



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:32 PM BST

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 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

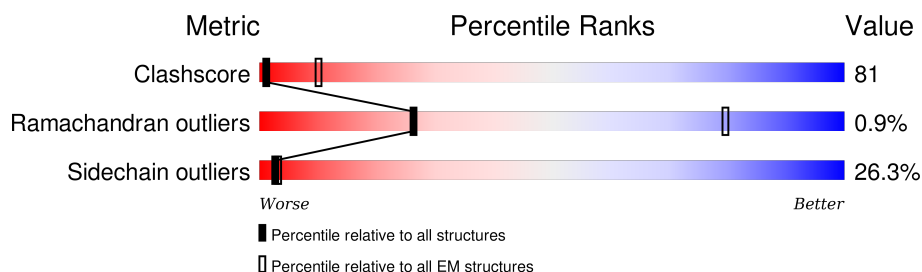
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	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	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	
1	L	1103	
1	M	1103	
1	N	1103	
1	O	1103	
1	P	1103	
1	Q	1103	

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.

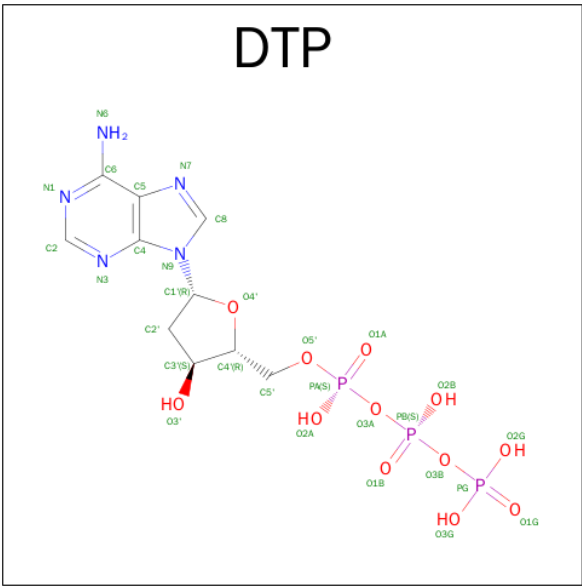
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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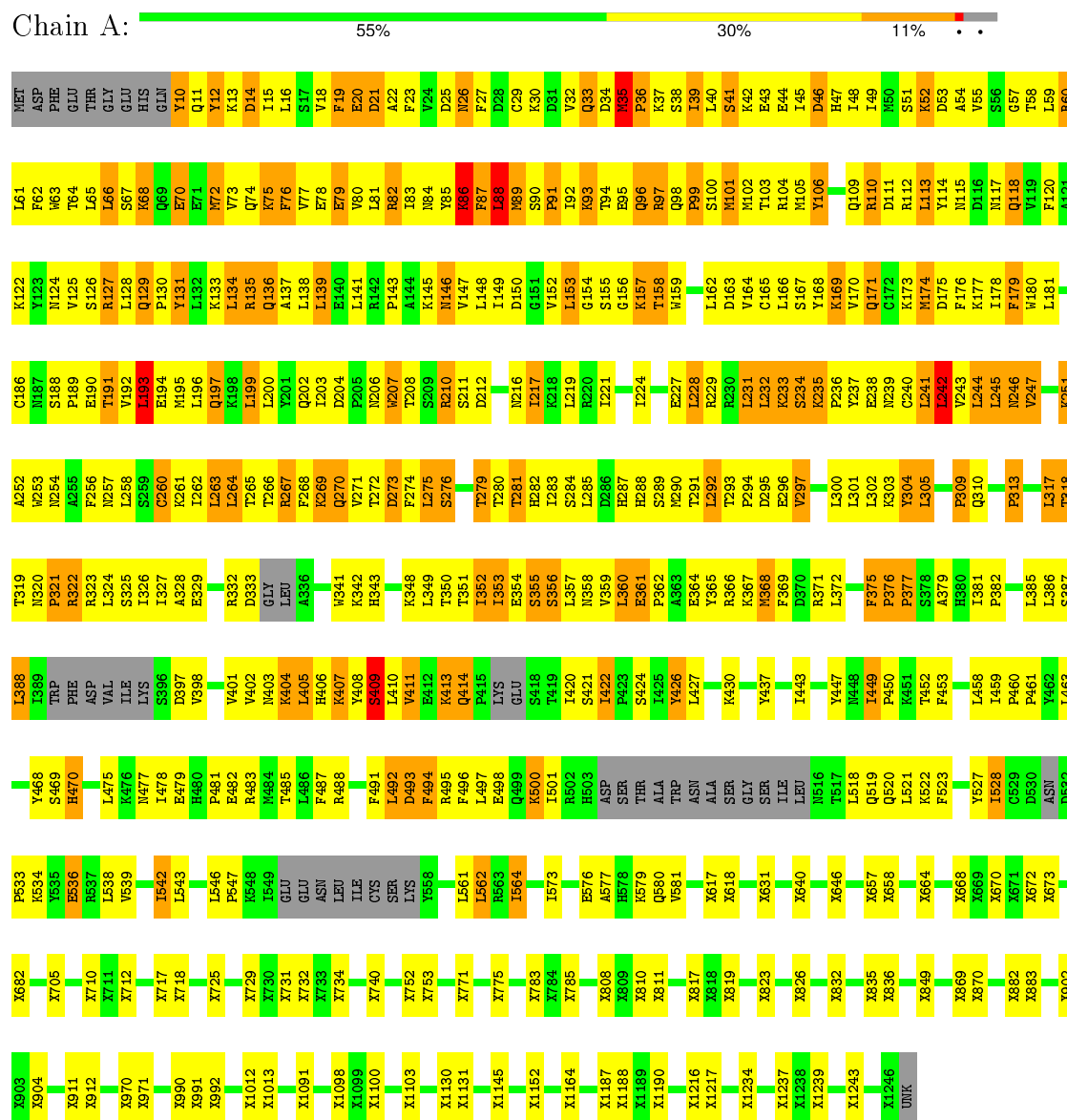
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Mol	Chain	Residues	Atoms					AltConf
2	P	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	Q	1	Total	C	N	O	P	0
			30	10	5	12	3	

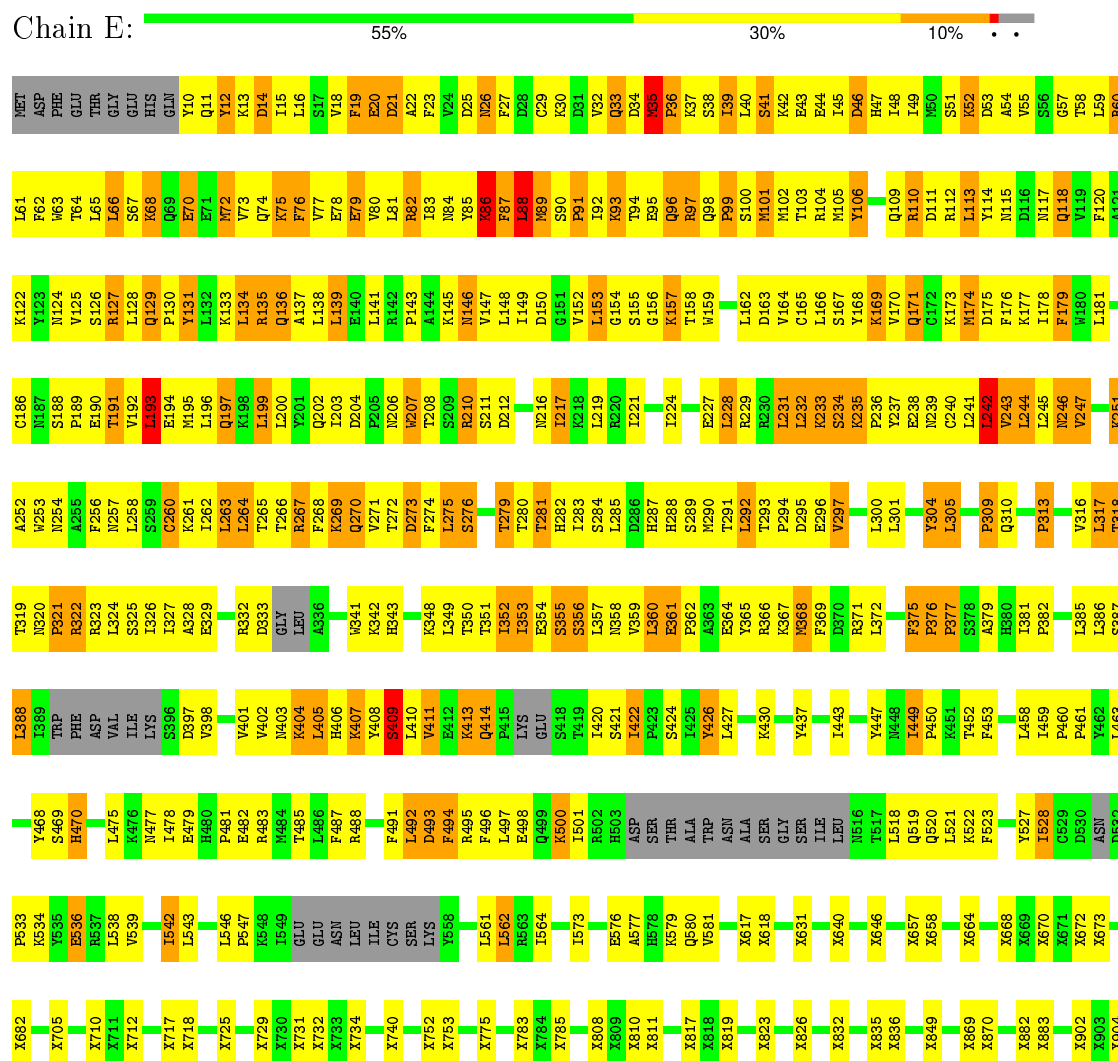
3 Residue-property plots

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



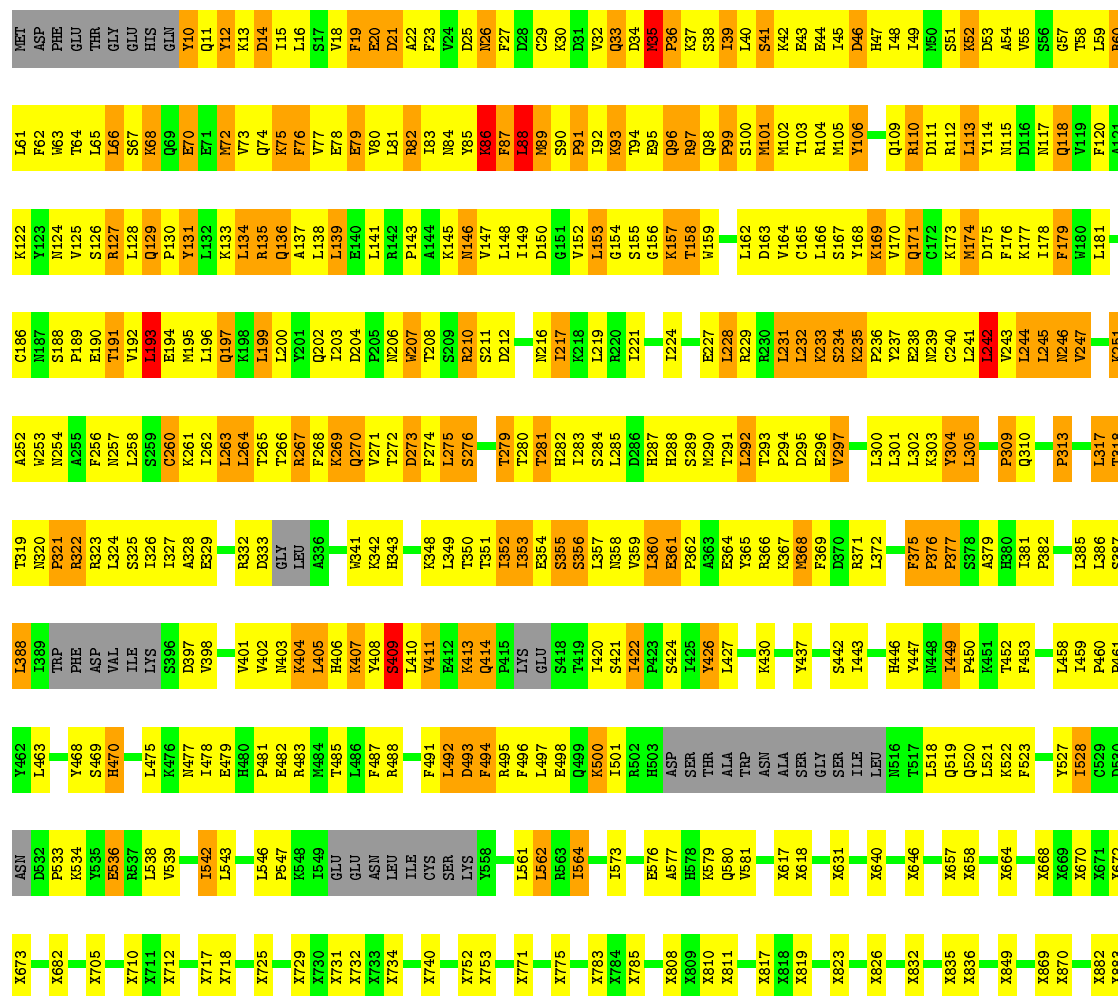
- Molecule 1: Apaf-1 related killer DARK





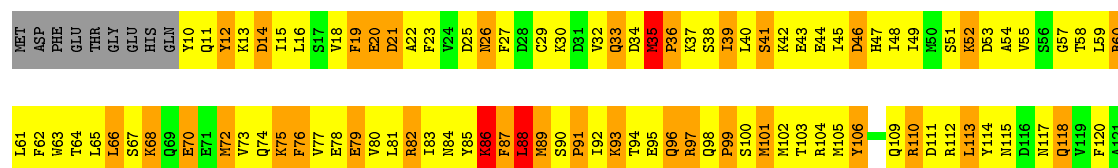
• Molecule 1: Apaf-1 related killer DARK

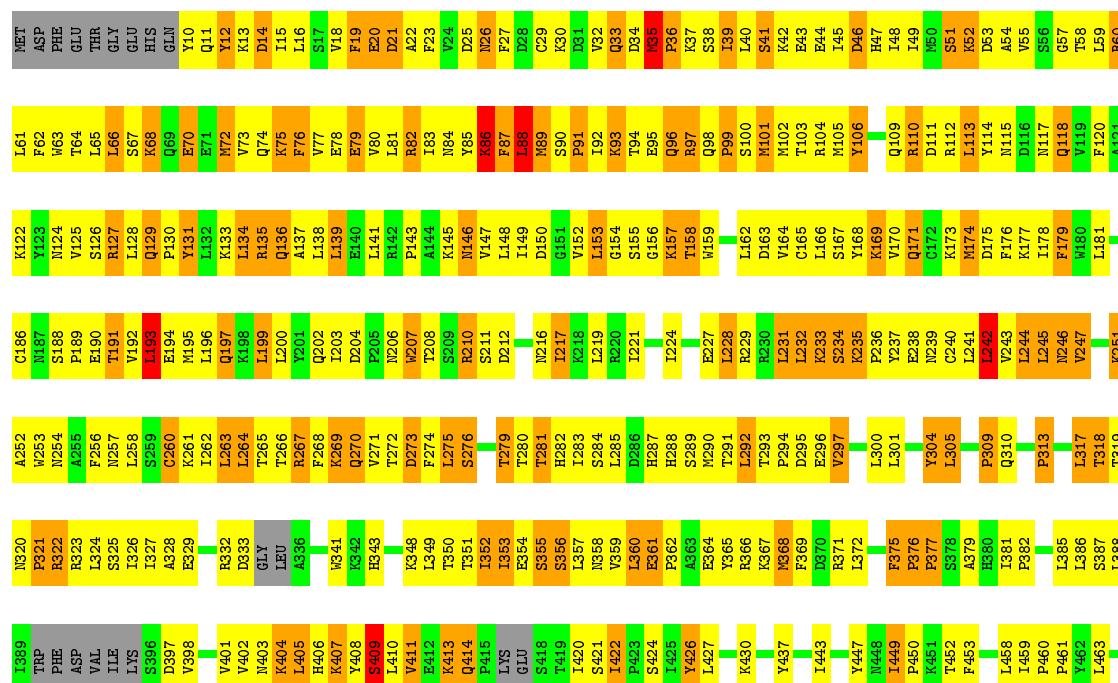
Chain F: 55% 30% 11% . .

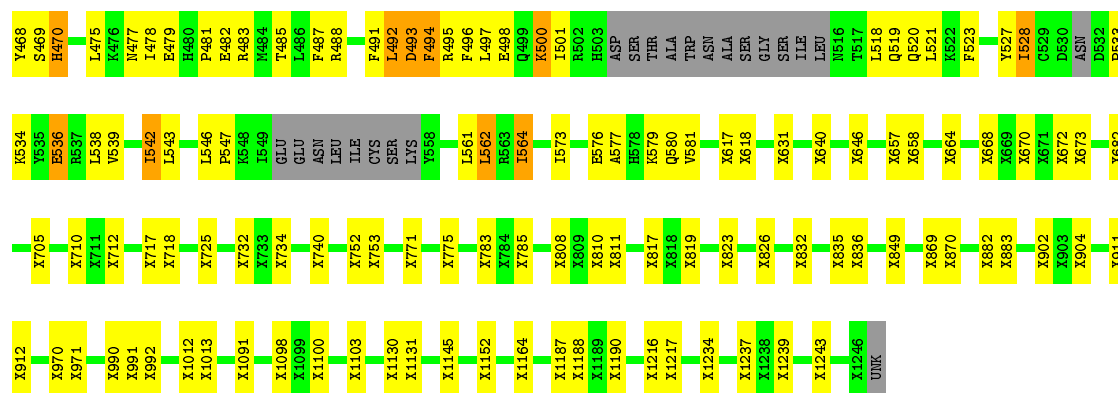


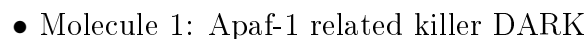
• Molecule 1: Apaf-1 related killer DARK

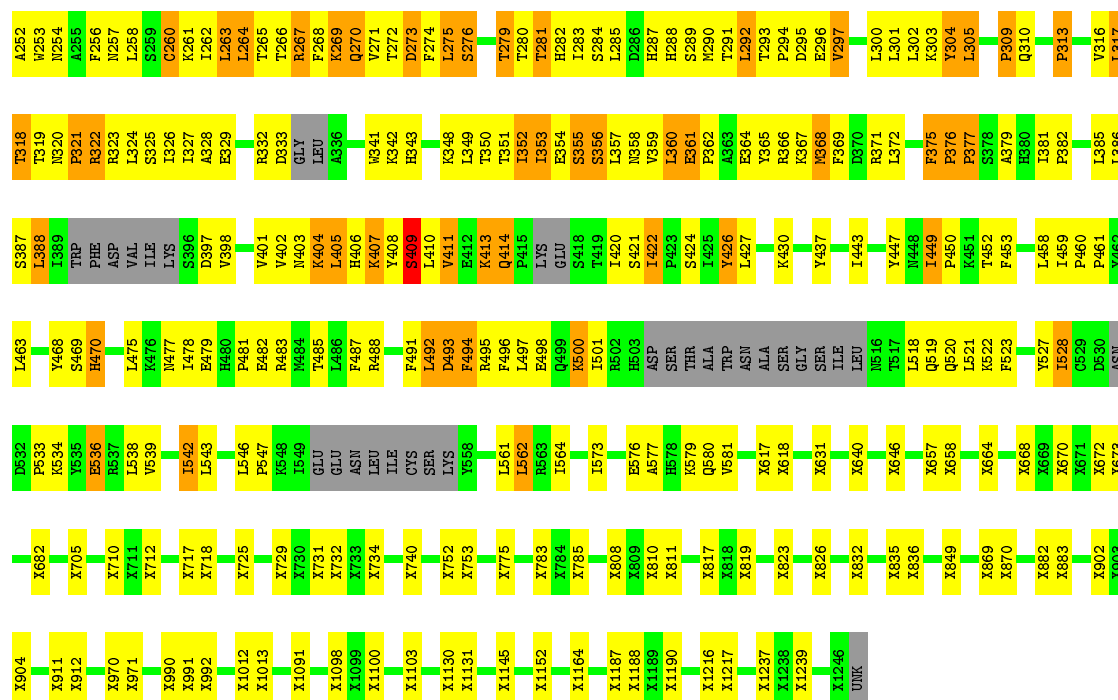
Chain G: 55% 30% 10% . .



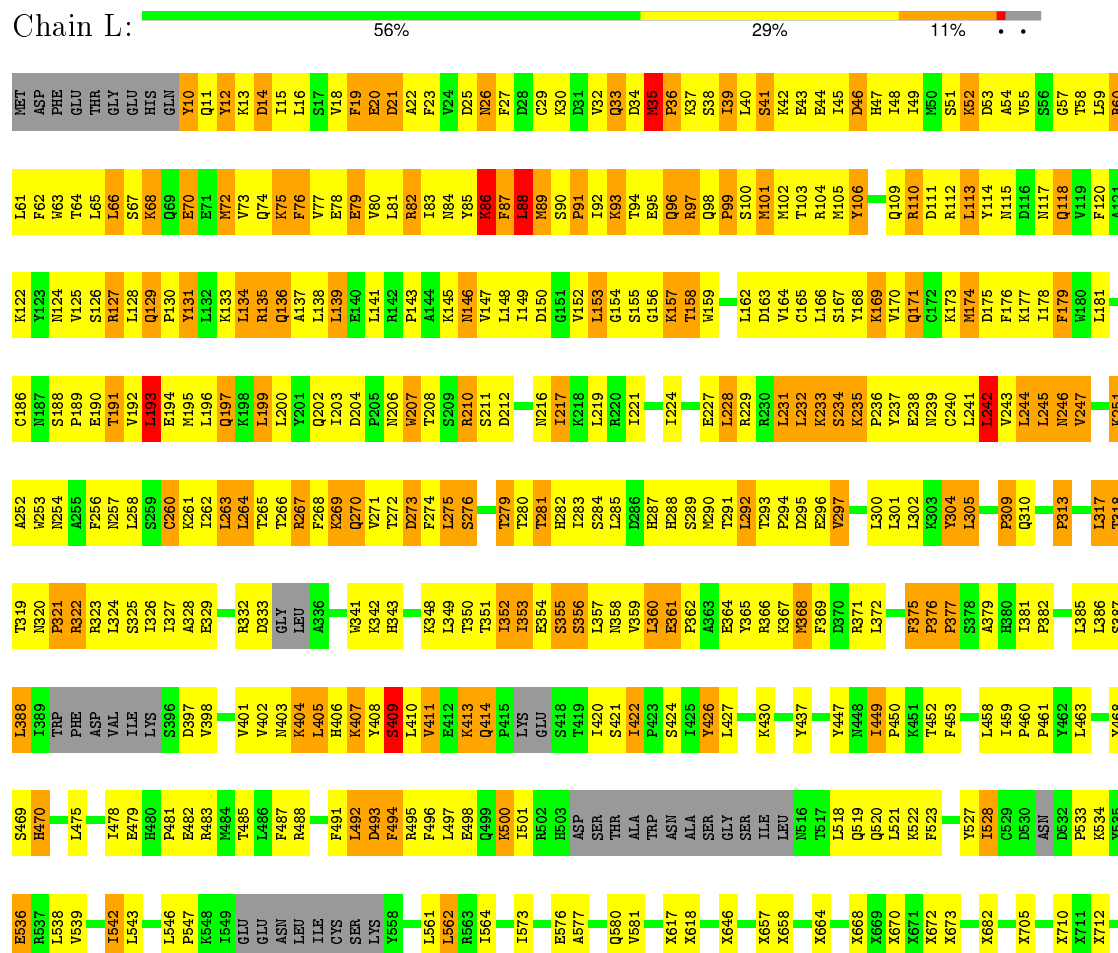


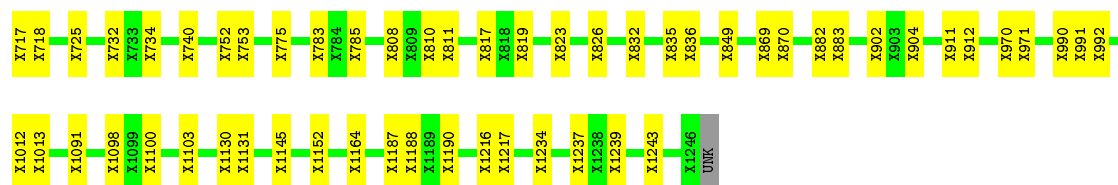






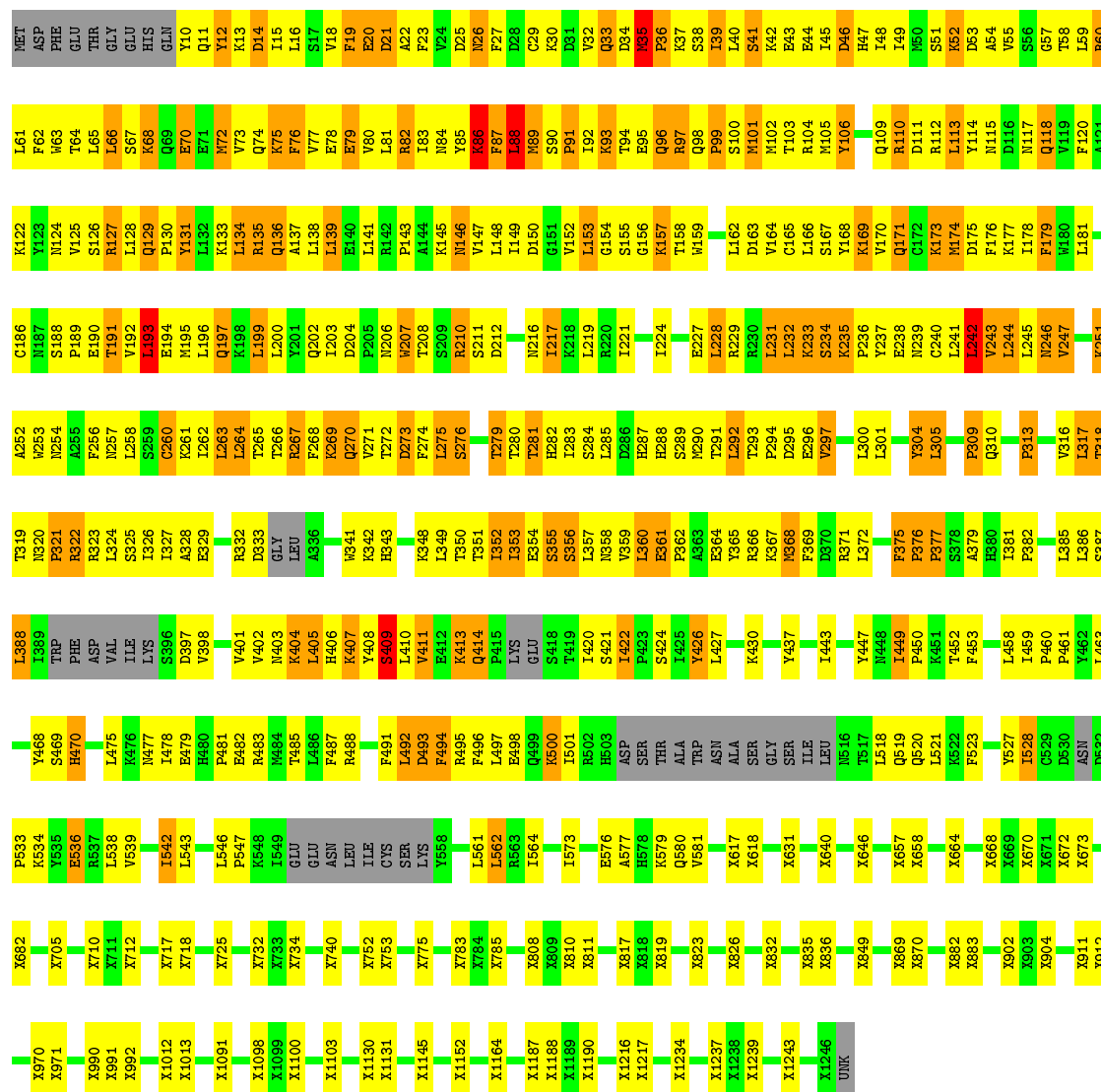
• Molecule 1: Apaf-1 related killer DARK





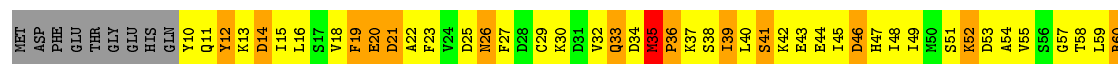
• Molecule 1: Apaf-1 related killer DARK

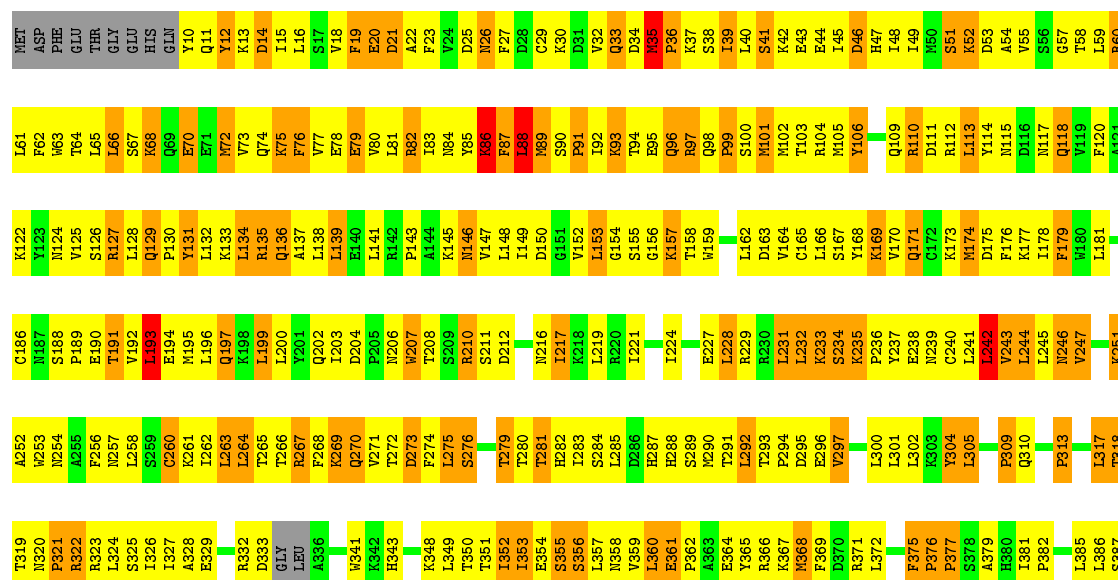
Chain M: 55% 30% 10%

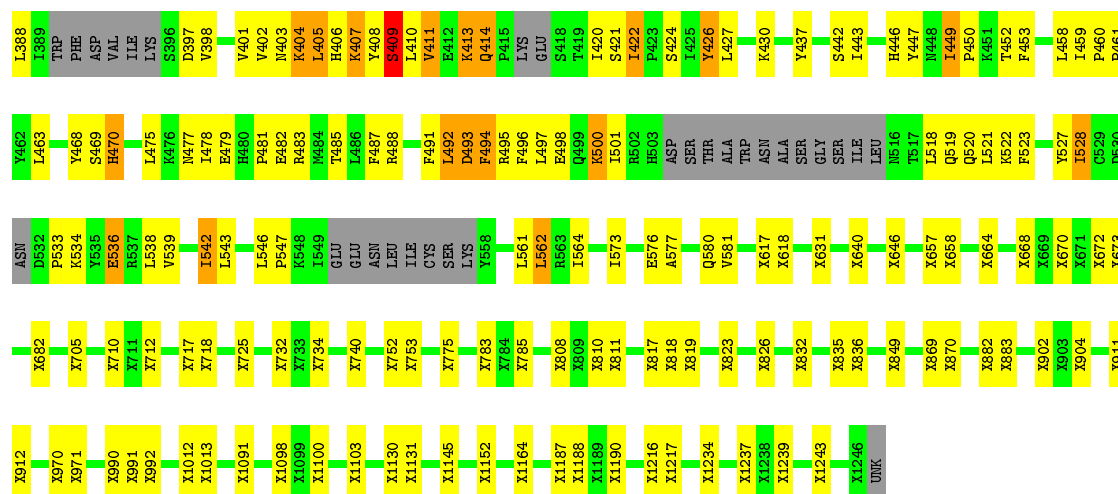


• Molecule 1: Apaf-1 related killer DARK

Chain N: 55% 30% 10%

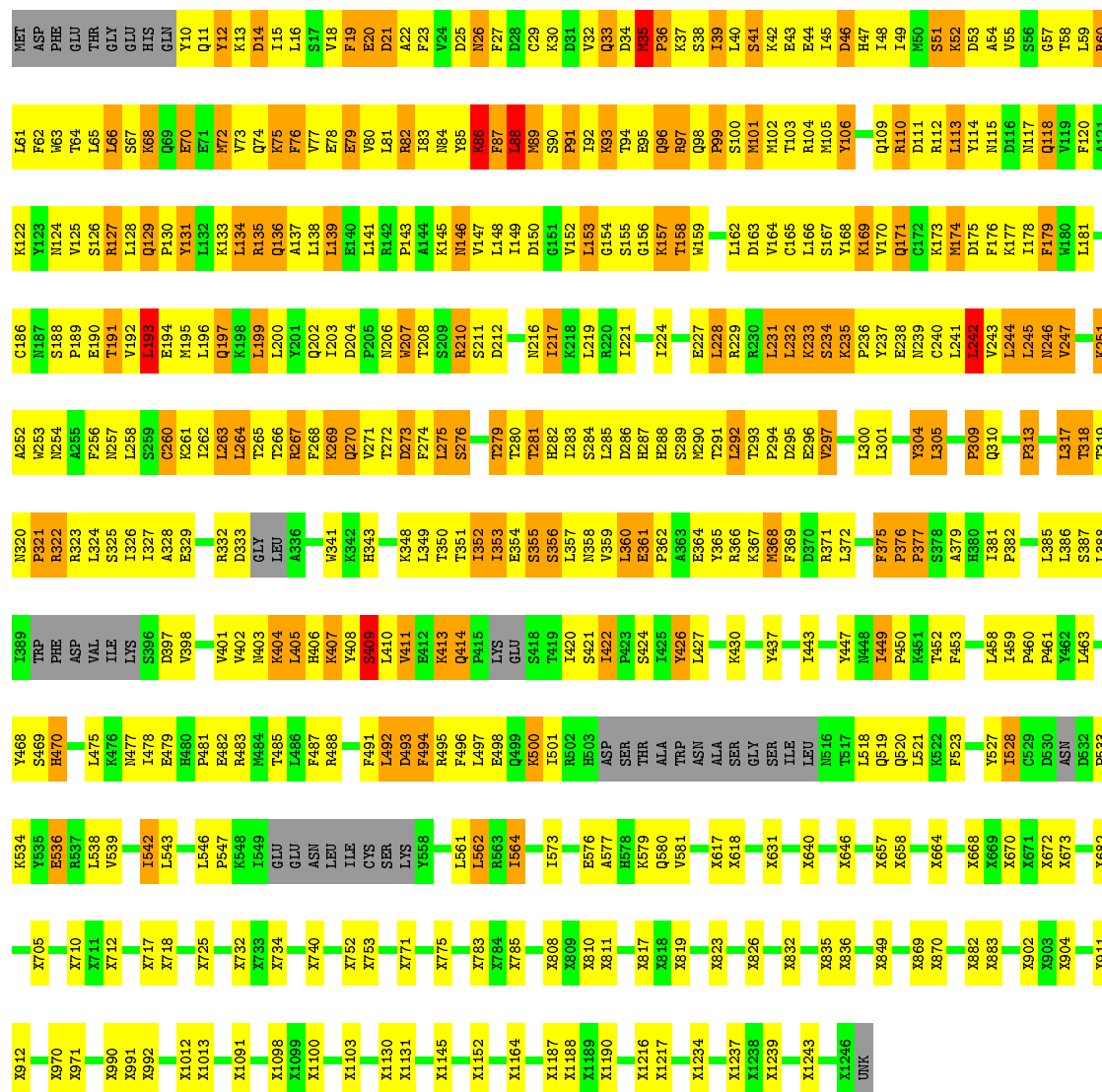




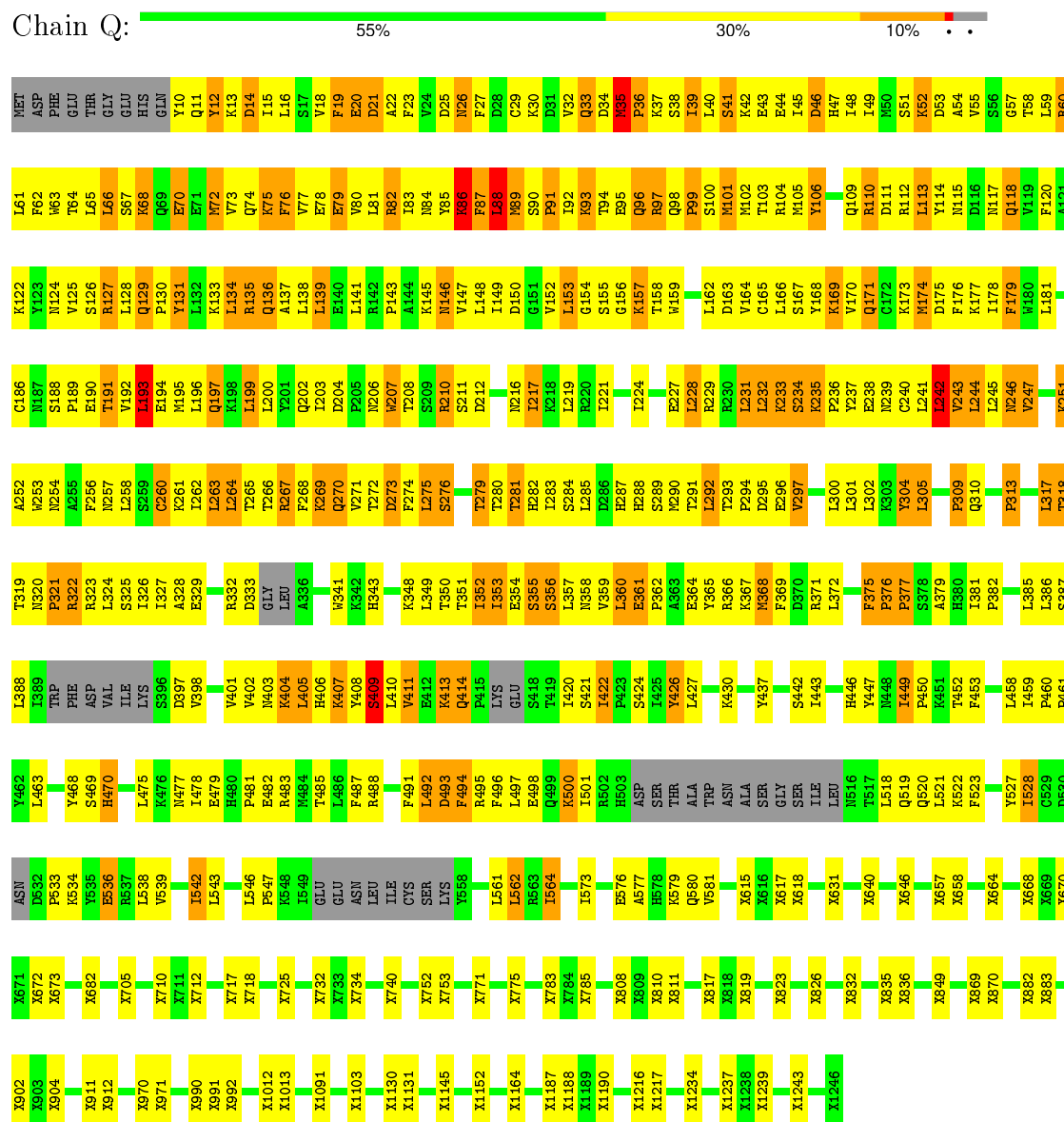


• Molecule 1: Apaf-1 related killer DARK

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 images	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	78000	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%)	21	66
1	C	529/1103 (48%)	469 (89%)	55 (10%)	5 (1%)	21	66
1	D	529/1103 (48%)	468 (88%)	56 (11%)	5 (1%)	21	66
1	E	529/1103 (48%)	469 (89%)	55 (10%)	5 (1%)	21	66
1	F	529/1103 (48%)	468 (88%)	56 (11%)	5 (1%)	21	66
1	G	529/1103 (48%)	469 (89%)	55 (10%)	5 (1%)	21	66
1	H	529/1103 (48%)	468 (88%)	56 (11%)	5 (1%)	21	66
1	I	529/1103 (48%)	469 (89%)	55 (10%)	5 (1%)	21	66
1	J	529/1103 (48%)	468 (88%)	56 (11%)	5 (1%)	21	66
1	K	529/1103 (48%)	469 (89%)	55 (10%)	5 (1%)	21	66
1	L	529/1103 (48%)	468 (88%)	56 (11%)	5 (1%)	21	66
1	M	529/1103 (48%)	469 (89%)	55 (10%)	5 (1%)	21	66
1	N	529/1103 (48%)	468 (88%)	56 (11%)	5 (1%)	21	66
1	O	529/1103 (48%)	469 (89%)	55 (10%)	5 (1%)	21	66
1	P	529/1103 (48%)	468 (88%)	56 (11%)	5 (1%)	21	66
1	Q	529/1103 (48%)	469 (89%)	55 (10%)	5 (1%)	21	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	8464/17648 (48%)	7496 (89%)	888 (10%)	80 (1%)	26	66

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	6
1	C	500/551 (91%)	369 (74%)	131 (26%)	0	6
1	D	500/551 (91%)	368 (74%)	132 (26%)	0	6
1	E	500/551 (91%)	369 (74%)	131 (26%)	0	6
1	F	500/551 (91%)	368 (74%)	132 (26%)	0	6
1	G	500/551 (91%)	369 (74%)	131 (26%)	0	6
1	H	500/551 (91%)	368 (74%)	132 (26%)	0	6
1	I	500/551 (91%)	369 (74%)	131 (26%)	0	6
1	J	500/551 (91%)	368 (74%)	132 (26%)	0	6
1	K	500/551 (91%)	369 (74%)	131 (26%)	0	6
1	L	500/551 (91%)	368 (74%)	132 (26%)	0	6
1	M	500/551 (91%)	369 (74%)	131 (26%)	0	6
1	N	500/551 (91%)	368 (74%)	132 (26%)	0	6
1	O	500/551 (91%)	369 (74%)	131 (26%)	0	6
1	P	500/551 (91%)	368 (74%)	132 (26%)	0	6
1	Q	500/551 (91%)	369 (74%)	131 (26%)	0	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	8000/8816 (91%)	5896 (74%)	2104 (26%)	3 6

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	-	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
2	DTP	D	1301	-	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
2	DTP	E	1301	-	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
2	DTP	F	1301	-	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
2	DTP	G	1301	-	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
2	DTP	H	1301	-	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
2	DTP	I	1301	-	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
2	DTP	J	1301	-	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
2	DTP	K	1301	-	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
2	DTP	L	1301	-	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
2	DTP	M	1301	-	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
2	DTP	N	1301	-	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
2	DTP	O	1301	-	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
2	DTP	P	1301	-	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)
2	DTP	Q	1301	-	25,32,32	0.92	1 (4%)	26,50,50	1.68	1 (3%)

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 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1301	DTP	N3-C2-N1	-6.57	123.71	128.87
2	P	1301	DTP	N3-C2-N1	-6.57	123.71	128.87
2	L	1301	DTP	N3-C2-N1	-6.57	123.71	128.87
2	H	1301	DTP	N3-C2-N1	-6.57	123.71	128.87
2	N	1301	DTP	N3-C2-N1	-6.57	123.71	128.87

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.