



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 21, 2017 – 11:32 PM EST

PDB ID : 5WVE
EMDB ID: : EMD-6690
Title : Apaf-1-Caspase-9 holoenzyme
Authors : Li, Y.; Zhou, M.; Hu, Q.; Shi, Y.
Deposited on : 2016-12-24
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.

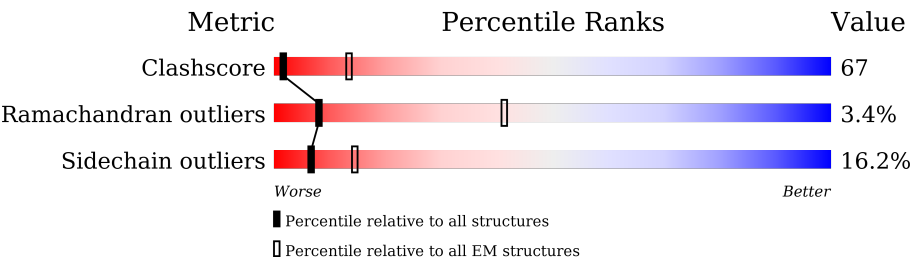
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

1 Overall quality at a glance i

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	1248	<div><div>32%</div><div>46%</div><div>13%</div><div>•</div><div>8%</div></div>
1	C	1248	<div><div>32%</div><div>46%</div><div>13%</div><div>•</div><div>8%</div></div>
1	E	1248	<div><div>31%</div><div>46%</div><div>13%</div><div>•</div><div>8%</div></div>
1	G	1248	<div><div>31%</div><div>46%</div><div>14%</div><div>•</div><div>8%</div></div>
1	I	1248	<div><div>32%</div><div>46%</div><div>13%</div><div>•</div><div>8%</div></div>
1	K	1248	<div><div>32%</div><div>46%</div><div>13%</div><div>•</div><div>8%</div></div>
1	M	1248	<div><div>32%</div><div>46%</div><div>13%</div><div>•</div><div>8%</div></div>
2	B	105	<div><div>82%</div><div>15%</div><div>••</div></div>
2	D	105	<div><div>83%</div><div>14%</div><div>••</div></div>

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Mol	Chain	Length	Quality of chain
2	F	105	 82% 15% ..
2	H	105	 83% 14% ..
2	J	105	 82% 15% ..
2	L	105	 83% 14% ..
2	N	105	 83% 14% ..
3	O	102	 50% 37% • 11%
3	P	102	 52% 34% • 11%
3	Q	102	 42% 44% • 11%
3	R	102	 47% 39% • 11%
3	W	102	 80% 13% 7%
3	X	102	 74% 16% • 10%
4	S	100	 51% 35% 10% •
4	T	100	 48% 45% • •
4	U	100	 45% 46% 5% •
4	V	100	 57% 33% 6% •
4	Y	100	 71% 19% 5% 5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 78605 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		

- Molecule 2 is a protein called Cytochrome c.

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

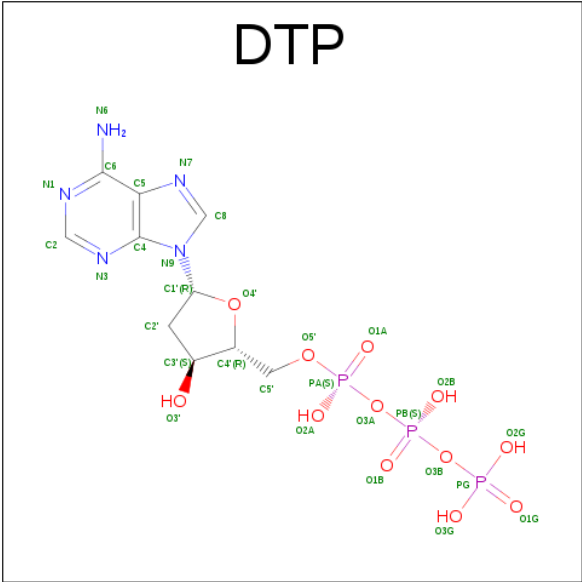
- Molecule 3 is a protein called Apoptotic protease-activating factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	91	Total	C	N	O	S	0	0
			735	461	127	141	6		
3	P	91	Total	C	N	O	S	0	0
			735	461	127	141	6		
3	Q	91	Total	C	N	O	S	0	0
			735	461	127	141	6		
3	R	91	Total	C	N	O	S	0	0
			735	461	127	141	6		
3	W	95	Total	C	N	O	S	0	0
			762	479	131	146	6		
3	X	92	Total	C	N	O	S	0	0
			742	466	128	142	6		

- Molecule 4 is a protein called Caspase.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	96	Total	C	N	O	S	0	0
			783	479	153	146	5		
4	T	96	Total	C	N	O	S	0	0
			783	479	153	146	5		
4	U	96	Total	C	N	O	S	0	0
			783	479	153	146	5		
4	V	96	Total	C	N	O	S	0	0
			783	479	153	146	5		
4	Y	95	Total	C	N	O	S	0	0
			777	475	152	145	5		

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



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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

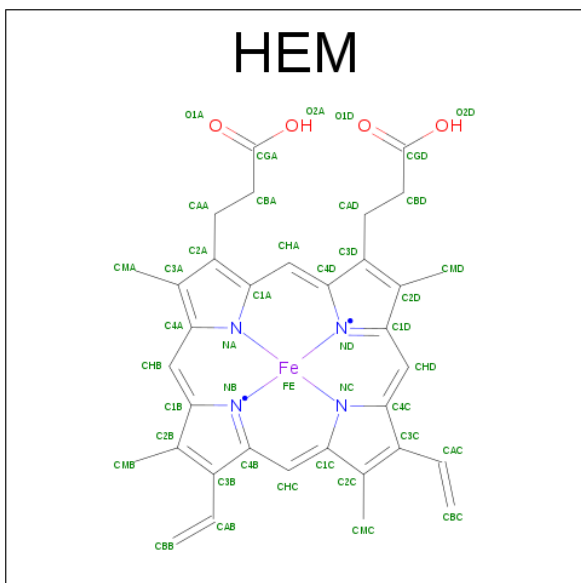
Mol	Chain	Residues	Atoms		AltConf
6	G	1	Total	Mg	0
			1	1	
6	K	1	Total	Mg	0
			1	1	
6	E	1	Total	Mg	0
			1	1	
6	I	1	Total	Mg	0
			1	1	
6	C	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Mg	0
			1	1	
6	M	1	Total	Mg	0
			1	1	

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

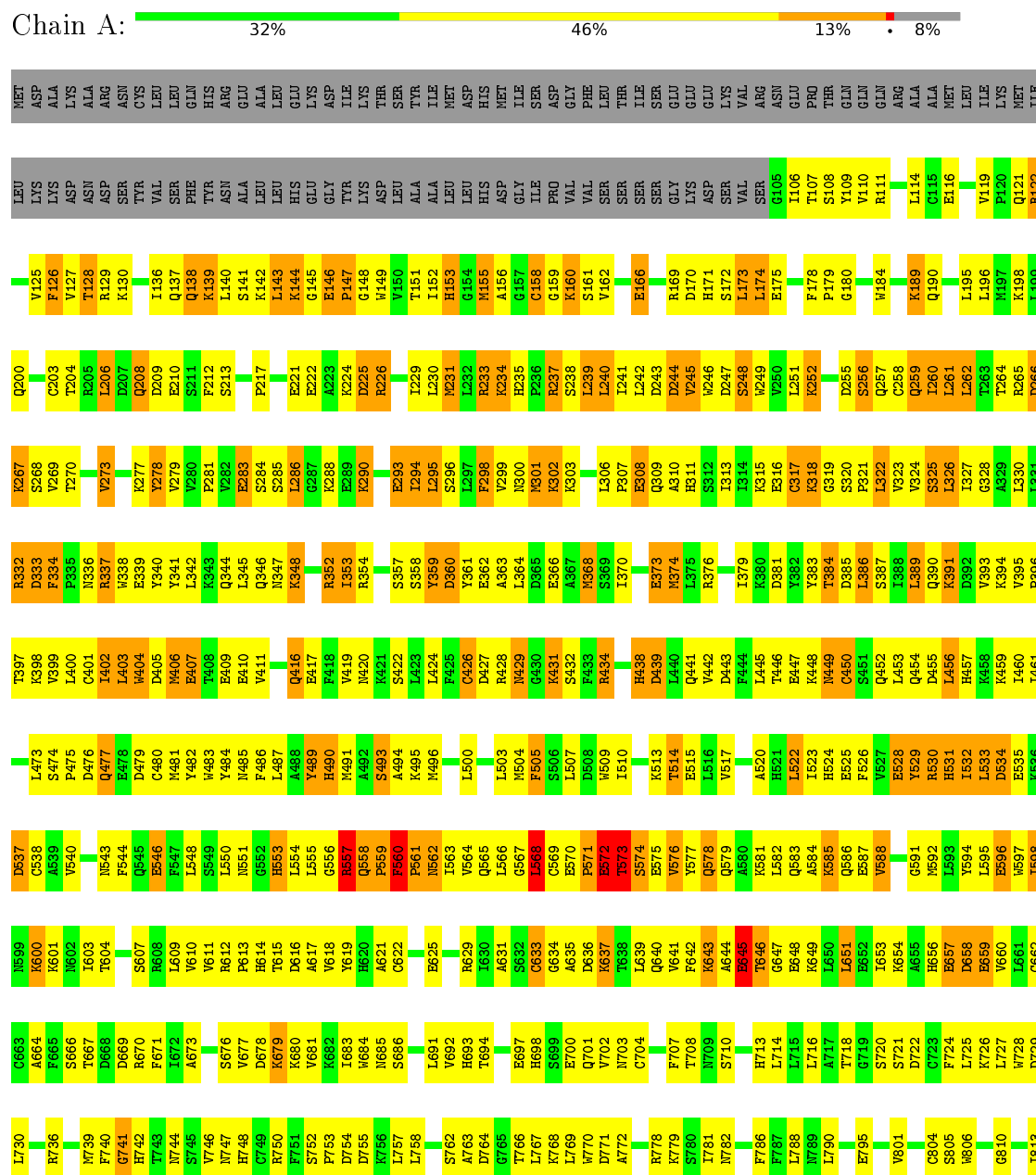


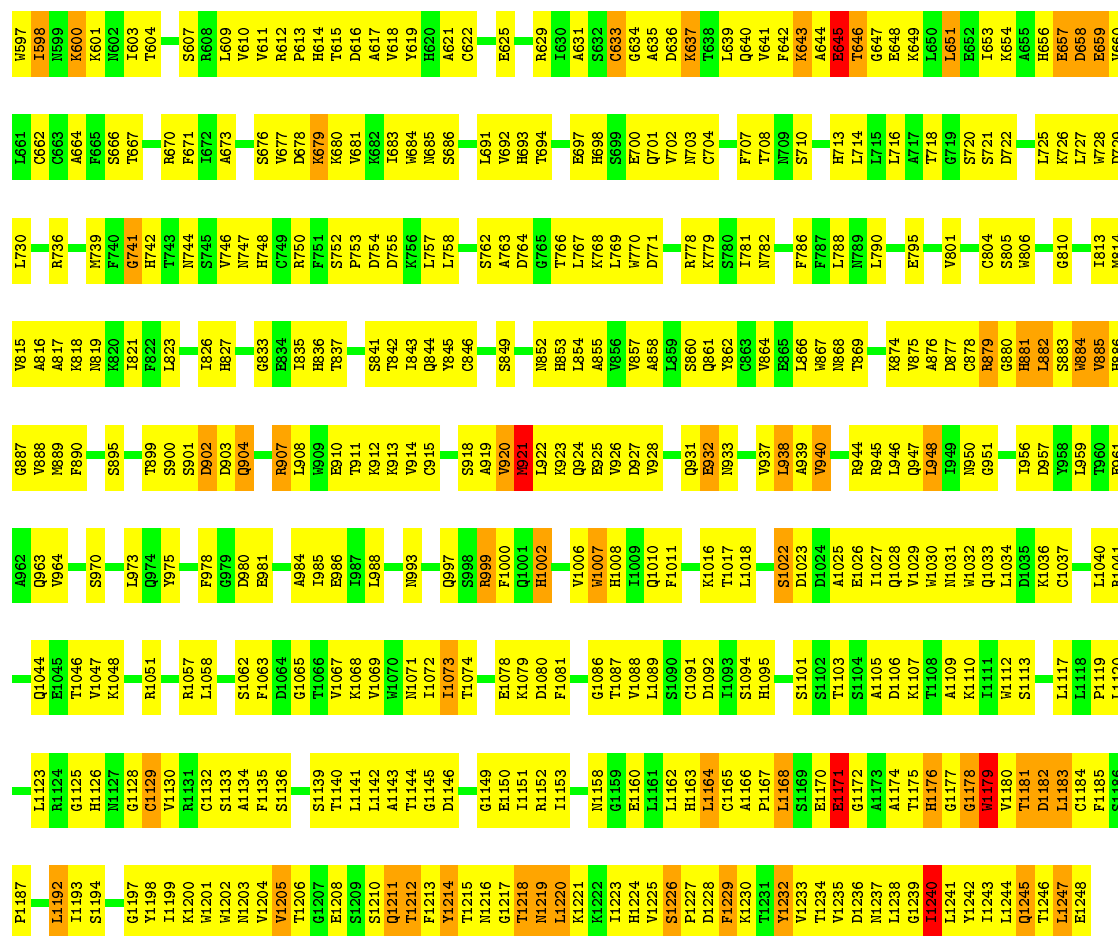
Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
7	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
7	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
7	H	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
7	J	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
7	L	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
7	N	1	Total	C	Fe	N	O	0
			43	34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

3 Residue-property plots

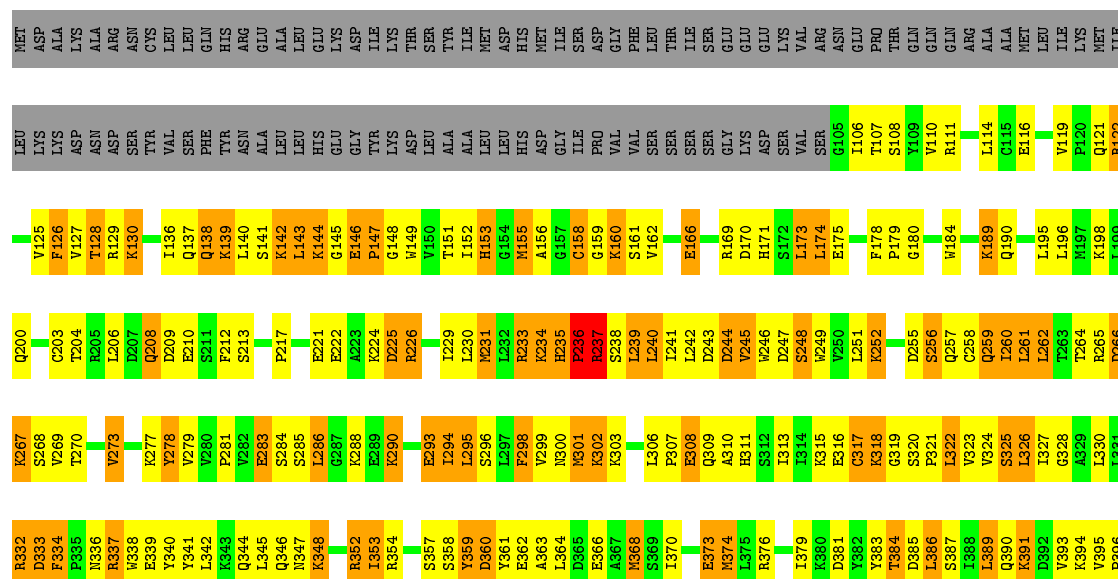
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric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

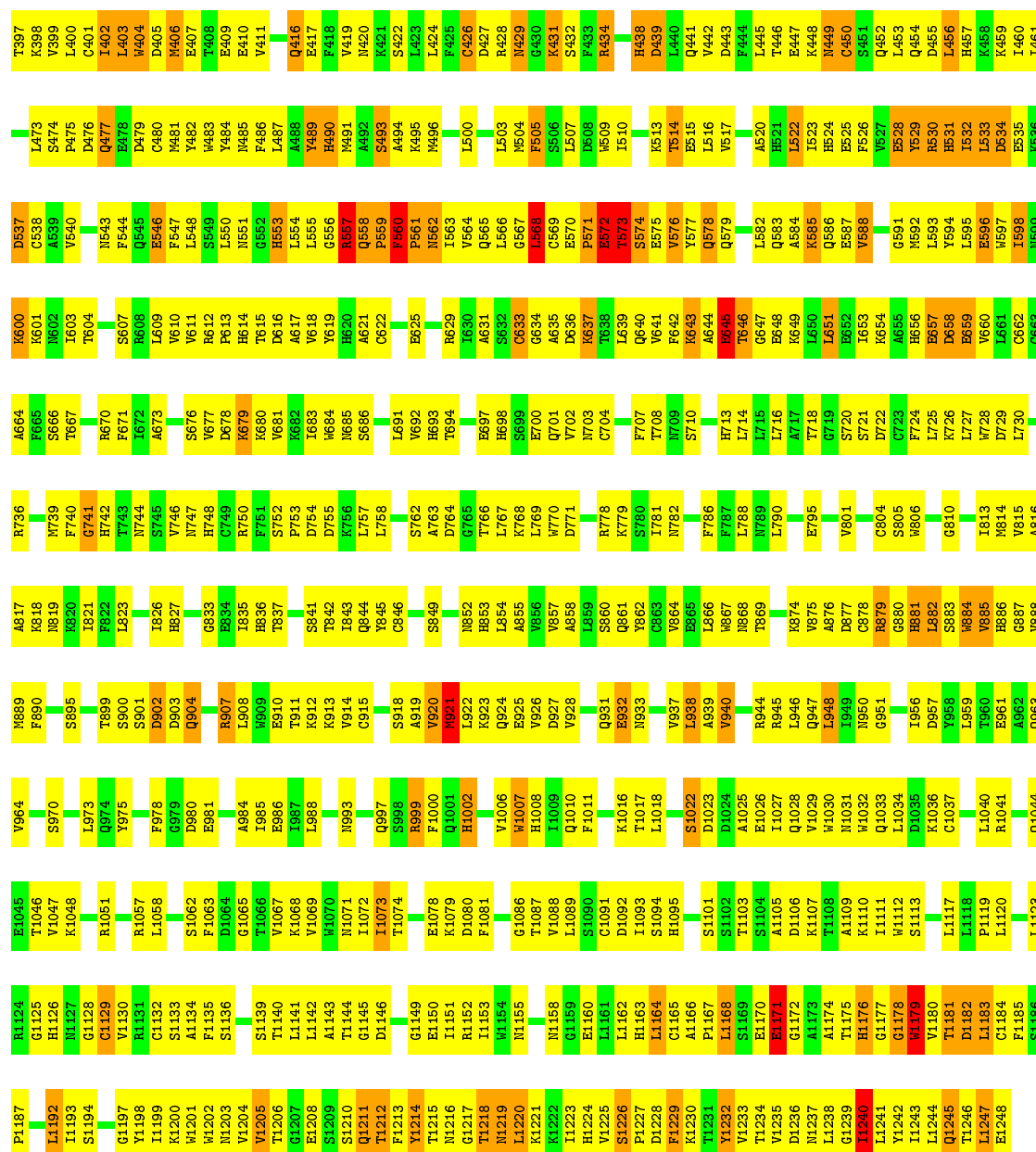
- Molecule 1: Apoptotic protease-activating factor 1



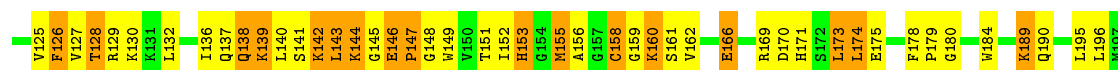
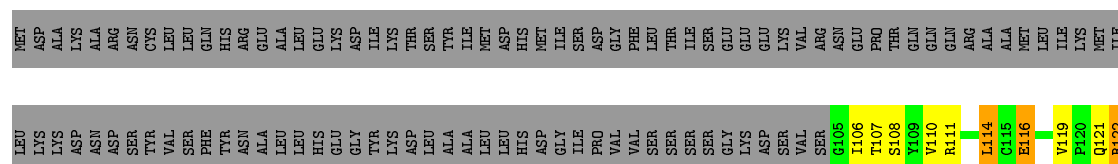


- Molecule 1: Apoptotic protease-activating factor 1



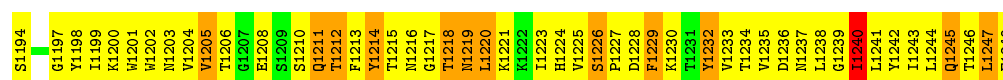


- Molecule 1: Apoptotic protease-activating factor 1



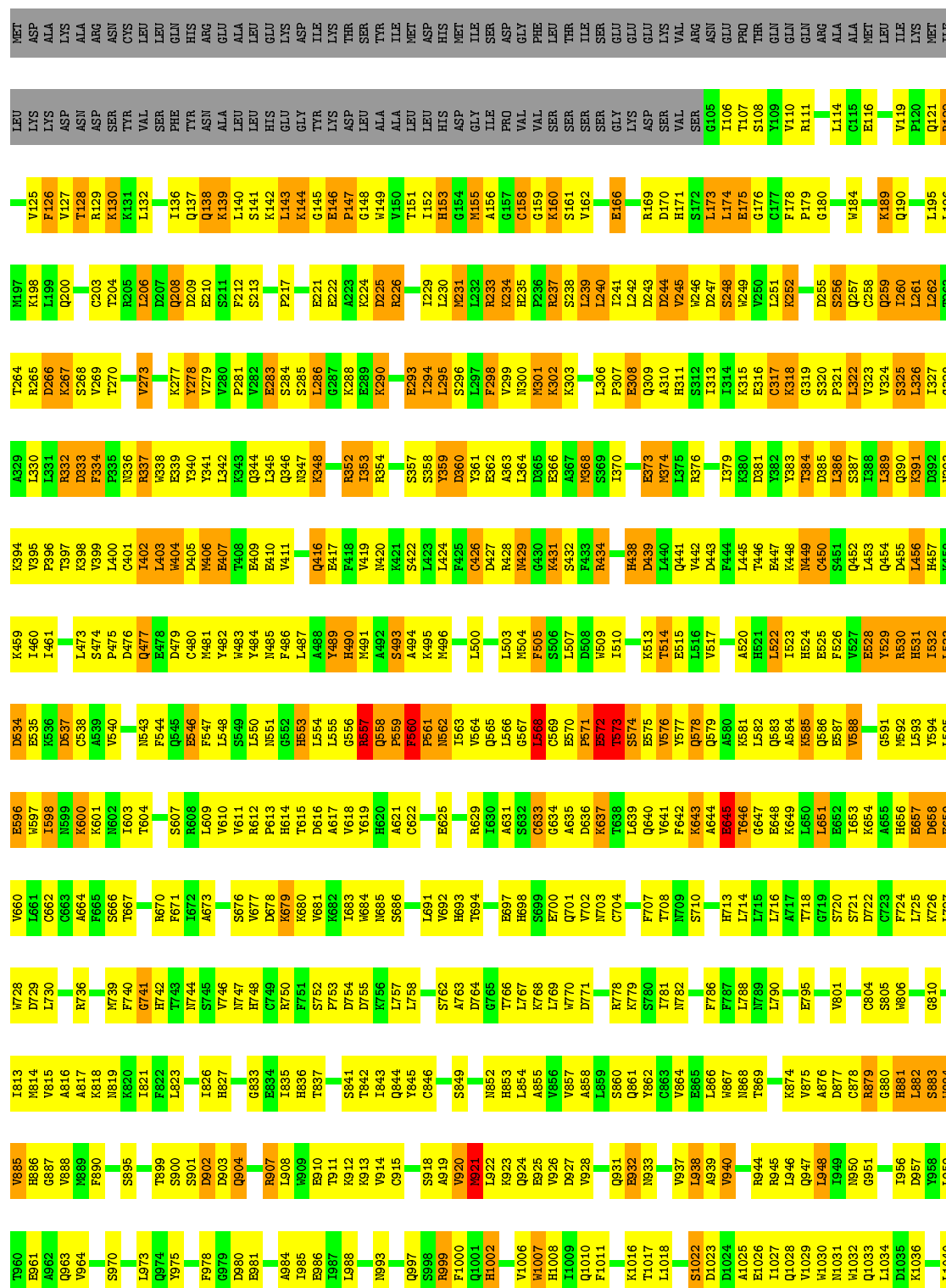
Chain I:  32% 46% 13% 8%

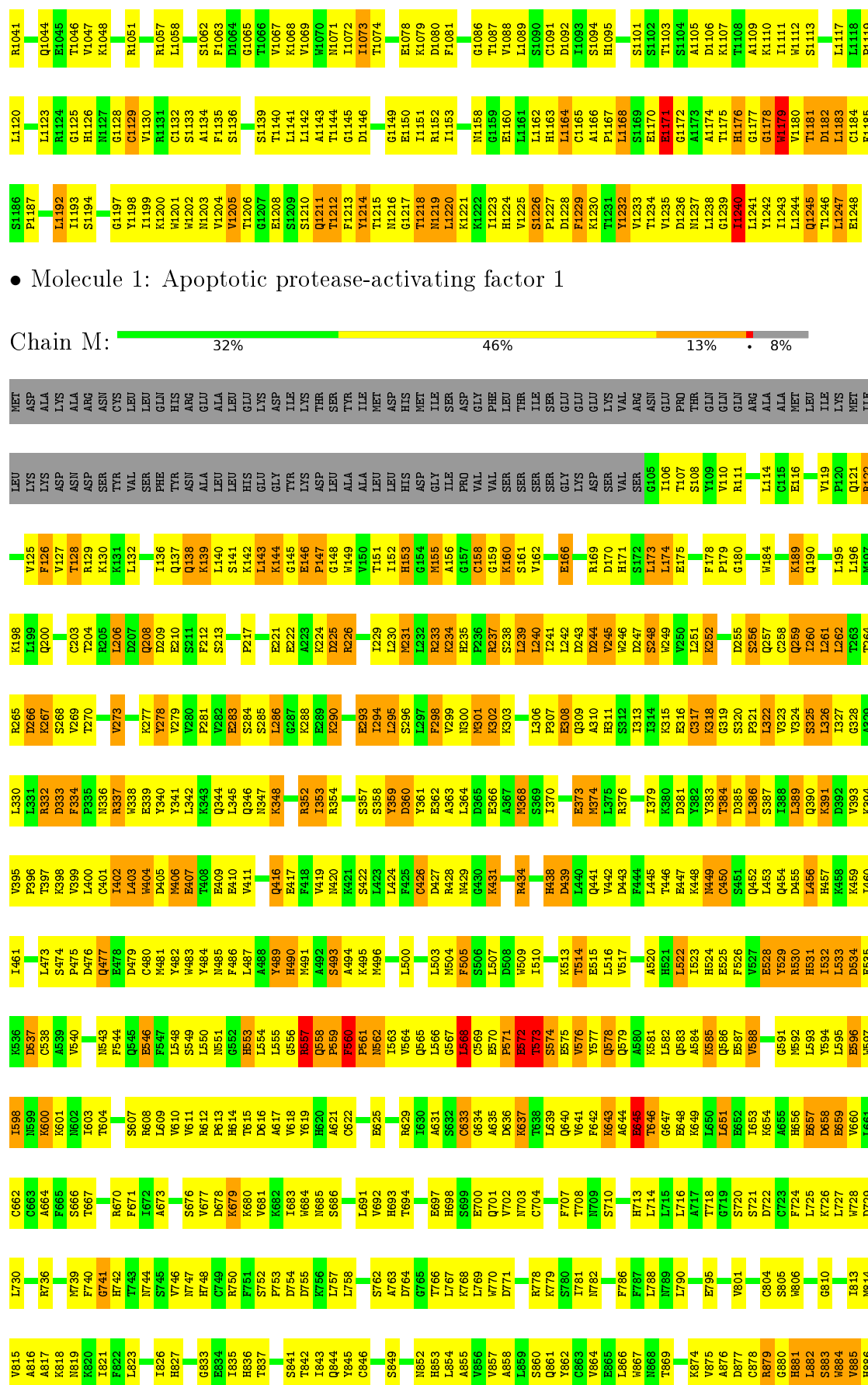
H1126	V1047	S970	F890	K818	A684	K800	C538	L473	T397	R332	K267	Q200	LEU	MET
H1127	K1048	S970	S895	H819	F695	K601	A589	S474	K398	D333	S268	Q200	LYS	ASP
G1128	R051	L973	S895	H820	S666	N602	V540	D475	V399	F334	V269	C203	LYS	ALA
C1129	R1051	L973	T899	H821	T687	T604	N543	Q477	C401	P335	T270	T204	ASP	LYS
V1130	R1057	Y975	T899	H822	H742	T604	N543	Q477	C401	P335	T270	T204	ASN	ALA
H1131	L1058	Y975	S901	H823	T743	T604	N543	Q477	C401	P335	T270	T204	ASP	ARG
C1132		F978	S901	L823	T743	T604	N543	Q477	C401	P335	T270	T204	SER	ASN
S1133		G979	D902	I826	S745	S607	Q545	D479	L403	V338	K277	Q208	TYR	CYS
A1134	S1062	G979	D903	H827	S745	S607	Q545	D479	L403	V338	K277	Q208	VAL	LEU
F1135	F1063	Q981	Q904	H827	S745	S607	Q545	D479	L403	V338	K277	Q208	SER	LEU
S1136	D1064	E981		H833	H748	V610	L548	Y482	N406	Y341	V279	E210	PHE	GLN
	G1065	E981		H833	H748	V610	L548	Y482	N406	Y341	V279	E210	TYR	HIS
S1139	T1066	A984	R907	H834	C749	R612	L550	Y484	T408	K343	P281	F212	ASN	ARG
T1140	V1067	I985	R909	H835	C749	R612	L550	Y484	T408	K343	P281	F212	ALA	GLU
K1068	K1068	E986	T910	H836	R750	R613	N551	N485	E409	K344	E283	S213	LEU	ALA
L1141	V1069	E986	T910	H837	R750	R613	N551	N485	E409	K344	E283	S213	LEU	LEU
V1069	F1069	E987	T911	H837	R750	R613	N551	N485	E409	K344	E283	S213	HIS	GLU
N1070	N1070	L988	K912	H841	D754	R616	L555	Y489	E416	K348	E221	E221	GLU	GLU
T1144	N1071	L988	K912	H842	D754	R616	L555	Y489	E416	K348	E221	E221	GLY	ASP
G1145	I1072	N993	V914	H843	D755	R616	L555	Y489	E416	K348	E221	E221	TYR	ILE
D1146	T1073	N993	C915	H844	D755	R616	L555	Y489	E416	K348	E221	E221	LYS	LYS
	T1074	Q997	C915	H844	D755	R616	L555	Y489	E416	K348	E221	E221	ASP	THR
G1149	E1078	Q997	S918	C846	S762	L691	F560	A494	K421	R354	K290	R226	LEU	SER
E1150	K1079	R999	A919	C846	S762	L691	F560	A494	K421	R354	K290	R226	ALA	TYR
I1151	F1080	R999	A919	C846	S762	L691	F560	A494	K421	R354	K290	R226	ALA	ILE
R1152	D1080	Q1001	N920	H849	D764	V692	N562	K495	S422	S357	E293	I229	LEU	MET
I1153	F1081	H1002	N920	H849	D764	V692	N562	K495	S422	S357	E293	I229	LEU	ASP
		H1002	N920	H849	D764	V692	N562	K495	S422	S357	E293	I229	LEU	HIS
G1086		V1006	K923	H852	T766	L692	F563	N496	L424	S358	I294	L230	ASP	MET
T1087		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	GLY	ILE
E1088		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	ILE	SER
H1088		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	PRO	ASP
L1161		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
L1162		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
H1163		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
L1164		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
C1165		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
A1166		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
P1167		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
L1168		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
S1169		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
E1170		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
E1171		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
G1172		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
A1173		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
A1174		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
T1175		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
H1176		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
G1177		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
G1178		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
H1179		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
V1180		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
T1181		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
D1182		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
L1183		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
C1184		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
F1185		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
S1186		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
P1187		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
L1192		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY
I1193		V1006	K923	H853	T766	L692	F563	N496	L424	S358	I294	L230	VAL	GLY

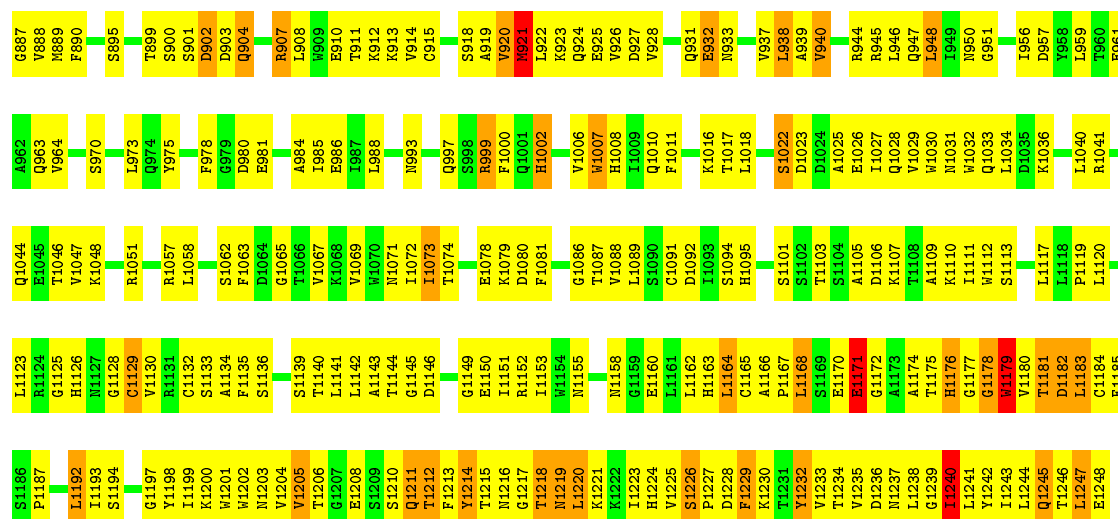


• Molecule 1: Apoptotic protease-activating factor 1

Chain K: 32% 46% 13% 8%







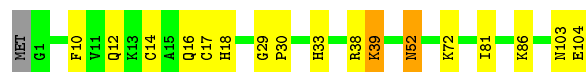
- Molecule 2: Cytochrome c

Chain B: 82% 15% ..



- Molecule 2: Cytochrome c

Chain D: 83% 14% ..



- Molecule 2: Cytochrome c

Chain F: 82% 15% ..



- Molecule 2: Cytochrome c

Chain H: 83% 14% ..

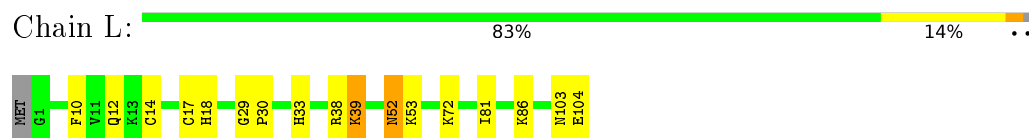


- Molecule 2: Cytochrome c

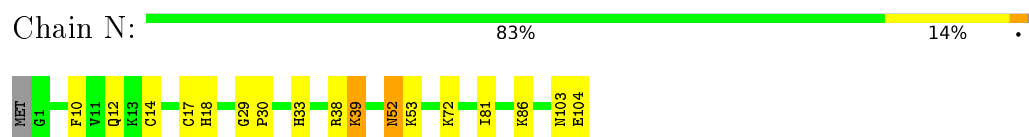
Chain J: 82% 15% ..



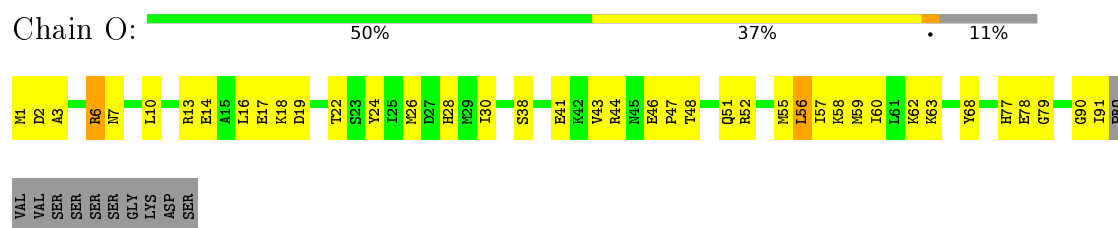
- Molecule 2: Cytochrome c



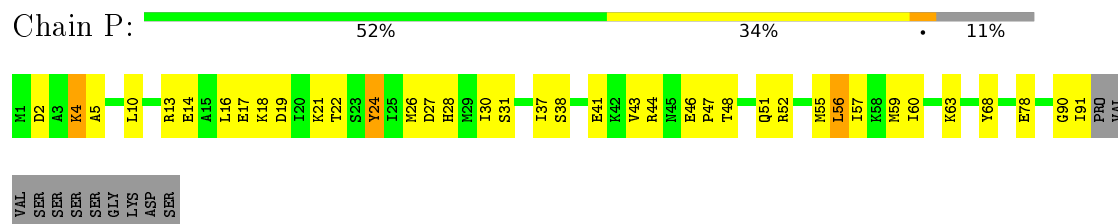
- Molecule 2: Cytochrome c



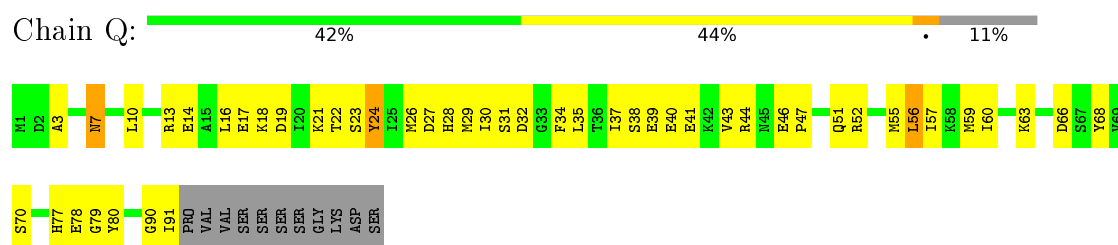
- Molecule 3: Apoptotic protease-activating factor 1



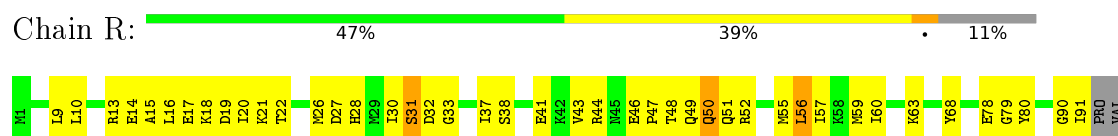
- Molecule 3: Apoptotic protease-activating factor 1



- Molecule 3: Apoptotic protease-activating factor 1



- Molecule 3: Apoptotic protease-activating factor 1



VAL
SER
SER
SER
SER
GLY
LYS
ASP
SER

• Molecule 3: Apoptotic protease-activating factor 1

Chain W: 80% 13% 7%

H1 D2 A3 R6 N7 L10 R13 E17 K18 D19 K21 P47 Q51 K58 L61 K81 S95 SER SER SER SER GLY ASP SER

• Molecule 3: Apoptotic protease-activating factor 1

Chain X: 74% 16% 10%

H1 R6 L9 E17 K18 D19 H28 F34 I37 E40 V43 R44 R45 E46 R52 A53 A54 D66 S67 Y68 L83 I91 P92 VAL SER SER SER SER GLY LYS ASP SER

• Molecule 4: Caspase

Chain S: 51% 35% 10%

H1 D2 R6 R7 L8 L9 R10 R11 C12 R13 R14 R15 L16 V17 E18 E19 L20 Q21 D27 V28 L29 L30 L31 R32 E33 L34 R35 R36 P37 H38 M39 I40 E41 D42 I43 Q44 R45 R51 R52 T64 R65 Q68 A69 L70 P71 L72 F73 I74 S75 C76 L77 E78 D79 T80 G81 Q82 L85 R93 A96 LYS LEU SER LYS

• Molecule 4: Caspase

Chain T: 48% 45%

H1 D2 R6 R7 L8 L9 R10 R11 R12 C12 R13 L14 V17 L20 Q21 V28 L29 R32 E33 L34 R35 R36 P37 H38 M39 I40 E41 Q44 R45 S50 R51 R52 R56 I59 I60 E63 T64 Q68 A69 L70 P71 L72 F73 I74 S75 C76 L77 E78 T80 G81 Q82 L85 R88 R93 A96 LYS LEU SER LYS

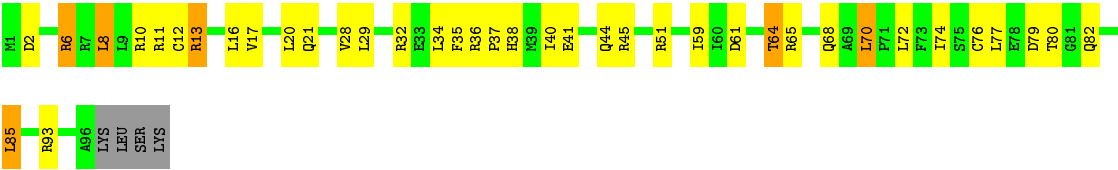
• Molecule 4: Caspase

Chain U: 45% 46% 5%

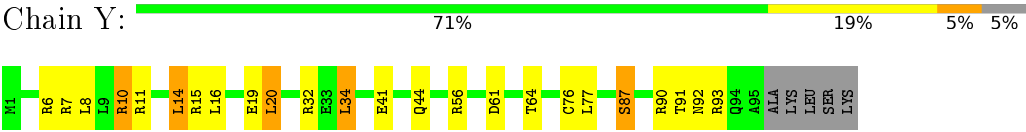
H1 D2 R6 R7 L8 L9 R10 R11 R12 C12 R13 L14 L15 L16 V17 E18 E19 L20 Q21 V28 L29 R32 E33 L34 R35 R36 P37 H38 M39 I40 E41 Q44 R45 R51 R52 R56 I59 I60 D61 E63 T64 R65 Q68 A69 L70 P71 L72 F73 I74 S75 C76 L77 E78 D79 T80 G81 Q82 L85 R88 R93 A96 LYS LEU SER LYS

• Molecule 4: Caspase

Chain V: 57% 33% 6%



● Molecule 4: Caspase



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	240130	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	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: 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	0.31	0/9337	0.52	2/12636 (0.0%)
1	C	0.30	0/9337	0.52	2/12636 (0.0%)
1	E	0.31	1/9337 (0.0%)	0.53	3/12636 (0.0%)
1	G	0.31	0/9337	0.52	2/12636 (0.0%)
1	I	0.31	0/9337	0.52	2/12636 (0.0%)
1	K	0.31	1/9337 (0.0%)	0.52	2/12636 (0.0%)
1	M	0.31	0/9337	0.52	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
3	O	0.41	0/745	0.64	0/998
3	P	0.42	0/745	0.64	0/998
3	Q	0.40	0/745	0.62	0/998
3	R	0.41	0/745	0.64	0/998
3	W	0.66	0/773	0.58	0/1038
3	X	0.74	0/753	0.61	0/1010
4	S	0.42	0/790	0.66	0/1059
4	T	0.42	0/790	0.64	0/1059
4	U	0.40	0/790	0.62	0/1059
4	V	0.43	0/790	0.67	0/1059
4	Y	0.60	0/784	0.61	0/1051
All	All	0.37	2/79682 (0.0%)	0.55	15/107605 (0.0%)

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
4	T	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	1179	TRP	C-N	-6.36	1.19	1.34
1	E	236	PRO	N-CD	5.21	1.55	1.47

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	560	PHE	C-N-CD	-6.44	106.43	120.60
1	K	560	PHE	C-N-CD	-6.43	106.45	120.60
1	A	560	PHE	C-N-CD	-6.42	106.48	120.60
1	C	560	PHE	C-N-CD	-6.39	106.54	120.60
1	E	560	PHE	C-N-CD	-6.39	106.54	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	T	52	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	9139	0	9004	1450	0
1	C	9139	0	9005	1398	0
1	E	9139	0	9005	1439	0
1	G	9139	0	9005	1410	0
1	I	9139	0	9005	1405	0
1	K	9139	0	9005	1410	0
1	M	9139	0	9005	1400	0
2	B	823	0	849	33	0
2	D	823	0	849	33	0
2	F	823	0	849	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	823	0	849	31	0
2	J	823	0	849	33	0
2	L	823	0	849	33	0
2	N	823	0	849	35	0
3	O	735	0	738	82	0
3	P	735	0	738	98	0
3	Q	735	0	738	124	0
3	R	735	0	738	101	0
3	W	762	0	768	36	0
3	X	742	0	745	17	0
4	S	783	0	792	109	0
4	T	783	0	792	115	0
4	U	783	0	792	119	0
4	V	783	0	792	67	0
4	Y	777	0	784	26	0
5	A	30	0	12	6	0
5	C	30	0	12	6	0
5	E	30	0	12	6	0
5	G	30	0	12	6	0
5	I	30	0	12	6	0
5	K	30	0	12	6	0
5	M	30	0	12	6	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
6	K	1	0	0	0	0
6	M	1	0	0	0	0
7	B	43	0	30	15	0
7	D	43	0	30	18	0
7	F	43	0	30	14	0
7	H	43	0	30	14	0
7	J	43	0	30	15	0
7	L	43	0	30	14	0
7	N	43	0	30	16	0
All	All	78605	0	77688	10505	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 67.

The worst 5 of 10505 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:C:862:TYR:CD1	1:C:885:VAL:HG12	1.35	1.62
1:M:862:TYR:CD1	1:M:885:VAL:HG12	1.35	1.60
1:K:862:TYR:CD1	1:K:885:VAL:HG12	1.35	1.60
1:C:862:TYR:CZ	1:C:881:HIS:HB2	1.06	1.59
1:I:862:TYR:CD1	1:I:885:VAL:HG12	1.35	1.59

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	1142/1248 (92%)	1002 (88%)	93 (8%)	47 (4%)	3	36
1	C	1142/1248 (92%)	1002 (88%)	94 (8%)	46 (4%)	4	37
1	E	1142/1248 (92%)	999 (88%)	95 (8%)	48 (4%)	3	35
1	G	1142/1248 (92%)	1002 (88%)	93 (8%)	47 (4%)	3	36
1	I	1142/1248 (92%)	1002 (88%)	93 (8%)	47 (4%)	3	36
1	K	1142/1248 (92%)	1002 (88%)	93 (8%)	47 (4%)	3	36
1	M	1142/1248 (92%)	1002 (88%)	93 (8%)	47 (4%)	3	36
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
2	L	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
2	N	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
3	O	89/102 (87%)	86 (97%)	3 (3%)	0	100	100
3	P	89/102 (87%)	87 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Q	89/102 (87%)	86 (97%)	3 (3%)	0	100	100
3	R	89/102 (87%)	87 (98%)	2 (2%)	0	100	100
3	W	93/102 (91%)	93 (100%)	0	0	100	100
3	X	90/102 (88%)	90 (100%)	0	0	100	100
4	S	94/100 (94%)	92 (98%)	2 (2%)	0	100	100
4	T	94/100 (94%)	91 (97%)	3 (3%)	0	100	100
4	U	94/100 (94%)	88 (94%)	6 (6%)	0	100	100
4	V	94/100 (94%)	92 (98%)	2 (2%)	0	100	100
4	Y	93/100 (93%)	92 (99%)	1 (1%)	0	100	100
All	All	9716/10583 (92%)	8695 (90%)	692 (7%)	329 (3%)	8	42

5 of 329 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	574	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	1027/1119 (92%)	840 (82%)	187 (18%)	2	16
1	C	1027/1119 (92%)	840 (82%)	187 (18%)	2	16
1	E	1027/1119 (92%)	840 (82%)	187 (18%)	2	16
1	G	1027/1119 (92%)	840 (82%)	187 (18%)	2	16
1	I	1027/1119 (92%)	840 (82%)	187 (18%)	2	16
1	K	1027/1119 (92%)	839 (82%)	188 (18%)	2	16
1	M	1027/1119 (92%)	840 (82%)	187 (18%)	2	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	86/87 (99%)	80 (93%)	6 (7%)	19	58
2	D	86/87 (99%)	81 (94%)	5 (6%)	25	64
2	F	86/87 (99%)	80 (93%)	6 (7%)	19	58
2	H	86/87 (99%)	81 (94%)	5 (6%)	25	64
2	J	86/87 (99%)	80 (93%)	6 (7%)	19	58
2	L	86/87 (99%)	80 (93%)	6 (7%)	19	58
2	N	86/87 (99%)	80 (93%)	6 (7%)	19	58
3	O	80/90 (89%)	77 (96%)	3 (4%)	40	74
3	P	80/90 (89%)	76 (95%)	4 (5%)	30	68
3	Q	80/90 (89%)	76 (95%)	4 (5%)	30	68
3	R	80/90 (89%)	76 (95%)	4 (5%)	30	68
3	W	84/90 (93%)	82 (98%)	2 (2%)	57	83
3	X	81/90 (90%)	79 (98%)	2 (2%)	55	82
4	S	85/89 (96%)	73 (86%)	12 (14%)	4	28
4	T	85/89 (96%)	80 (94%)	5 (6%)	24	63
4	U	85/89 (96%)	79 (93%)	6 (7%)	18	58
4	V	85/89 (96%)	77 (91%)	8 (9%)	11	45
4	Y	84/89 (94%)	77 (92%)	7 (8%)	14	51
All	All	8700/9427 (92%)	7293 (84%)	1407 (16%)	7	22

5 of 1407 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	308	GLU
1	I	173	LEU
1	M	619	TYR
1	G	362	GLU
1	G	586	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 242 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	709	ASN
1	I	579	GLN
3	R	49	GLN

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Mol	Chain	Res	Type
1	G	904	GLN
1	I	183	HIS

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 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$
5	DTP	A	1301	6	25,32,32	0.93	1 (4%)	26,50,50	1.66	1 (3%)
7	HEM	B	201	2	24,50,50	0.86	1 (4%)	16,82,82	1.65	2 (12%)
5	DTP	C	1301	6	25,32,32	0.92	1 (4%)	26,50,50	1.69	1 (3%)
7	HEM	D	201	2	24,50,50	0.86	1 (4%)	16,82,82	1.64	2 (12%)
5	DTP	E	1301	6	25,32,32	0.93	1 (4%)	26,50,50	1.69	1 (3%)
7	HEM	F	201	2	24,50,50	0.86	1 (4%)	16,82,82	1.65	2 (12%)
5	DTP	G	1301	6	25,32,32	0.92	1 (4%)	26,50,50	1.67	1 (3%)
7	HEM	H	201	2	24,50,50	0.86	1 (4%)	16,82,82	1.65	2 (12%)
5	DTP	I	1301	6	25,32,32	0.92	1 (4%)	26,50,50	1.66	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	HEM	J	201	2	24,50,50	0.86	1 (4%)	16,82,82	1.64	2 (12%)
5	DTP	K	1301	6	25,32,32	0.91	1 (4%)	26,50,50	1.68	1 (3%)
7	HEM	L	201	2	24,50,50	0.84	1 (4%)	16,82,82	1.65	2 (12%)
5	DTP	M	1301	6	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
7	HEM	N	201	2	24,50,50	0.85	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
5	DTP	A	1301	6	-	0/18/34/34	0/3/3/3
7	HEM	B	201	2	-	0/6/54/54	0/0/8/8
5	DTP	C	1301	6	-	0/18/34/34	0/3/3/3
7	HEM	D	201	2	-	0/6/54/54	0/0/8/8
5	DTP	E	1301	6	-	0/18/34/34	0/3/3/3
7	HEM	F	201	2	-	0/6/54/54	0/0/8/8
5	DTP	G	1301	6	-	0/18/34/34	0/3/3/3
7	HEM	H	201	2	-	0/6/54/54	0/0/8/8
5	DTP	I	1301	6	-	0/18/34/34	0/3/3/3
7	HEM	J	201	2	-	0/6/54/54	0/0/8/8
5	DTP	K	1301	6	-	0/18/34/34	0/3/3/3
7	HEM	L	201	2	-	0/6/54/54	0/0/8/8
5	DTP	M	1301	6	-	0/18/34/34	0/3/3/3
7	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)
7	H	201	HEM	C3B-C2B	-2.80	1.36	1.40
7	B	201	HEM	C3B-C2B	-2.79	1.36	1.40
7	J	201	HEM	C3B-C2B	-2.78	1.36	1.40
7	N	201	HEM	C3B-C2B	-2.77	1.36	1.40
7	D	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(°)
5	E	1301	DTP	N3-C2-N1	-6.61	123.68	128.87
5	C	1301	DTP	N3-C2-N1	-6.59	123.69	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1301	DTP	N3-C2-N1	-6.56	123.72	128.87
5	K	1301	DTP	N3-C2-N1	-6.53	123.74	128.87
5	A	1301	DTP	N3-C2-N1	-6.45	123.80	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 148 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1301	DTP	6	0
7	B	201	HEM	15	0
5	C	1301	DTP	6	0
7	D	201	HEM	18	0
5	E	1301	DTP	6	0
7	F	201	HEM	14	0
5	G	1301	DTP	6	0
7	H	201	HEM	14	0
5	I	1301	DTP	6	0
7	J	201	HEM	15	0
5	K	1301	DTP	6	0
7	L	201	HEM	14	0
5	M	1301	DTP	6	0
7	N	201	HEM	16	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	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	1179:TRP	C	1180:VAL	N	1.19