/9337	0.51	2/12636 (0.0%)
1	I	0.30	0/9337	0.51	2/12636 (0.0%)
1	K	0.30	0/9337	0.51	2/12636 (0.0%)
1	M	0.30	0/9337	0.51	2/12636 (0.0%)
2	B	0.65	0/839	0.73	0/1118
2	D	0.65	0/839	0.73	0/1118
2	F	0.65	0/839	0.73	0/1118
2	H	0.65	0/839	0.73	0/1118
2	J	0.65	0/839	0.73	0/1118
2	L	0.65	0/839	0.73	0/1118
2	N	0.65	0/839	0.73	0/1118
All	All	0.34	0/71232	0.53	14/96278 (0.0%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	880	GLY	N-CA-C	5.73	127.43	113.10
1	I	880	GLY	N-CA-C	5.73	127.43	113.10
1	K	880	GLY	N-CA-C	5.73	127.43	113.10
1	M	880	GLY	N-CA-C	5.73	127.42	113.10
1	E	880	GLY	N-CA-C	5.72	127.41	113.10

There are no chirality outliers.

There are no planarity outliers.

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	9139	0	9005	1372	0
1	C	9139	0	9005	1371	0
1	E	9139	0	9005	1360	0
1	G	9139	0	9005	1382	0
1	I	9139	0	9005	1358	0
1	K	9139	0	9005	1357	0
1	M	9139	0	9005	1366	0
2	B	823	0	849	31	0
2	D	823	0	849	33	0
2	F	823	0	849	30	0
2	H	823	0	849	34	0
2	J	823	0	849	32	0
2	L	823	0	849	33	0
2	N	823	0	849	31	0
3	A	30	0	12	6	0
3	C	30	0	12	6	0
3	E	30	0	12	6	0
3	G	30	0	12	6	0
3	I	30	0	12	7	0
3	K	30	0	12	6	0
3	M	30	0	12	6	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
5	B	43	0	30	15	0
5	D	43	0	30	16	0
5	F	43	0	30	14	0
5	H	43	0	30	16	0
5	J	43	0	30	15	0
5	L	43	0	30	15	0
5	N	43	0	30	13	0
All	All	70252	0	69272	9596	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 69.

The worst 5 of 9596 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:E:544:PHE:CE1	1:E:576:VAL:HG13	1.28	1.68
1:G:544:PHE:CE1	1:G:576:VAL:HG13	1.28	1.67
1:C:544:PHE:CE1	1:C:576:VAL:HG13	1.28	1.65
1:C:862:TYR:CD1	1:C:885:VAL:HG12	1.26	1.64
1:A:544:PHE:CE1	1:A:576:VAL:HG13	1.28	1.64

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	1142/1260 (91%)	999 (88%)	98 (9%)	45 (4%)	4	38
1	C	1142/1260 (91%)	999 (88%)	98 (9%)	45 (4%)	4	38
1	E	1142/1260 (91%)	999 (88%)	98 (9%)	45 (4%)	4	38
1	G	1142/1260 (91%)	999 (88%)	98 (9%)	45 (4%)	4	38
1	I	1142/1260 (91%)	999 (88%)	98 (9%)	45 (4%)	4	38
1	K	1142/1260 (91%)	999 (88%)	97 (8%)	46 (4%)	4	38
1	M	1142/1260 (91%)	999 (88%)	97 (8%)	46 (4%)	4	38
2	B	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
2	D	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
2	F	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
2	H	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
2	J	102/105 (97%)	100 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
2	N	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
All	All	8708/9555 (91%)	7693 (88%)	698 (8%)	317 (4%)	7	41

5 of 317 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	PRO
1	A	557	ARG
1	A	560	PHE
1	A	562	ASN
1	A	645	GLU

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	1027/1131 (91%)	838 (82%)	189 (18%)	2	15
1	C	1027/1131 (91%)	838 (82%)	189 (18%)	2	15
1	E	1027/1131 (91%)	838 (82%)	189 (18%)	2	15
1	G	1027/1131 (91%)	838 (82%)	189 (18%)	2	15
1	I	1027/1131 (91%)	838 (82%)	189 (18%)	2	15
1	K	1027/1131 (91%)	838 (82%)	189 (18%)	2	15
1	M	1027/1131 (91%)	838 (82%)	189 (18%)	2	15
2	B	86/87 (99%)	80 (93%)	6 (7%)	19	60
2	D	86/87 (99%)	80 (93%)	6 (7%)	19	60
2	F	86/87 (99%)	80 (93%)	6 (7%)	19	60
2	H	86/87 (99%)	80 (93%)	6 (7%)	19	60
2	J	86/87 (99%)	81 (94%)	5 (6%)	25	66
2	L	86/87 (99%)	80 (93%)	6 (7%)	19	60
2	N	86/87 (99%)	80 (93%)	6 (7%)	19	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7791/8526 (91%)	6427 (82%)	1364 (18%)	6 17

5 of 1364 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	243	ASP
1	G	1192	LEU
1	M	405	ASP
1	G	290	LYS
1	G	473	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 208 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	259	GLN
1	G	1245	GLN
1	M	490	HIS
1	G	416	GLN
1	G	583	GLN

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](#)

Of 21 ligands modelled in this entry, 7 are monoatomic - leaving 14 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	1301	4	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
5	HEM	B	201	2	24,50,50	0.86	1 (4%)	16,82,82	1.64	2 (12%)
3	DTP	C	1301	4	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
5	HEM	D	201	2	24,50,50	0.85	1 (4%)	16,82,82	1.64	2 (12%)
3	DTP	E	1301	4	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
5	HEM	F	201	2	24,50,50	0.86	1 (4%)	16,82,82	1.64	2 (12%)
3	DTP	G	1301	4	25,32,32	0.93	1 (4%)	26,50,50	1.68	1 (3%)
5	HEM	H	201	2	24,50,50	0.86	1 (4%)	16,82,82	1.65	2 (12%)
3	DTP	I	1301	4	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
5	HEM	J	201	2	24,50,50	0.86	1 (4%)	16,82,82	1.65	2 (12%)
3	DTP	K	1301	4	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
5	HEM	L	201	2	24,50,50	0.85	1 (4%)	16,82,82	1.65	2 (12%)
3	DTP	M	1301	4	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
5	HEM	N	201	2	24,50,50	0.84	1 (4%)	16,82,82	1.65	2 (12%)

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	1301	4	-	0/18/34/34	0/3/3/3
5	HEM	B	201	2	-	0/6/54/54	0/0/8/8
3	DTP	C	1301	4	-	0/18/34/34	0/3/3/3
5	HEM	D	201	2	-	0/6/54/54	0/0/8/8
3	DTP	E	1301	4	-	0/18/34/34	0/3/3/3
5	HEM	F	201	2	-	0/6/54/54	0/0/8/8
3	DTP	G	1301	4	-	0/18/34/34	0/3/3/3
5	HEM	H	201	2	-	0/6/54/54	0/0/8/8
3	DTP	I	1301	4	-	0/18/34/34	0/3/3/3
5	HEM	J	201	2	-	0/6/54/54	0/0/8/8
3	DTP	K	1301	4	-	0/18/34/34	0/3/3/3
5	HEM	L	201	2	-	0/6/54/54	0/0/8/8
3	DTP	M	1301	4	-	0/18/34/34	0/3/3/3
5	HEM	N	201	2	-	0/6/54/54	0/0/8/8

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	201	HEM	C3B-C2B	-2.82	1.36	1.40
5	J	201	HEM	C3B-C2B	-2.79	1.36	1.40
5	D	201	HEM	C3B-C2B	-2.79	1.36	1.40
5	H	201	HEM	C3B-C2B	-2.77	1.36	1.40
5	F	201	HEM	C3B-C2B	-2.76	1.36	1.40

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1301	DTP	N3-C2-N1	-6.59	123.70	128.87
3	A	1301	DTP	N3-C2-N1	-6.58	123.71	128.87
3	G	1301	DTP	N3-C2-N1	-6.57	123.71	128.87
3	E	1301	DTP	N3-C2-N1	-6.56	123.72	128.87
3	M	1301	DTP	N3-C2-N1	-6.56	123.72	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 147 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1301	DTP	6	0
5	B	201	HEM	15	0
3	C	1301	DTP	6	0
5	D	201	HEM	16	0
3	E	1301	DTP	6	0
5	F	201	HEM	14	0
3	G	1301	DTP	6	0
5	H	201	HEM	16	0
3	I	1301	DTP	7	0
5	J	201	HEM	15	0
3	K	1301	DTP	6	0
5	L	201	HEM	15	0
3	M	1301	DTP	6	0
5	N	201	HEM	13	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.