



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:06 PM BST

PDB ID : 4APW  
EMDB ID: : EMD-2068  
Title : Alp12 filament structure  
Authors : Popp, D.; Narita, A.; Lee, L.J.; Ghoshdastider, U.; Xue, B.; Srinivasan, R.;  
Balasubramanian, M.K.; Tanaka, T.; Robinson, R.C.  
Deposited on : 2012-04-06  
Resolution : 19.70 Å(reported)  
Based on PDB ID : 3JS6

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
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



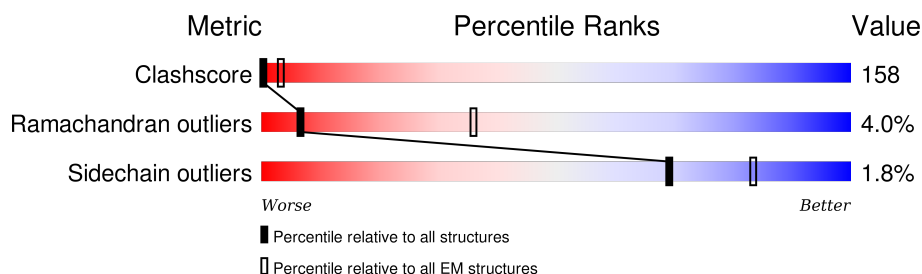
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 19.70 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  $\geq 3$ , 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	329	20% 63% 10% 5% •
1	B	329	19% 64% 10% 5% •
1	C	329	19% 64% 10% 5% •
1	D	329	24% 59% 11% 5% •
1	E	329	23% 60% 10% 5% •
1	F	329	20% 64% 10% 5% •
1	G	329	21% 63% 10% 5% •
1	H	329	23% 61% 10% 5% •
1	I	329	23% 60% 10% 5% •

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Mol	Chain	Length	Quality of chain
1	J	329	<div><div></div><div>21%63%10%5%</div></div>
1	K	329	<div><div></div><div>22%62%10%5%</div></div>
1	L	329	<div><div></div><div>24%60%10%5%</div></div>
1	M	329	<div><div></div><div>24%59%11%5%</div></div>
1	N	329	<div><div></div><div>19%64%10%5%</div></div>
1	O	329	<div><div></div><div>19%64%10%5%</div></div>
1	P	329	<div><div></div><div>21%63%10%5%</div></div>



## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 40752 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 ALP12.

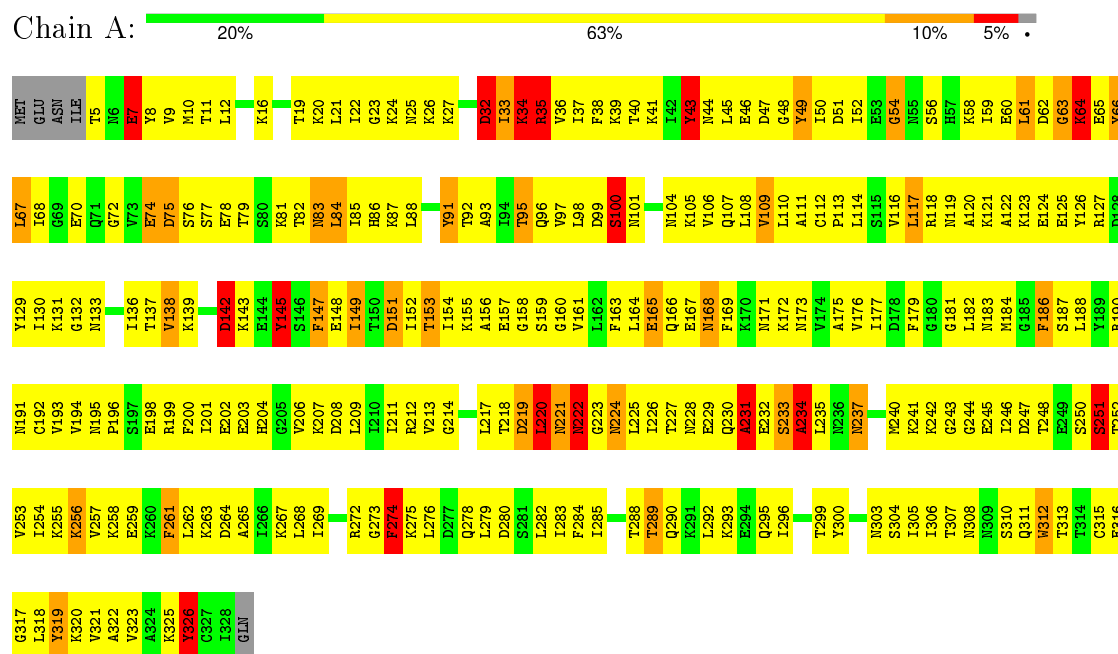
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	324	Total	C	N	O	S	0	1
			2547	1607	425	508	7		
1	B	324	Total	C	N	O	S	0	1
			2547	1607	425	508	7		
1	C	324	Total	C	N	O	S	0	1
			2547	1607	425	508	7		
1	D	324	Total	C	N	O	S	0	1
			2547	1607	425	508	7		
1	E	324	Total	C	N	O	S	0	1
			2547	1607	425	508	7		
1	F	324	Total	C	N	O	S	0	1
			2547	1607	425	508	7		
1	G	324	Total	C	N	O	S	0	1
			2547	1607	425	508	7		
1	H	324	Total	C	N	O	S	0	1
			2547	1607	425	508	7		
1	I	324	Total	C	N	O	S	0	1
			2547	1607	425	508	7		
1	J	324	Total	C	N	O	S	0	1
			2547	1607	425	508	7		
1	K	324	Total	C	N	O	S	0	1
			2547	1607	425	508	7		
1	L	324	Total	C	N	O	S	0	1
			2547	1607	425	508	7		
1	M	324	Total	C	N	O	S	0	1
			2547	1607	425	508	7		
1	N	324	Total	C	N	O	S	0	1
			2547	1607	425	508	7		
1	O	324	Total	C	N	O	S	0	1
			2547	1607	425	508	7		
1	P	324	Total	C	N	O	S	0	1
			2547	1607	425	508	7		



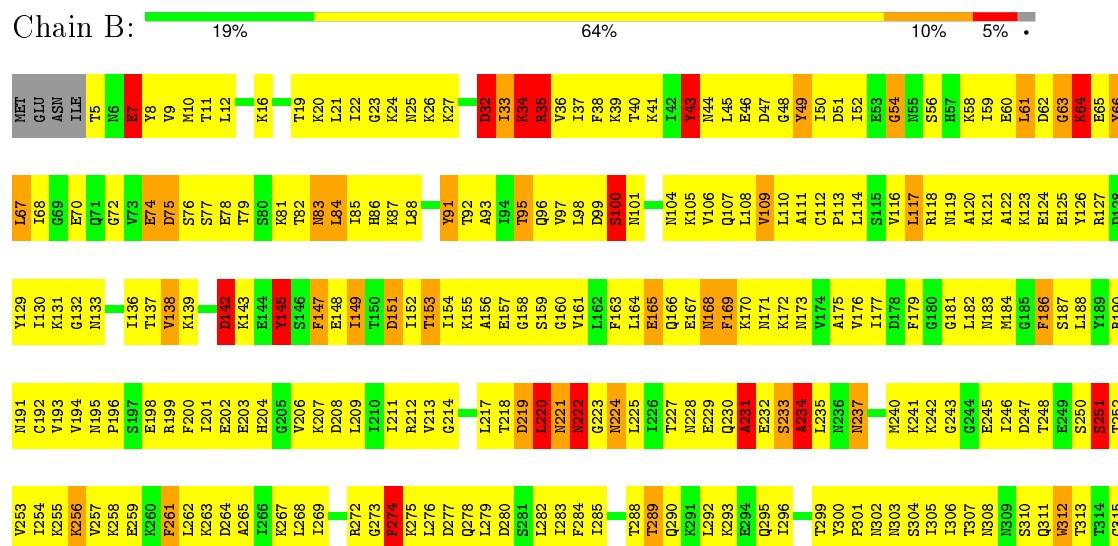
### 3 Residue-property plots

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: ALP12



#### • Molecule 1: ALP12



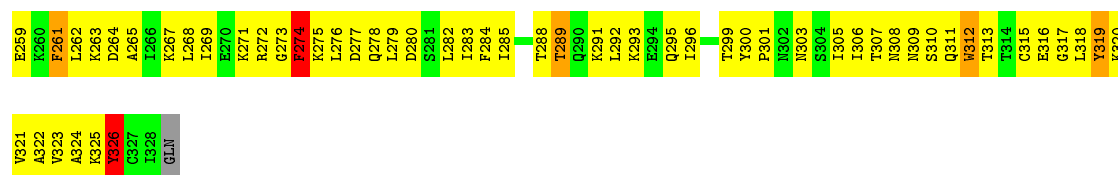






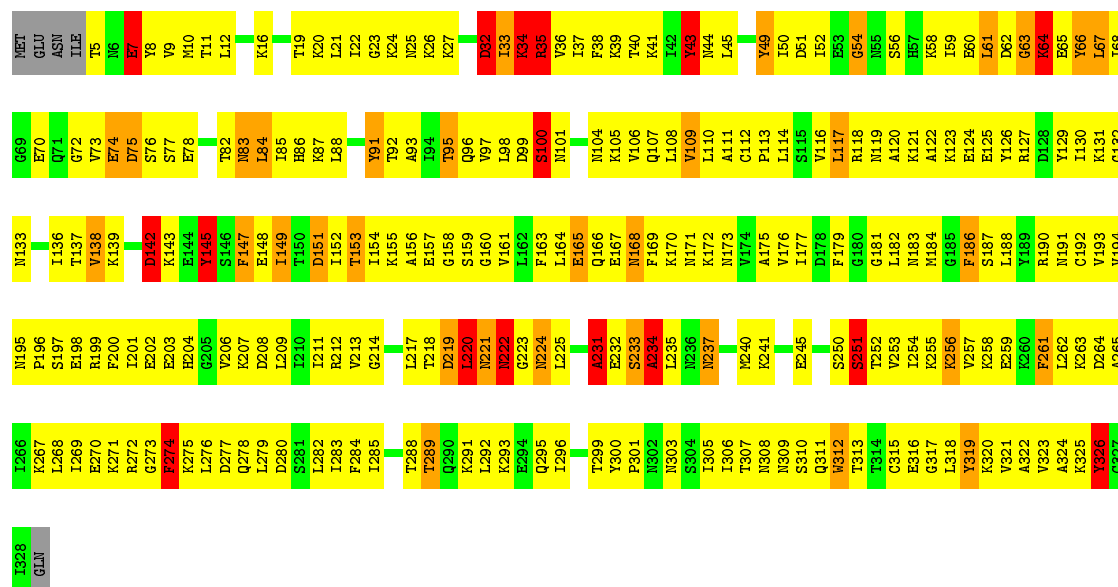






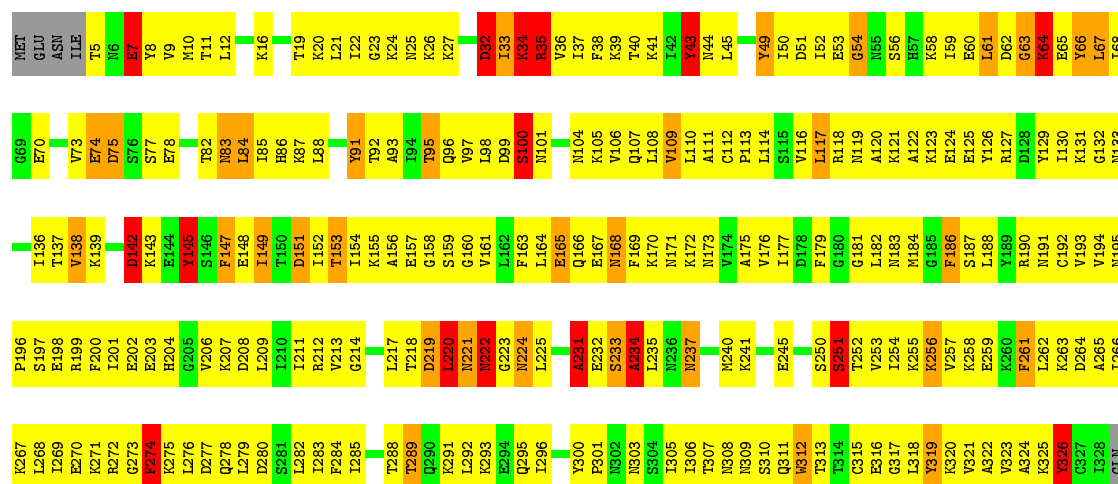
- Molecule 1: ALP12

Chain H: 23% 61% 10% 5% .



- Molecule 1: ALP12

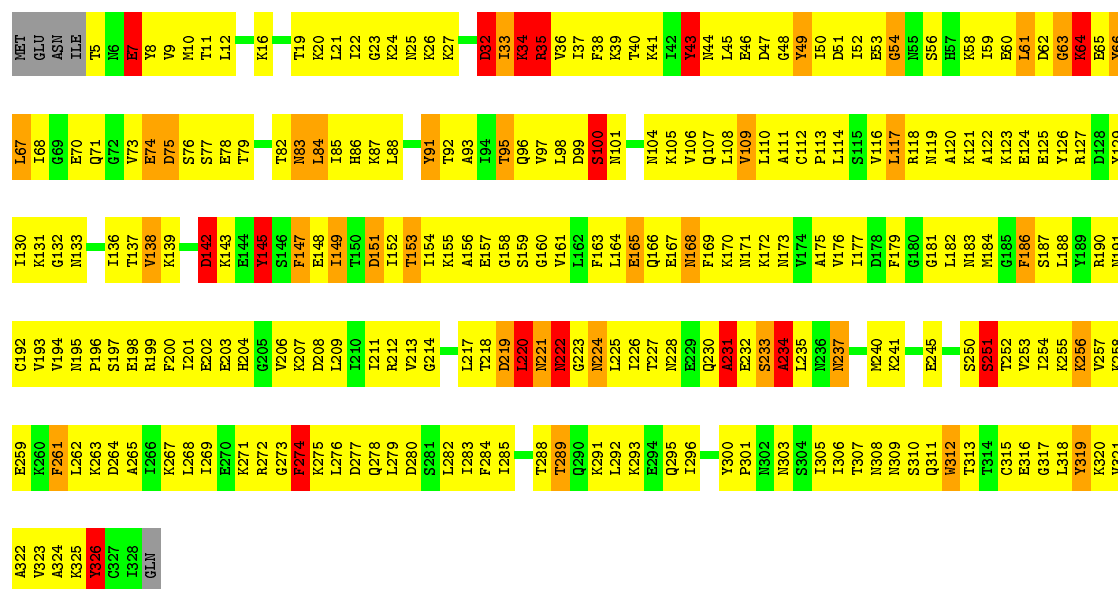
Chain I: 23% 60% 10% 5% .



- Molecule 1: ALP12

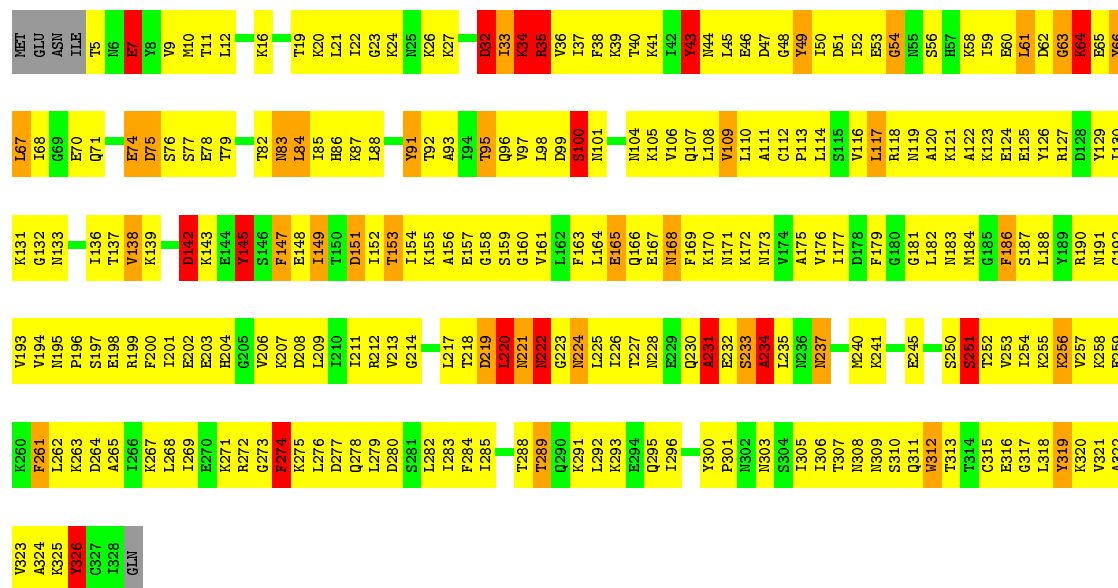
Chain J: 21% 63% 10% 5% .





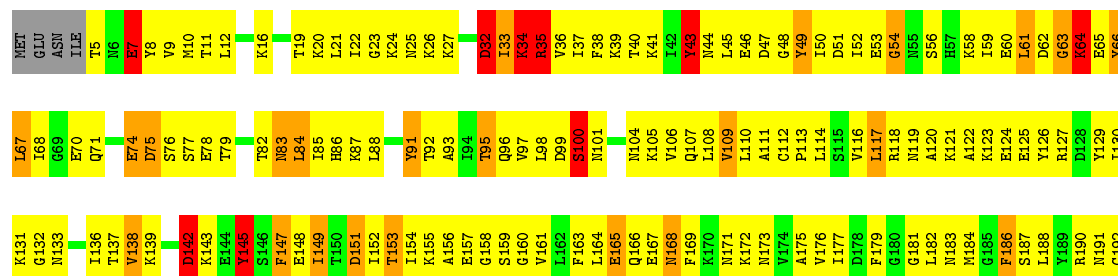
## • Molecule 1: ALP12

Chain K: 22% 62% 10% 5%

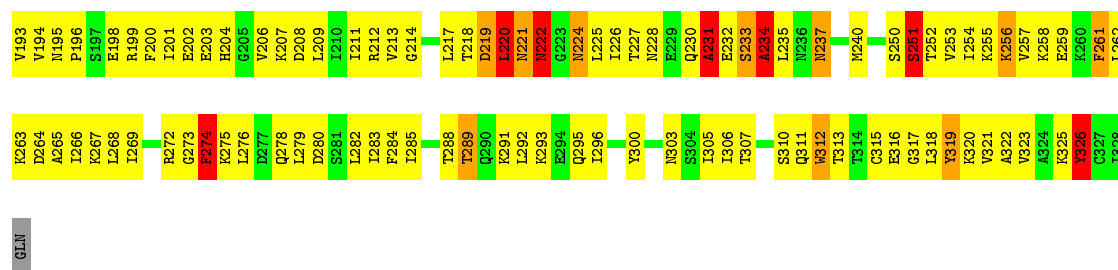


## • Molecule 1: ALP12

Chain L: 24% 60% 10% 5%

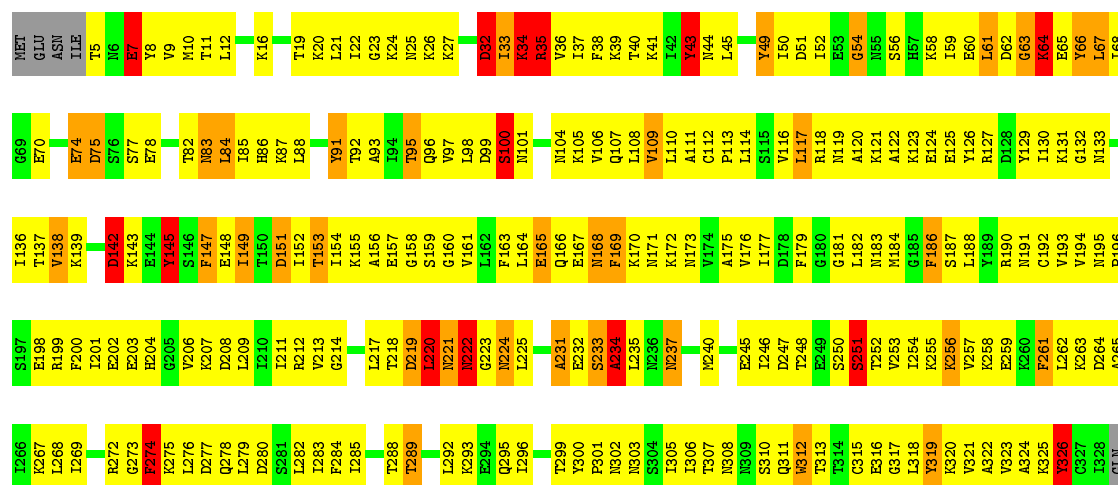






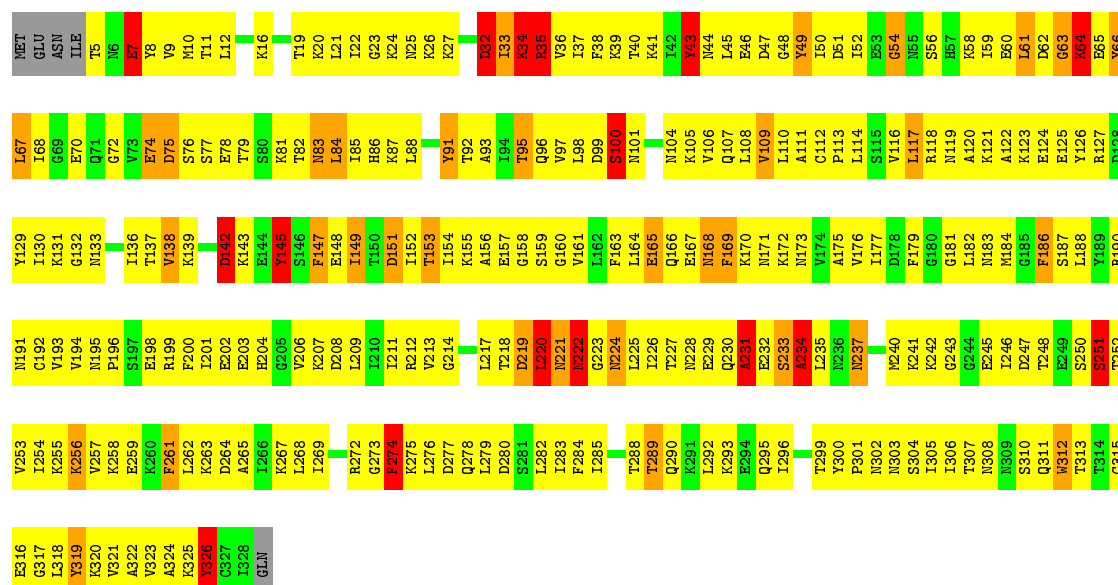
- Molecule 1: ALP12

Chain M: 24% 59% 11% 5%



- Molecule 1: ALP12

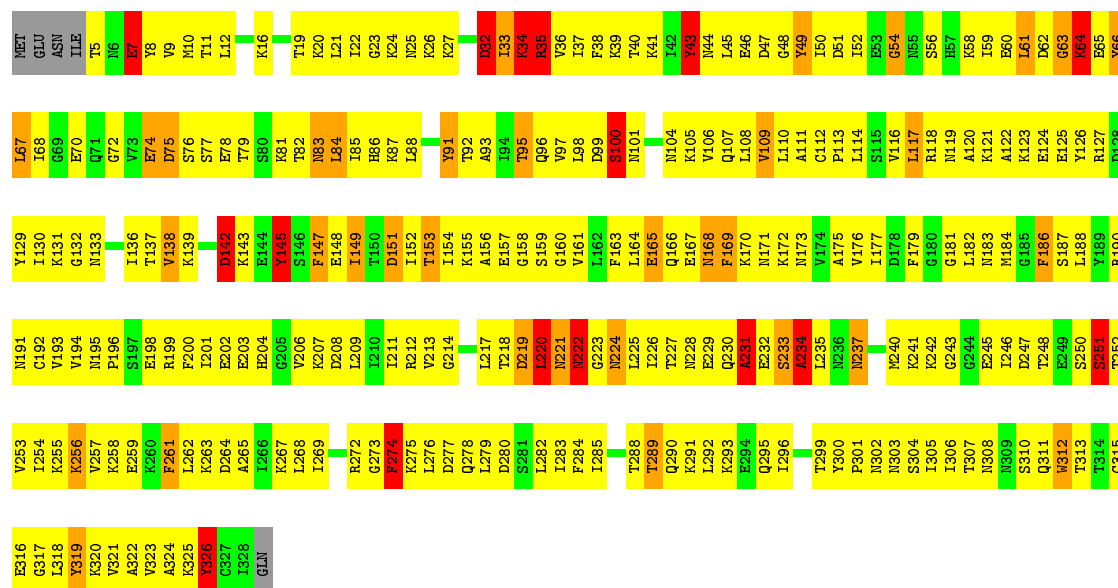
Chain N: 19% 64% 10% 5%



- Molecule 1: ALP12

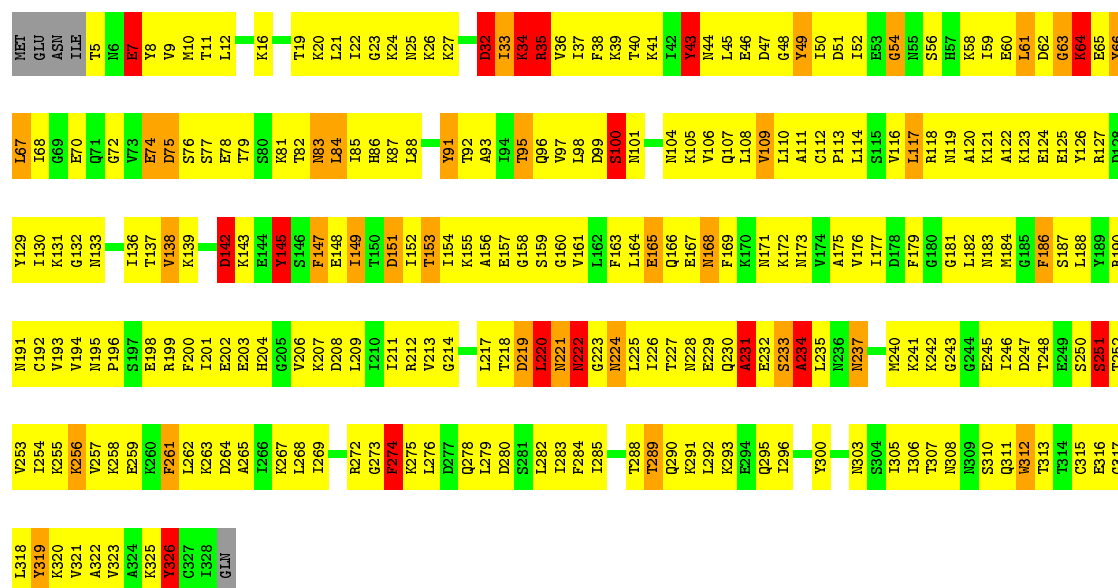


Chain O:  19% 64% 10% 5%



• Molecule 1: ALP12

Chain P:  21% 63% 10% 5%





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH SCANNED IMAGE	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	100	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	40000	Depositor
Image detector	KODAK SO163 FILM	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.71	1/2578 (0.0%)	1.64	70/3467 (2.0%)
1	B	0.71	1/2578 (0.0%)	1.64	70/3467 (2.0%)
1	C	0.71	1/2578 (0.0%)	1.64	70/3467 (2.0%)
1	D	0.71	1/2578 (0.0%)	1.64	69/3467 (2.0%)
1	E	0.71	1/2578 (0.0%)	1.64	68/3467 (2.0%)
1	F	0.71	1/2578 (0.0%)	1.64	69/3467 (2.0%)
1	G	0.71	1/2578 (0.0%)	1.64	68/3467 (2.0%)
1	H	0.71	1/2578 (0.0%)	1.64	70/3467 (2.0%)
1	I	0.71	1/2578 (0.0%)	1.64	69/3467 (2.0%)
1	J	0.71	1/2578 (0.0%)	1.64	69/3467 (2.0%)
1	K	0.71	1/2578 (0.0%)	1.64	70/3467 (2.0%)
1	L	0.71	1/2578 (0.0%)	1.64	69/3467 (2.0%)
1	M	0.71	1/2578 (0.0%)	1.64	70/3467 (2.0%)
1	N	0.71	1/2578 (0.0%)	1.64	70/3467 (2.0%)
1	O	0.71	1/2578 (0.0%)	1.64	70/3467 (2.0%)
1	P	0.71	1/2578 (0.0%)	1.64	70/3467 (2.0%)
All	All	0.71	16/41248 (0.0%)	1.64	1111/55472 (2.0%)

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
1	A	1	17
1	B	1	17
1	C	1	17
1	D	1	17
1	E	1	17
1	F	1	17
1	G	1	17
1	H	1	17
1	I	1	17

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	1	17
1	K	1	17
1	L	1	17
1	M	1	17
1	N	1	17
1	O	1	17
1	P	1	17
All	All	16	272

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	145	TYR	CE1-CZ	-6.69	1.29	1.38
1	D	145	TYR	CE1-CZ	-6.68	1.29	1.38
1	P	145	TYR	CE1-CZ	-6.66	1.29	1.38
1	A	145	TYR	CE1-CZ	-6.65	1.29	1.38
1	L	145	TYR	CE1-CZ	-6.64	1.29	1.38

The worst 5 of 1111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	222	ASN	N-CA-CB	-18.65	77.03	110.60
1	K	222	ASN	N-CA-CB	-18.63	77.07	110.60
1	I	222	ASN	N-CA-CB	-18.61	77.11	110.60
1	E	222	ASN	N-CA-CB	-18.60	77.11	110.60
1	H	222	ASN	N-CA-CB	-18.60	77.12	110.60

5 of 16 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	34	LYS	CA
1	B	34	LYS	CA
1	C	34	LYS	CA
1	D	34	LYS	CA
1	E	34	LYS	CA

5 of 272 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	33	ILE	Mainchain
1	A	34	LYS	Mainchain
1	A	35	ARG	Mainchain

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Mol	Chain	Res	Type	Group
1	A	43	TYR	Sidechain
1	A	54	GLY	Peptide

## 5.2 Too-close contacts [i](#)

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	2547	0	2571	895	0
1	B	2547	0	2566	1086	0
1	C	2547	0	2566	1091	0
1	D	2547	0	2573	795	0
1	E	2547	0	2569	813	0
1	F	2547	0	2556	1325	0
1	G	2547	0	2554	1296	0
1	H	2547	0	2564	1122	0
1	I	2547	0	2563	1066	0
1	J	2547	0	2553	1244	0
1	K	2547	0	2554	1273	0
1	L	2547	0	2569	822	0
1	M	2547	0	2573	807	0
1	N	2547	0	2563	1042	0
1	O	2547	0	2565	1048	0
1	P	2547	0	2572	902	0
All	All	40752	0	41031	12900	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 158.

The worst 5 of 12900 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:225:LEU:HD22	1:D:300:TYR:CE2	1.35	1.62
1:O:300:TYR:CA	1:P:227:THR:HG23	1.19	1.61
1:B:46:GLU:HB2	1:C:324:ALA:CB	1.30	1.61
1:A:46:GLU:HB2	1:B:324:ALA:CB	1.30	1.61
1:C:46:GLU:HB2	1:D:324:ALA:CB	1.30	1.61



There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	322/329 (98%)	283 (88%)	26 (8%)	13 (4%)	4	35
1	B	322/329 (98%)	283 (88%)	26 (8%)	13 (4%)	4	35
1	C	322/329 (98%)	283 (88%)	26 (8%)	13 (4%)	4	35
1	D	322/329 (98%)	283 (88%)	26 (8%)	13 (4%)	4	35
1	E	322/329 (98%)	283 (88%)	26 (8%)	13 (4%)	4	35
1	F	322/329 (98%)	284 (88%)	25 (8%)	13 (4%)	4	35
1	G	322/329 (98%)	283 (88%)	26 (8%)	13 (4%)	4	35
1	H	322/329 (98%)	284 (88%)	25 (8%)	13 (4%)	4	35
1	I	322/329 (98%)	283 (88%)	26 (8%)	13 (4%)	4	35
1	J	322/329 (98%)	283 (88%)	26 (8%)	13 (4%)	4	35
1	K	322/329 (98%)	283 (88%)	26 (8%)	13 (4%)	4	35
1	L	322/329 (98%)	283 (88%)	26 (8%)	13 (4%)	4	35
1	M	322/329 (98%)	283 (88%)	26 (8%)	13 (4%)	4	35
1	N	322/329 (98%)	283 (88%)	26 (8%)	13 (4%)	4	35
1	O	322/329 (98%)	283 (88%)	26 (8%)	13 (4%)	4	35
1	P	322/329 (98%)	283 (88%)	26 (8%)	13 (4%)	4	35
All	All	5152/5264 (98%)	4530 (88%)	414 (8%)	208 (4%)	6	35

5 of 208 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	34	LYS
1	A	118	ARG
1	A	221	ASN

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Mol	Chain	Res	Type
1	A	234	ALA

### 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	283/289 (98%)	278 (98%)	5 (2%)	66	87
1	B	283/289 (98%)	278 (98%)	5 (2%)	66	87
1	C	283/289 (98%)	278 (98%)	5 (2%)	66	87
1	D	283/289 (98%)	278 (98%)	5 (2%)	66	87
1	E	283/289 (98%)	278 (98%)	5 (2%)	66	87
1	F	283/289 (98%)	278 (98%)	5 (2%)	66	87
1	G	283/289 (98%)	278 (98%)	5 (2%)	66	87
1	H	283/289 (98%)	278 (98%)	5 (2%)	66	87
1	I	283/289 (98%)	278 (98%)	5 (2%)	66	87
1	J	283/289 (98%)	278 (98%)	5 (2%)	66	87
1	K	283/289 (98%)	278 (98%)	5 (2%)	66	87
1	L	283/289 (98%)	278 (98%)	5 (2%)	66	87
1	M	283/289 (98%)	278 (98%)	5 (2%)	66	87
1	N	283/289 (98%)	278 (98%)	5 (2%)	66	87
1	O	283/289 (98%)	278 (98%)	5 (2%)	66	87
1	P	283/289 (98%)	278 (98%)	5 (2%)	66	87
All	All	4528/4624 (98%)	4448 (98%)	80 (2%)	69	87

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	34	LYS
1	I	256	LYS
1	O	222	ASN
1	H	61	LEU

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Mol	Chain	Res	Type
1	I	7	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 167 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	6	ASN
1	J	71	GLN
1	O	204	HIS
1	H	96	GLN
1	I	57	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](#)

There are no ligands in this entry.

## 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.