



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:47 am GMT

PDB ID : 3J9L
EMDB ID: : EMD-2871
Title : Structure of Dark apoptosome from *Drosophila melanogaster*
Authors : Pang, Y.; Bai, X.; Yan, C.; Hao, Q.; Chen, Z.; Wang, J.; Scheres, S.H.W.; Shi, Y.
Deposited on : 2015-02-04
Resolution : 4.00 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.

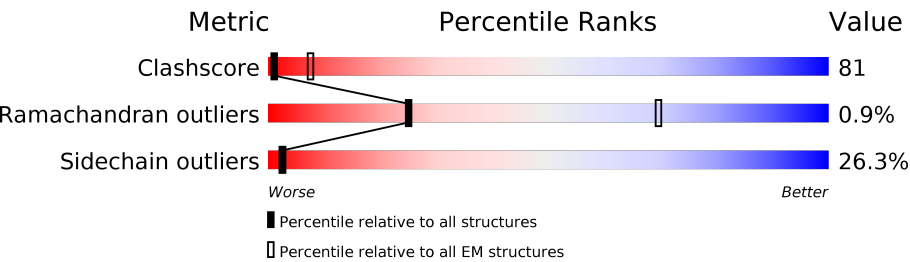
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

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 4.00 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	1103	55% 30% 11% . .
1	C	1103	55% 30% 10% . .
1	D	1103	56% 29% 11% . .
1	E	1103	55% 30% 10% . .
1	F	1103	55% 30% 11% . .
1	G	1103	55% 30% 10% . .
1	H	1103	56% 30% 11% . .
1	I	1103	55% 30% 10% . .
1	J	1103	55% 30% 10% . .

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Mol	Chain	Length	Quality of chain
1	K	1103	 55% 30% 10% . .
1	L	1103	 56% 29% 11% . .
1	M	1103	 55% 30% 10% . .
1	N	1103	 55% 30% 10% . .
1	O	1103	 55% 30% 10% . .
1	P	1103	 55% 30% 11% . .
1	Q	1103	 55% 30% 10% . .

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
2	DTP	C	1301	-	-	X	-
2	DTP	D	1301	-	-	X	-
2	DTP	E	1301	-	-	X	-
2	DTP	F	1301	-	-	X	-
2	DTP	G	1301	-	-	X	-
2	DTP	H	1301	-	-	X	-
2	DTP	I	1301	-	-	X	-
2	DTP	J	1301	-	-	X	-
2	DTP	K	1301	-	-	X	-
2	DTP	L	1301	-	-	X	-
2	DTP	M	1301	-	-	X	-
2	DTP	N	1301	-	-	X	-
2	DTP	O	1301	-	-	X	-
2	DTP	P	1301	-	-	X	-
2	DTP	Q	1301	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 112951 atoms, of which 0 are hydrogens and 0 are deuteriums.

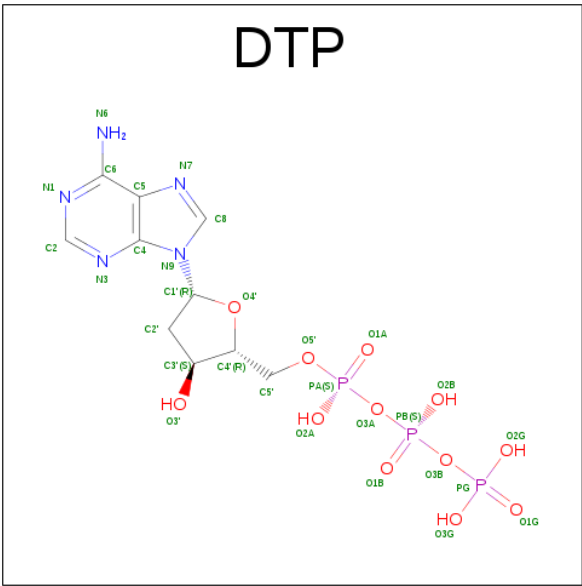
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	C	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	D	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	E	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	F	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	G	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	H	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	I	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	J	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	K	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	L	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	M	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	N	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	O	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	P	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	Q	1063	Total 7036	C 4411	N 1276	O 1326	S 23	0	0

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

mula: C₁₀H₁₆N₅O₁₂P₃).



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

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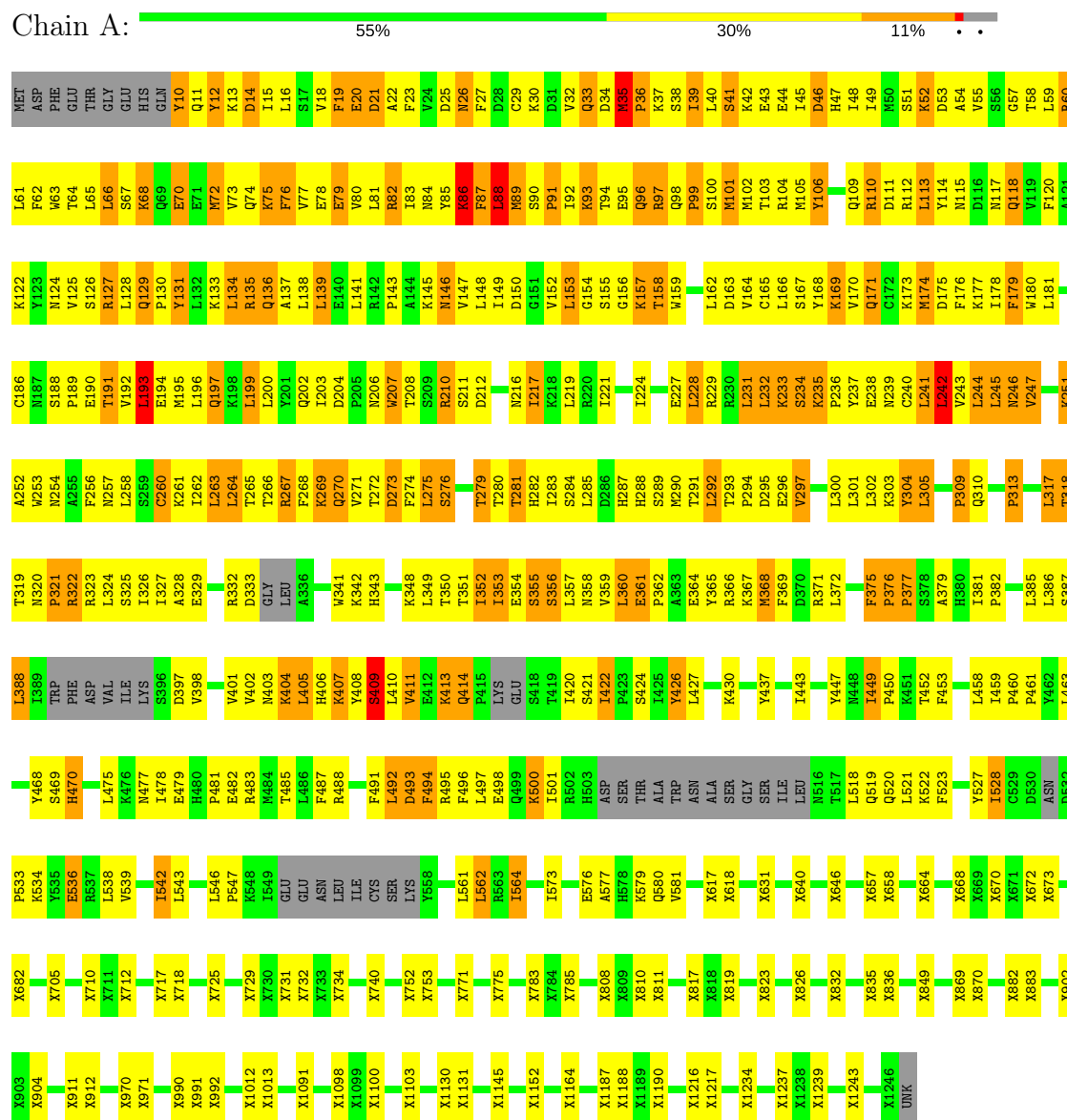
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Mol	Chain	Residues	Atoms					AltConf
2	P	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	Q	1	Total	C	N	O	P	0
			30	10	5	12	3	

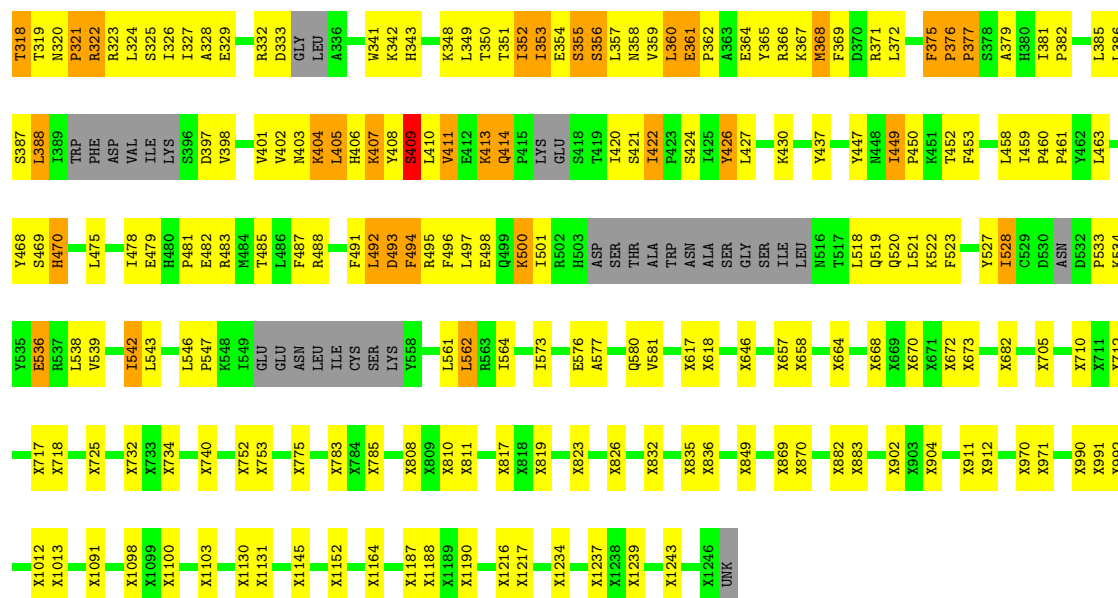
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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

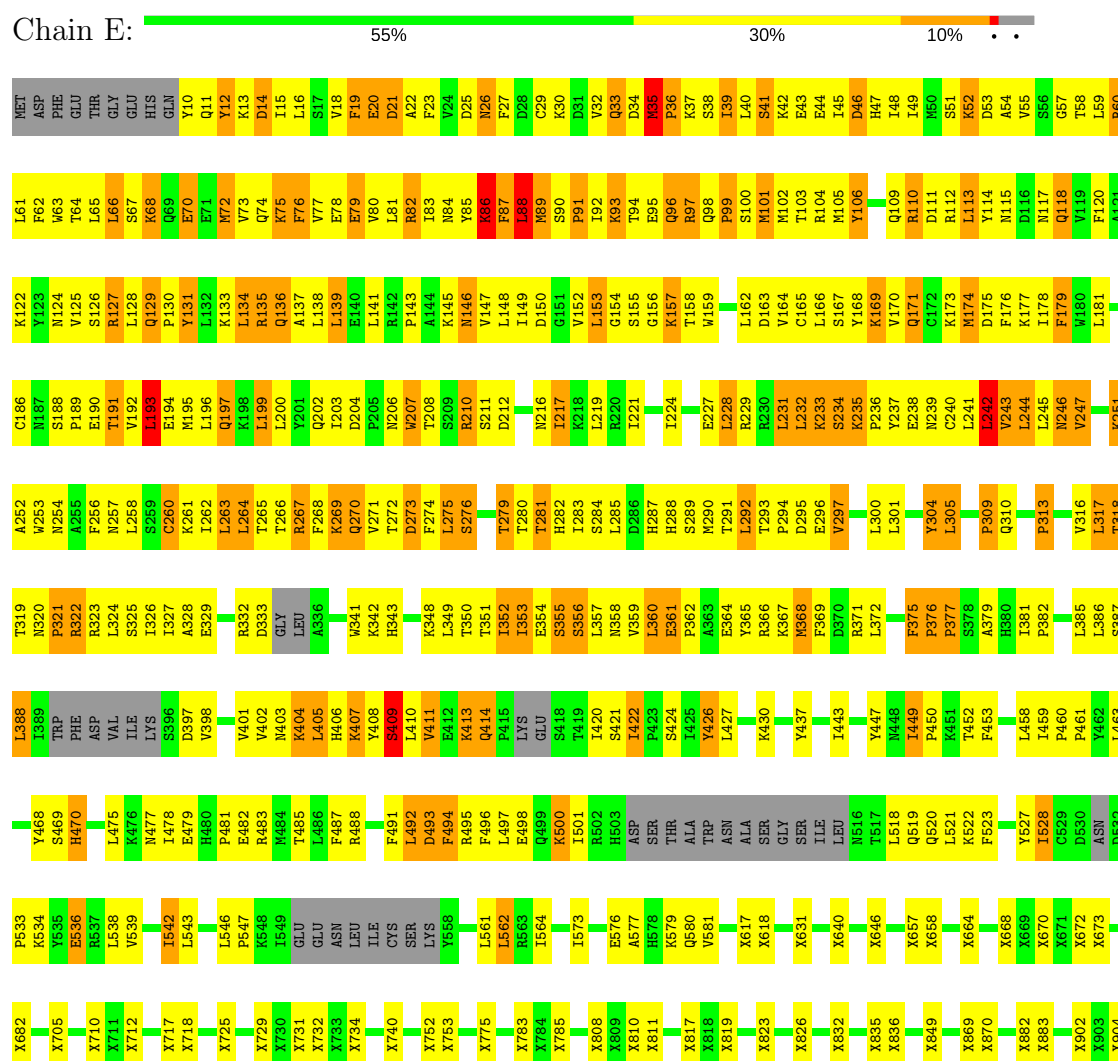


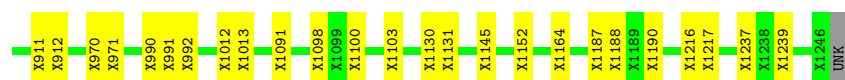
- Molecule 1: Apaf-1 related killer DARK



• Molecule 1: Apaf-1 related killer DARK

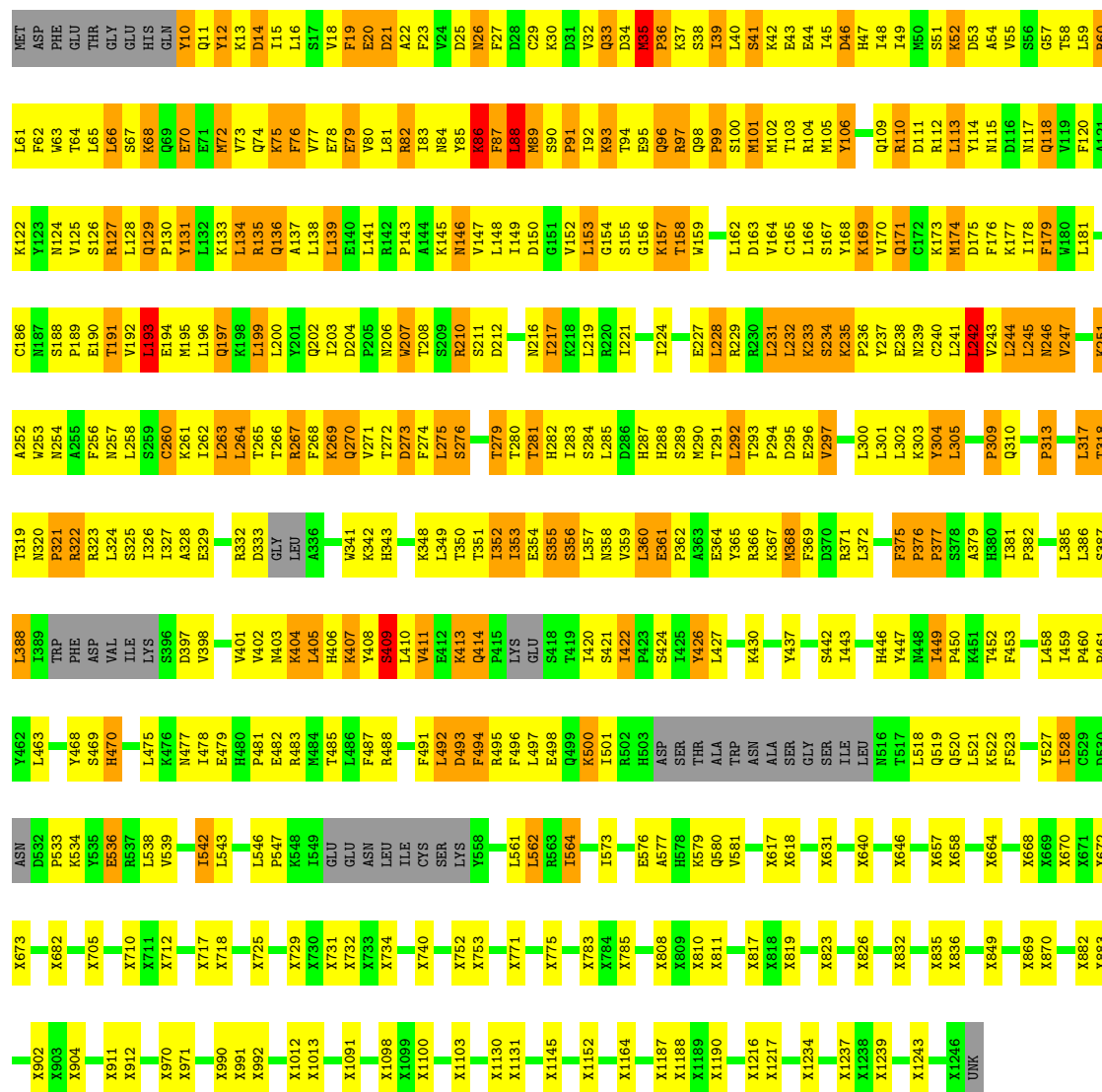
Chain E:





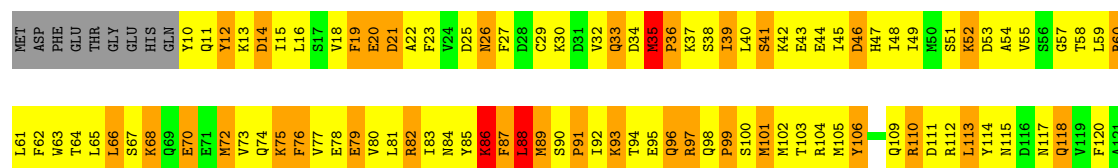
• Molecule 1: Apaf-1 related killer DARK

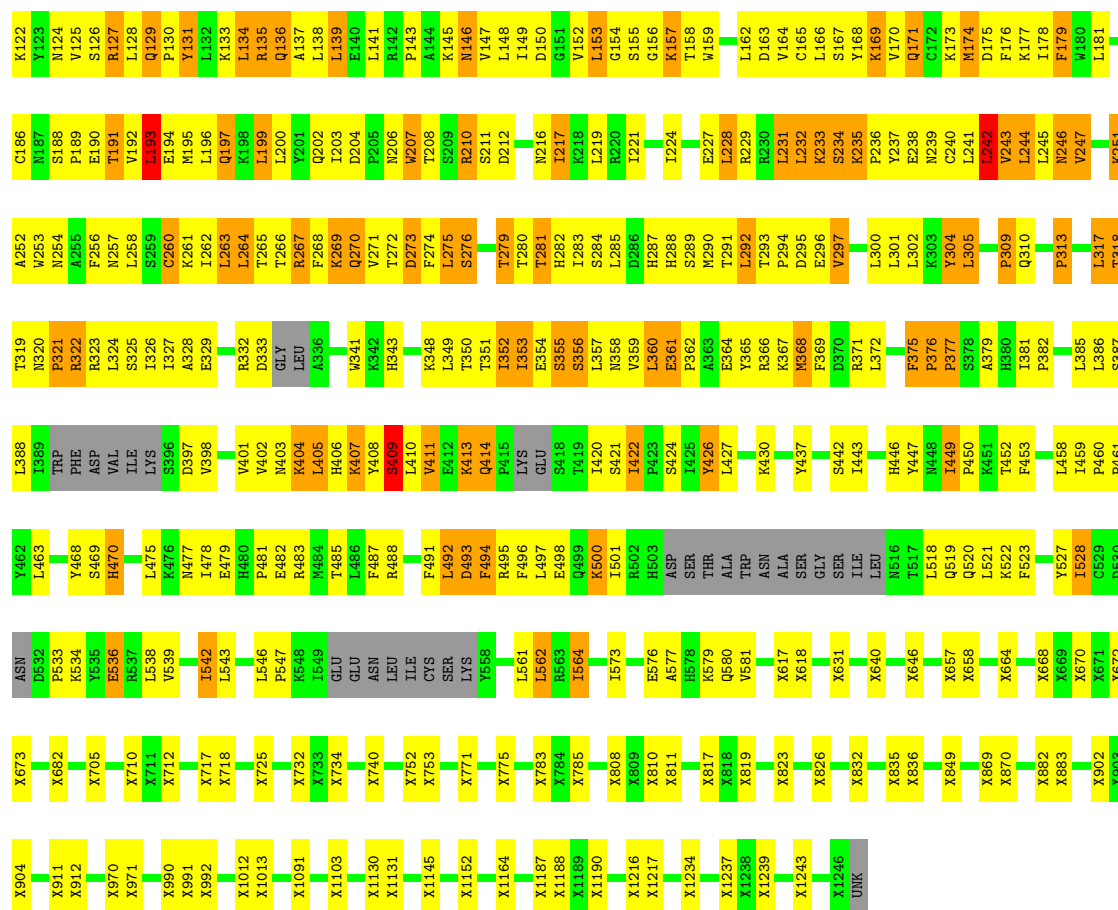
Chain F: 55% 30% 11% . .



• Molecule 1: Apaf-1 related killer DARK

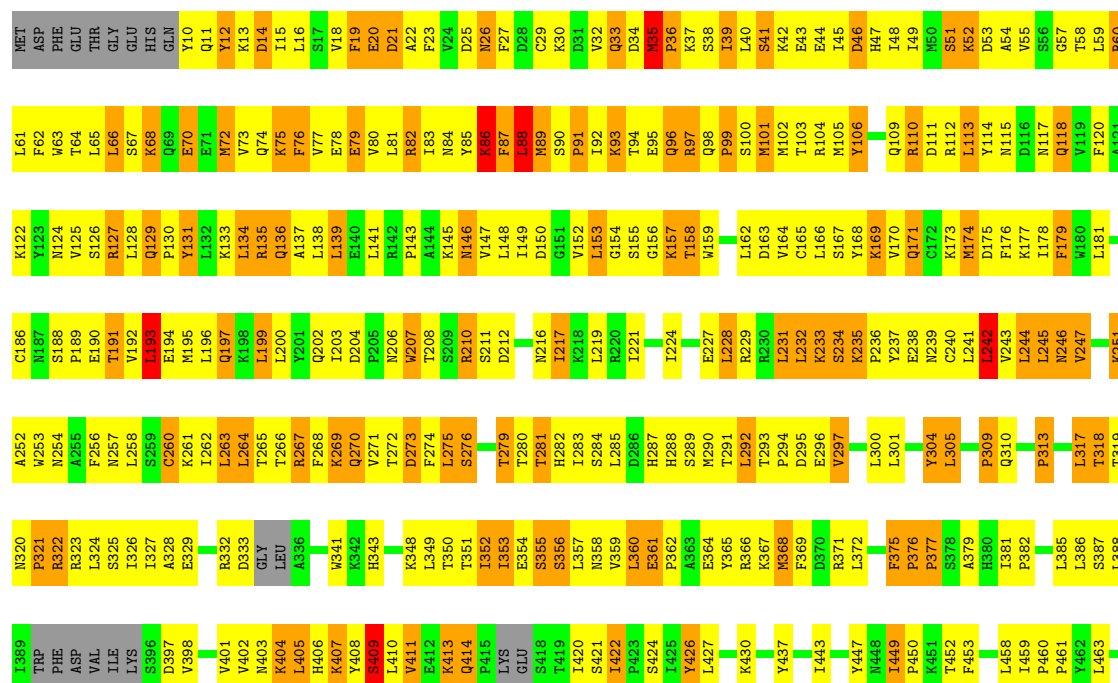
Chain G: 55% 30% 10% . .



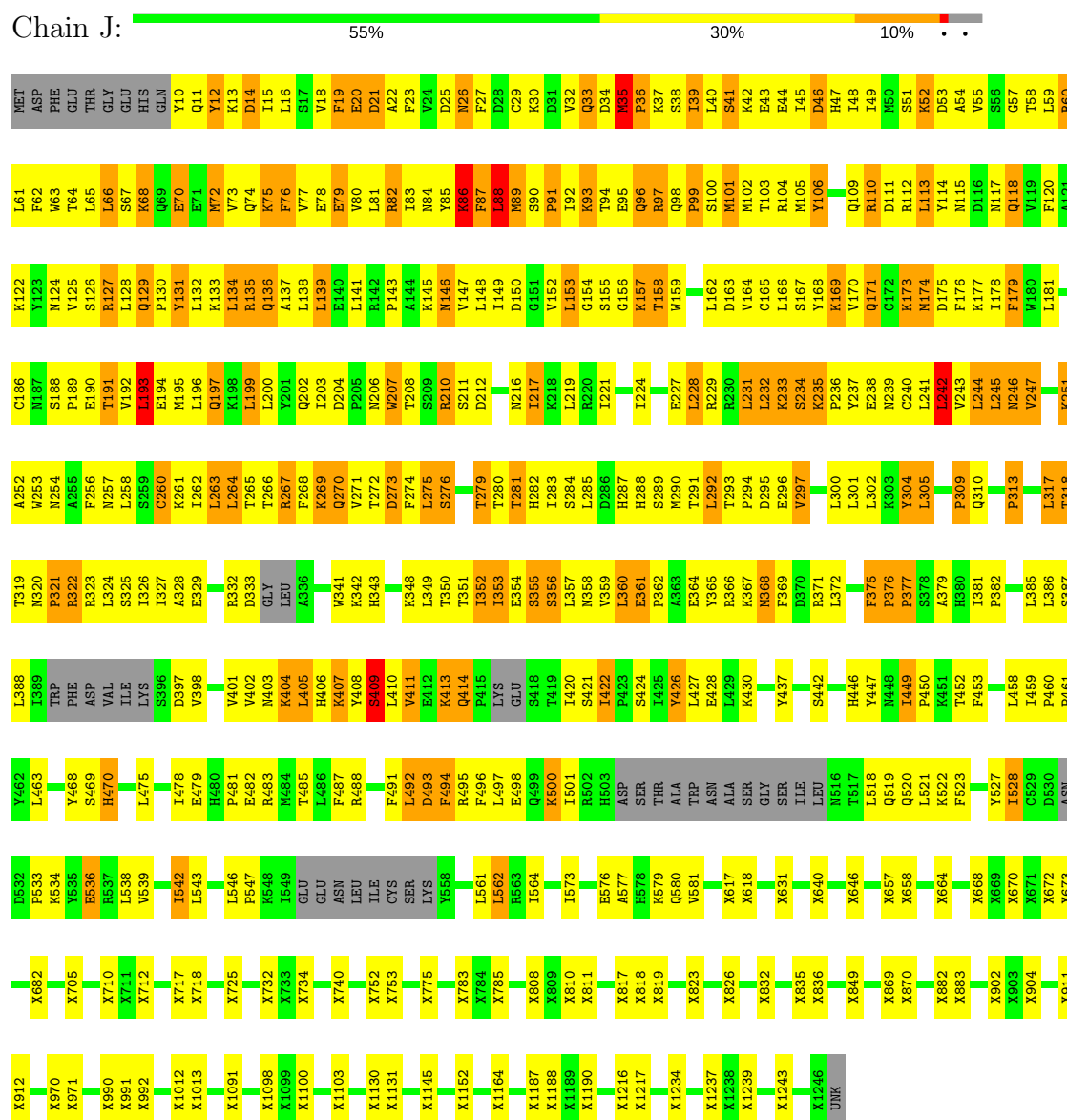


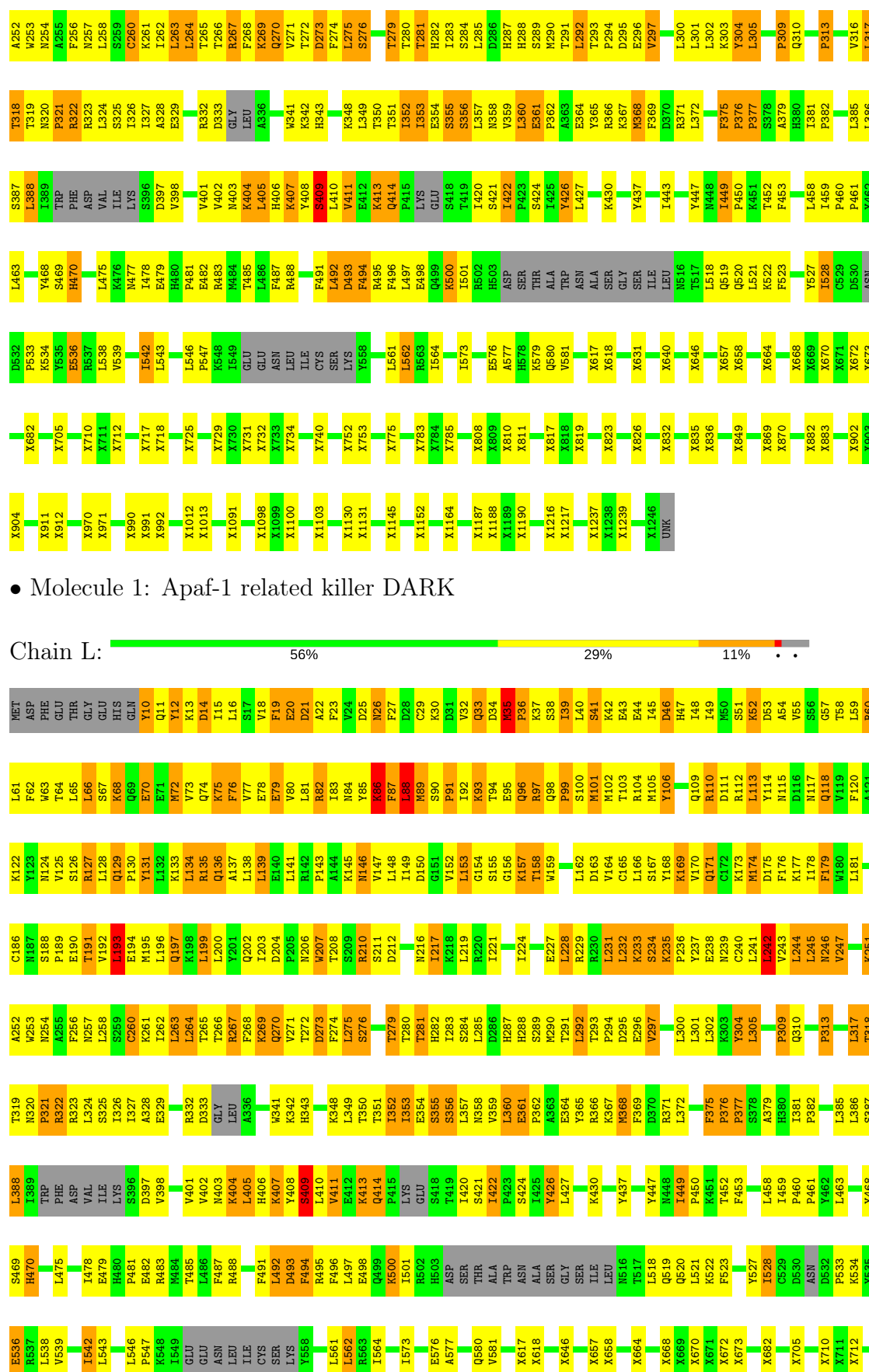
• Molecule 1: Apaf-1 related killer DARK

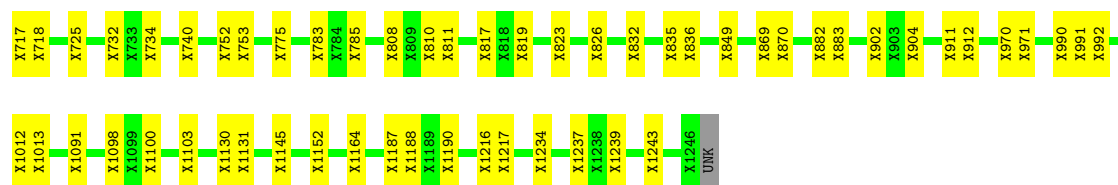
Chain H: 56% 30% 11% . .



Chain J:

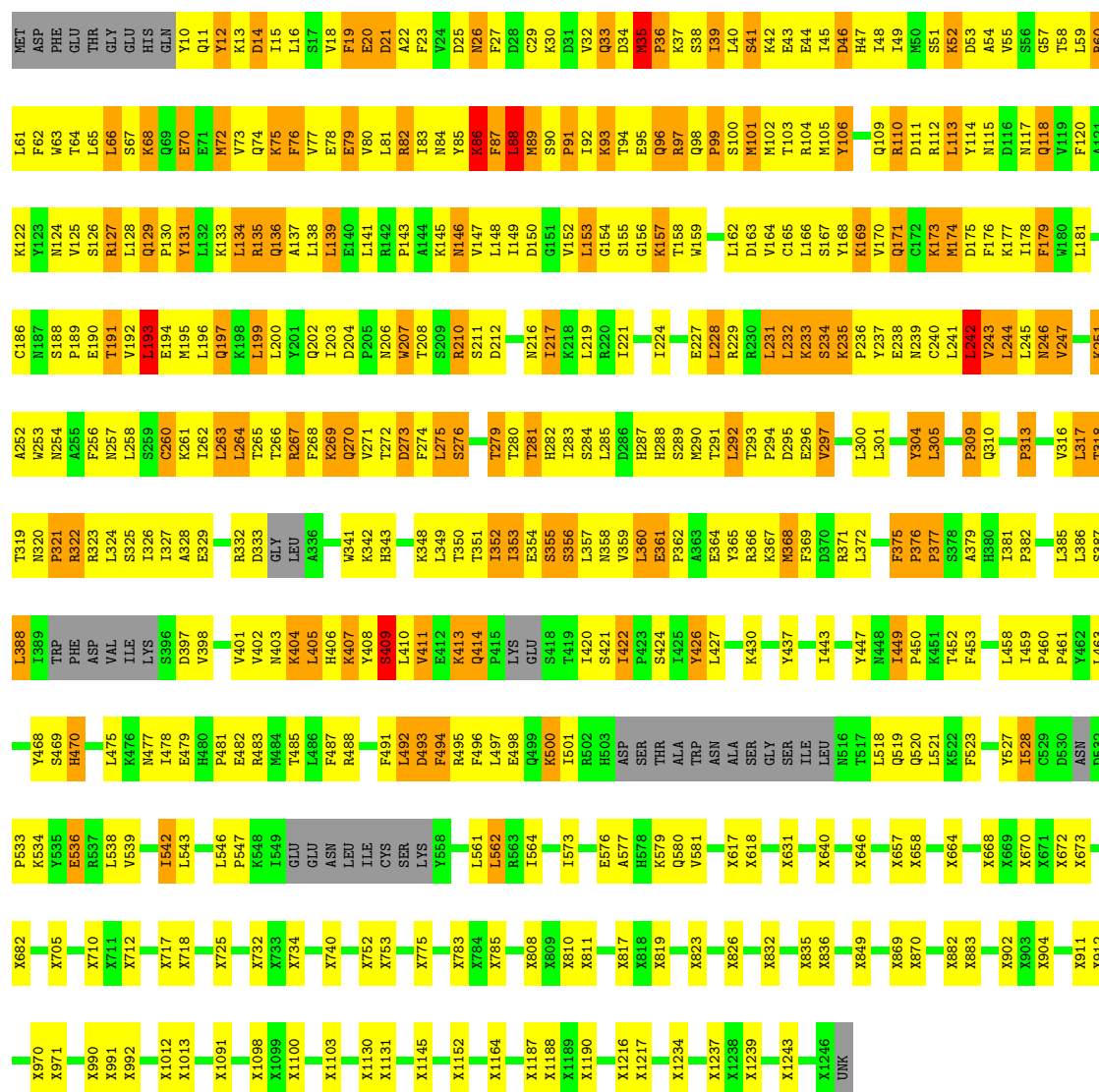






• Molecule 1: Apaf-1 related killer DARK

Chain M: 55% 30% 10%



• Molecule 1: Apaf-1 related killer DARK

Chain N: 55% 30% 10%

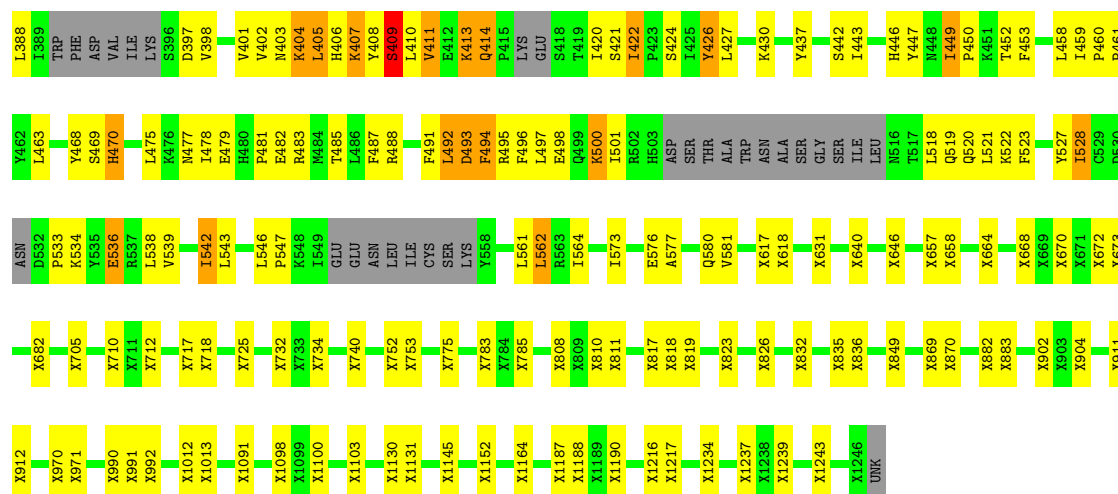


X912	X682	D532	Y462	L388	T319	A252	C186	K122	L61
X970	X705	K534	L463	L389	N320	W253	N187	Y123	F62
X971	X706	K535	Y468	TRP	P321	N254	P189	V125	W63
X990	X710	E536	H469	ASP	R323	A255	P189	V126	T64
X991	X711	L538	H470	VAL	L324	N257	T191	R127	L65
X992	X712	V539	L475	ILE	S325	L258	V192	L128	L66
X1012	X717	I542	L478	S396	LVS	S259	L193	Q129	K68
X1013	X718	L543	E479	V398	A328	L262	E194	P130	Q69
X1091	X725	L546	H480	V401	R332	L263	K198	L134	W72
X1098	X732	P547	E482	V402	D333	T265	L199	R135	V73
X1099	X733	K548	R483	N403	GLY	T266	L200	Q136	K75
X1100	X734	I549	H484	K404	LEU	R267	Y201	A137	F76
X1103	X740	GLU	H485	L405	A336	F268	Q202	L138	V77
X1130	X745	GLU	L486	H406		K269	L203	L139	E78
X1131	X752	LEU	R488	Y407	K341	Q270	D204	E140	E79
X1133	X753	ILE	F491	Y408	K342	T272	P205	L141	V80
X1145	X755	CVS	L492	L410	H343	D273	N206	R142	L81
X1152	X763	LYS	D493	V411	K348	L274	T208	P143	T83
X1164	X784	Y558	F494	E412	L349	L275	S209	K145	T83
X1187	X808	L561	R496	Q414	T351	S276	R210	K146	N84
X1188	X809	L562	L497	P415	L352			Y147	K86
X1190	X811	R563	E498	L415	L353	T280	D212	L148	F87
X1216	X817	L564	Q499	GLU	E354	T281	N216	D150	N89
X1217	X818	R577	ASP	S418	S355	H282	L217	G151	S90
X1237	X819	H578	SER	T419	S356	L283	K218	V152	P91
X1238	X823	K579	THR	I420	L357	S284	L219	L153	I92
X1239	X826	Q580	TRP	Y426	N358	L285	R220	G154	K93
X1246	X832	V581	ALA	L427	V359	D286	I221	S155	T94
UNK	X835	X617	ALA	E428	L360	H287	T224	K156	E95
	X836	X618	SER	K430	E361	H288		T157	Q96
	X837	X631	GLY	K430	S362	S289	E227	T158	R97
	X838	X631	ILE	K430	E364	M290	L228	W159	Q98
	X839	X640	LEU	K430	Y365	T291	R229		P99
	X849	X646	LEU	L429	R366	L292	R230	L162	S100
	X869	X657	SER	L429	K367	T293	R230	D163	M101
	X870	X658	GLY	K430	K367	P294	L231	V164	M102
	X879	X664	ILE	K430	M368	D295	L232	C165	T103
	X882	X668	LEU	K430	F369	E296	K233	L166	R104
	X883	X669	LEU	K430	D370	V297	S234	S167	M105
	X902	X670	LEU	K430	R371	L300	K235	Y168	Y106
	X903	X671	LEU	K430	L372	L301	P236	K169	
	X904	X672	LEU	K430	L372	L302	Y237	V170	Q109
	X911	X672	LEU	K430	L372	L302	Y237	Q171	R110
								C172	D111
								K173	R112
								M174	L113
								D175	Y114
								F176	N115
								K177	D116
								L178	N117
								F179	Q118
								W180	V119
								L181	F120
									A121

• Molecule 1: Apaf-1 related killer DARK

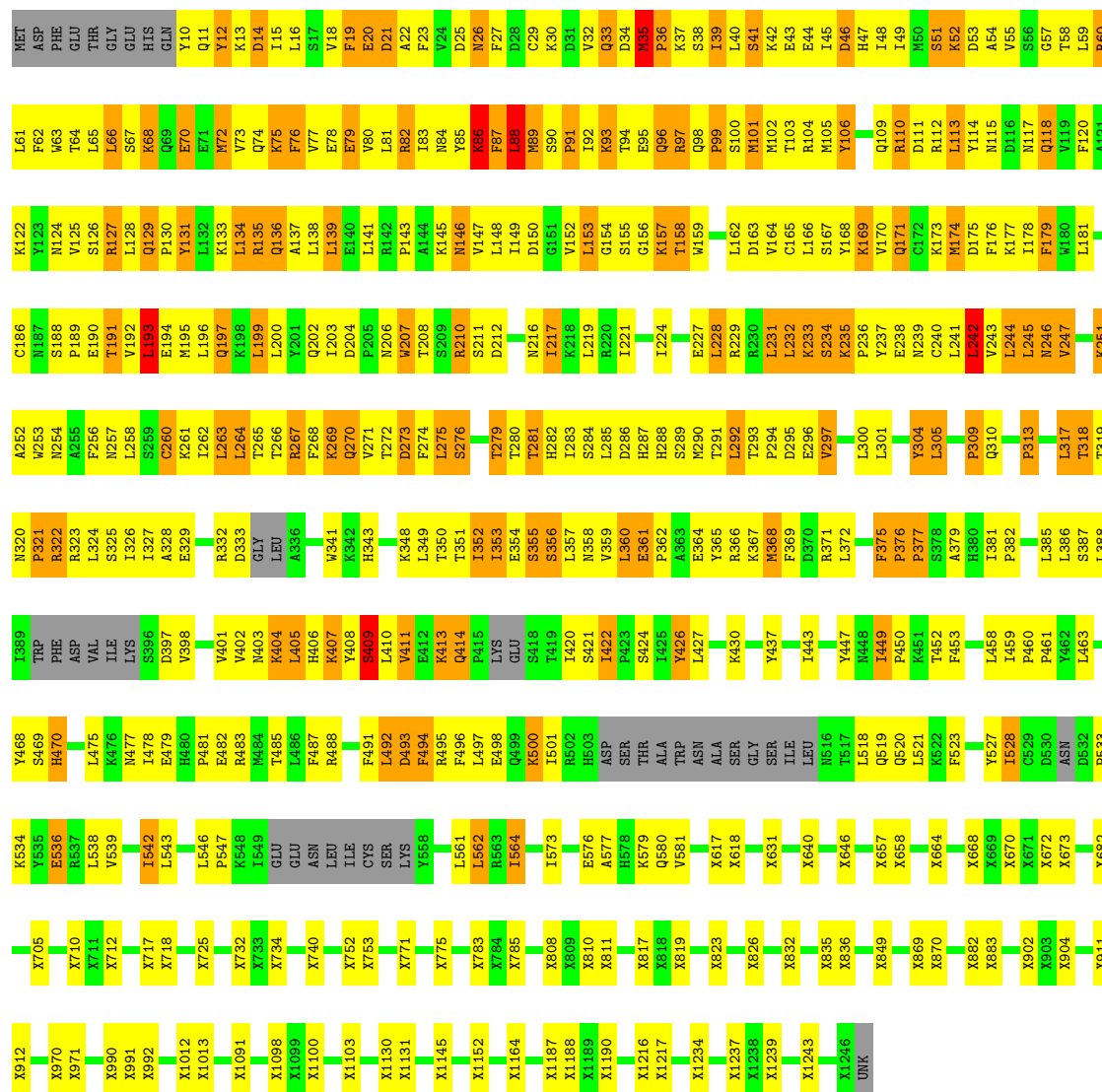
Chain O:  55% 30% 10%

T319	A252	C186	K122	L61	MET
N320	N253	N187	Y123	F62	ASP
P321	N254	S188	N124	W63	PHE
R322	A255	P189	V125	T64	GLU
R323	F256	E190	S126	L65	THR
L324	N257	T191	R127	L66	GLY
S325	L258	V192	L128	S67	GLU
I326	S259	L193	Q129	K68	GLN
A327	C260	E194	P130	Q69	
A328	K261	M195	Y131	E70	Y10
E329	L262	L196	L132	F71	Q11
	L263	Q197	K133	W72	Y12
R332	L264	K198	L134	V73	K13
D333	T265	L199	R135	Q74	D14
GLY	T266	L200	Q136	K75	I15
LEU	R267	Y201	A137	F76	L16
A336	F268	Q202	L138	V77	S17
	K269	L203	L139	E78	V18
W341	Q270	D204	E140	E79	F19
K342	V271	P205	L141	V80	E20
H343	T272	N206	R142	L81	D21
	D273	W207	P143	R82	A22
K348	F274	T208	A144	I83	F23
L349	L275	S209	K145	N84	V24
T350	S276	R210	N146	Y85	D25
	T279	S211	V147	K86	N26
I352	T280	D212	L148	F87	F27
K353	T281	N216	I149	L88	D28
S354	R282	L217	D150	M89	G29
S355	H283	K218	G151	S90	K30
S356	L283	L219	V152	P91	D31
N358	S284	L219	L153	I92	V32
S359	L285	R220	G154	K93	Q33
	D286	I221	S155	T94	D34
L360	H287		G156	E95	M35
E361	H288	I224	K157	Q96	K36
P362	T289	E227	T158	R97	R37
E364	N290	L228	W159	Q98	S38
T365	T291	R229	L162	P99	I39
R366	L292	V365	D163	S100	L40
K367	T293	R230	V164	M101	S41
M368	D295	L231	L162	M102	K42
F369	E296	L232	C165	T103	E43
	V297	K233	L166	R104	E44
D370		S234	S167	M105	I45
R371	L300	K235	Y168	Y106	D46
L372	L301	P236	K169		H47
	L302	Y237	V170	Q109	I48
F375	K303	E238	Q171	R110	I49
P377	Y304	N239	C172	D111	M50
S378	L305	C240	K173	R112	S51
A379		L241	M174	L113	K52
H380	P309	L242	D175	Y114	D53
L381	Q310	V243	F176	N115	A54
P382		L244	K177	D116	S55
	P313	L245	I178	N117	V56
		N246	F179	Q118	T57
L385	P313	V247	Y180	V119	G58
L386	L317		L181	F120	L59
R387		Y251		E121	D60

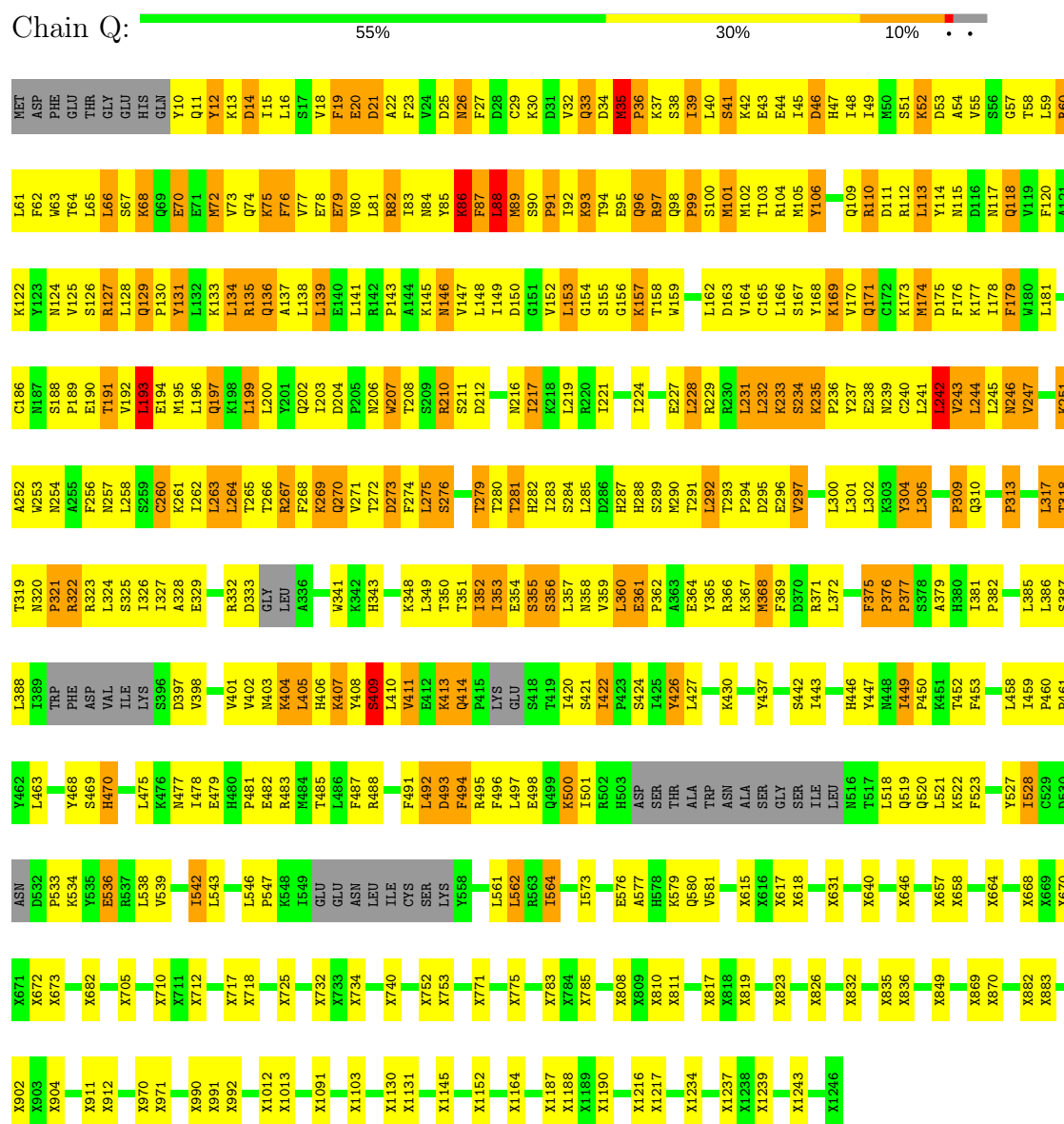


• Molecule 1: Apaf-1 related killer DARK

Chain P: 55% 30% 11%



• Molecule 1: Apaf-1 related killer DARK



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	9354	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each particle	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	6600	Depositor
Magnification	104748	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.58	4/4548 (0.1%)	0.77	12/6149 (0.2%)
1	C	0.57	3/4548 (0.1%)	0.77	13/6149 (0.2%)
1	D	0.57	3/4548 (0.1%)	0.77	12/6149 (0.2%)
1	E	0.57	3/4548 (0.1%)	0.77	13/6149 (0.2%)
1	F	0.57	3/4548 (0.1%)	0.77	12/6149 (0.2%)
1	G	0.57	3/4548 (0.1%)	0.77	13/6149 (0.2%)
1	H	0.57	3/4548 (0.1%)	0.77	12/6149 (0.2%)
1	I	0.57	3/4548 (0.1%)	0.77	13/6149 (0.2%)
1	J	0.57	3/4548 (0.1%)	0.77	12/6149 (0.2%)
1	K	0.57	3/4548 (0.1%)	0.77	13/6149 (0.2%)
1	L	0.57	3/4548 (0.1%)	0.77	12/6149 (0.2%)
1	M	0.57	3/4548 (0.1%)	0.77	13/6149 (0.2%)
1	N	0.57	3/4548 (0.1%)	0.77	12/6149 (0.2%)
1	O	0.57	3/4548 (0.1%)	0.77	13/6149 (0.2%)
1	P	0.57	3/4548 (0.1%)	0.77	12/6149 (0.2%)
1	Q	0.57	3/4548 (0.1%)	0.77	13/6149 (0.2%)
All	All	0.57	49/72768 (0.1%)	0.77	200/98384 (0.2%)

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
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
1	Q	0	6
All	All	0	81

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	86	LYS	CA-CB	-12.08	1.27	1.53
1	E	86	LYS	CA-CB	-12.08	1.27	1.53
1	G	86	LYS	CA-CB	-12.08	1.27	1.53
1	I	86	LYS	CA-CB	-12.08	1.27	1.53
1	K	86	LYS	CA-CB	-12.08	1.27	1.53

The worst 5 of 200 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	411	VAL	N-CA-CB	-10.46	88.48	111.50
1	E	411	VAL	N-CA-CB	-10.46	88.48	111.50
1	G	411	VAL	N-CA-CB	-10.46	88.48	111.50
1	I	411	VAL	N-CA-CB	-10.46	88.48	111.50
1	K	411	VAL	N-CA-CB	-10.46	88.48	111.50

There are no chirality outliers.

5 of 81 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	276	SER	Peptide
1	A	281	THR	Mainchain
1	A	33	GLN	Peptide
1	A	36	PRO	Peptide
1	A	75	LYS	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7031	0	5108	1000	0
1	C	7031	0	5108	1007	0
1	D	7031	0	5108	1010	0
1	E	7031	0	5108	1010	0
1	F	7031	0	5108	1022	0
1	G	7031	0	5108	1007	0
1	H	7031	0	5108	1018	0
1	I	7031	0	5108	1008	0
1	J	7031	0	5108	1024	0
1	K	7031	0	5108	1010	0
1	L	7031	0	5108	1009	0
1	M	7031	0	5108	1004	0
1	N	7031	0	5108	1021	0
1	O	7031	0	5108	1007	0
1	P	7031	0	5108	1021	0
1	Q	7036	0	5106	1003	0
2	C	30	0	12	19	0
2	D	30	0	12	20	0
2	E	30	0	12	19	0
2	F	30	0	12	19	0
2	G	30	0	12	19	0
2	H	30	0	12	20	0
2	I	30	0	12	18	0
2	J	30	0	12	19	0
2	K	30	0	12	20	0
2	L	30	0	12	20	0
2	M	30	0	12	19	0
2	N	30	0	12	18	0
2	O	30	0	12	18	0
2	P	30	0	12	19	0
2	Q	30	0	12	19	0
All	All	112951	0	81906	15693	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 81.

The worst 5 of 15693 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:N:174:MET:CE	1:N:241:LEU:HB2	1.26	1.66
1:J:174:MET:CE	1:J:241:LEU:HB2	1.26	1.66
1:M:174:MET:CE	1:M:241:LEU:HB2	1.26	1.64
1:C:174:MET:CE	1:C:241:LEU:HB2	1.26	1.64
1:I:174:MET:CE	1:I:241:LEU:HB2	1.26	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	529/1103 (48%)	468 (88%)	56 (11%)	5 (1%)	20	63
1	C	529/1103 (48%)	469 (89%)	55 (10%)	5 (1%)	20	63
1	D	529/1103 (48%)	468 (88%)	56 (11%)	5 (1%)	20	63
1	E	529/1103 (48%)	469 (89%)	55 (10%)	5 (1%)	20	63
1	F	529/1103 (48%)	468 (88%)	56 (11%)	5 (1%)	20	63
1	G	529/1103 (48%)	469 (89%)	55 (10%)	5 (1%)	20	63
1	H	529/1103 (48%)	468 (88%)	56 (11%)	5 (1%)	20	63
1	I	529/1103 (48%)	469 (89%)	55 (10%)	5 (1%)	20	63
1	J	529/1103 (48%)	468 (88%)	56 (11%)	5 (1%)	20	63
1	K	529/1103 (48%)	469 (89%)	55 (10%)	5 (1%)	20	63
1	L	529/1103 (48%)	468 (88%)	56 (11%)	5 (1%)	20	63
1	M	529/1103 (48%)	469 (89%)	55 (10%)	5 (1%)	20	63
1	N	529/1103 (48%)	468 (88%)	56 (11%)	5 (1%)	20	63
1	O	529/1103 (48%)	469 (89%)	55 (10%)	5 (1%)	20	63
1	P	529/1103 (48%)	468 (88%)	56 (11%)	5 (1%)	20	63
1	Q	529/1103 (48%)	469 (89%)	55 (10%)	5 (1%)	20	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	8464/17648 (48%)	7496 (89%)	888 (10%)	80 (1%)	25	63

5 of 80 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	PRO
1	A	409	SER
1	C	99	PRO
1	C	409	SER
1	D	99	PRO

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	500/551 (91%)	368 (74%)	132 (26%)	0	5
1	C	500/551 (91%)	369 (74%)	131 (26%)	0	5
1	D	500/551 (91%)	368 (74%)	132 (26%)	0	5
1	E	500/551 (91%)	369 (74%)	131 (26%)	0	5
1	F	500/551 (91%)	368 (74%)	132 (26%)	0	5
1	G	500/551 (91%)	369 (74%)	131 (26%)	0	5
1	H	500/551 (91%)	368 (74%)	132 (26%)	0	5
1	I	500/551 (91%)	369 (74%)	131 (26%)	0	5
1	J	500/551 (91%)	368 (74%)	132 (26%)	0	5
1	K	500/551 (91%)	369 (74%)	131 (26%)	0	5
1	L	500/551 (91%)	368 (74%)	132 (26%)	0	5
1	M	500/551 (91%)	369 (74%)	131 (26%)	0	5
1	N	500/551 (91%)	368 (74%)	132 (26%)	0	5
1	O	500/551 (91%)	369 (74%)	131 (26%)	0	5
1	P	500/551 (91%)	368 (74%)	132 (26%)	0	5
1	Q	500/551 (91%)	369 (74%)	131 (26%)	0	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	8000/8816 (91%)	5896 (74%)	2104 (26%)	2 5

5 of 2104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	93	LYS
1	J	500	LYS
1	P	353	ILE
1	I	191	THR
1	J	52	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 190 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	117	ASN
1	J	406	HIS
1	P	288	HIS
1	I	146	ASN
1	J	47	HIS

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](#)

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DTP	C	1301	-	26,32,32	0.91	1 (3%)	26,50,50	1.66	2 (7%)
2	DTP	D	1301	-	26,32,32	0.91	1 (3%)	26,50,50	1.66	2 (7%)
2	DTP	E	1301	-	26,32,32	0.91	1 (3%)	26,50,50	1.66	2 (7%)
2	DTP	F	1301	-	26,32,32	0.91	1 (3%)	26,50,50	1.66	2 (7%)
2	DTP	G	1301	-	26,32,32	0.91	1 (3%)	26,50,50	1.66	2 (7%)
2	DTP	H	1301	-	26,32,32	0.91	1 (3%)	26,50,50	1.66	2 (7%)
2	DTP	I	1301	-	26,32,32	0.91	1 (3%)	26,50,50	1.66	2 (7%)
2	DTP	J	1301	-	26,32,32	0.91	1 (3%)	26,50,50	1.66	2 (7%)
2	DTP	K	1301	-	26,32,32	0.91	1 (3%)	26,50,50	1.66	2 (7%)
2	DTP	L	1301	-	26,32,32	0.91	1 (3%)	26,50,50	1.66	2 (7%)
2	DTP	M	1301	-	26,32,32	0.91	1 (3%)	26,50,50	1.66	2 (7%)
2	DTP	N	1301	-	26,32,32	0.91	1 (3%)	26,50,50	1.66	2 (7%)
2	DTP	O	1301	-	26,32,32	0.91	1 (3%)	26,50,50	1.66	2 (7%)
2	DTP	P	1301	-	26,32,32	0.91	1 (3%)	26,50,50	1.66	2 (7%)
2	DTP	Q	1301	-	26,32,32	0.91	1 (3%)	26,50,50	1.66	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DTP	C	1301	-	-	0/18/34/34	0/3/3/3
2	DTP	D	1301	-	-	0/18/34/34	0/3/3/3
2	DTP	E	1301	-	-	0/18/34/34	0/3/3/3
2	DTP	F	1301	-	-	0/18/34/34	0/3/3/3
2	DTP	G	1301	-	-	0/18/34/34	0/3/3/3
2	DTP	H	1301	-	-	0/18/34/34	0/3/3/3
2	DTP	I	1301	-	-	0/18/34/34	0/3/3/3
2	DTP	J	1301	-	-	0/18/34/34	0/3/3/3
2	DTP	K	1301	-	-	0/18/34/34	0/3/3/3
2	DTP	L	1301	-	-	0/18/34/34	0/3/3/3
2	DTP	M	1301	-	-	0/18/34/34	0/3/3/3
2	DTP	N	1301	-	-	0/18/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DTP	O	1301	-	-	0/18/34/34	0/3/3/3
2	DTP	P	1301	-	-	0/18/34/34	0/3/3/3
2	DTP	Q	1301	-	-	0/18/34/34	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	1301	DTP	C5-C4	3.11	1.47	1.40
2	O	1301	DTP	C5-C4	3.11	1.47	1.40
2	M	1301	DTP	C5-C4	3.11	1.47	1.40
2	K	1301	DTP	C5-C4	3.11	1.47	1.40
2	I	1301	DTP	C5-C4	3.11	1.47	1.40

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1301	DTP	N3-C2-N1	-5.91	123.71	128.86
2	P	1301	DTP	N3-C2-N1	-5.91	123.71	128.86
2	L	1301	DTP	N3-C2-N1	-5.91	123.71	128.86
2	H	1301	DTP	N3-C2-N1	-5.91	123.71	128.86
2	N	1301	DTP	N3-C2-N1	-5.91	123.71	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 286 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1301	DTP	19	0
2	D	1301	DTP	20	0
2	E	1301	DTP	19	0
2	F	1301	DTP	19	0
2	G	1301	DTP	19	0
2	H	1301	DTP	20	0
2	I	1301	DTP	18	0
2	J	1301	DTP	19	0
2	K	1301	DTP	20	0
2	L	1301	DTP	20	0
2	M	1301	DTP	19	0
2	N	1301	DTP	18	0
2	O	1301	DTP	18	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	1301	DTP	19	0
2	Q	1301	DTP	19	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.