



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Nov 29, 2017 – 09:08 PM EST

PDB ID : 6AP1
EMDB ID: : EMD-8887
Title : Vps4p-Vta1p complex with peptide binding to the central pore of Vps4p
Authors : Han, H.; Monroe, N.; Shen, P.; Sundquist, W.I.; Hill, C.P.
Deposited on : unknown
Resolution : 3.20 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) : rb-20030345

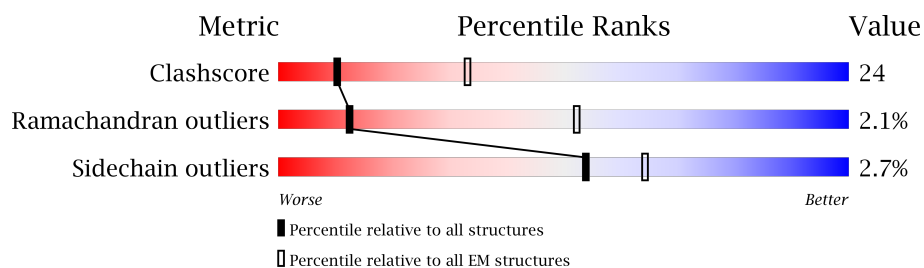
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	519	
1	B	519	
1	C	519	
1	D	519	
1	E	519	
1	F	519	
2	G	10	
3	H	330	
3	I	330	

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Mol	Chain	Length	Quality of chain
3	J	330	<div><div><div></div><div></div><div></div></div><div>5%8%</div><div>87%</div></div>
3	K	330	<div><div><div></div><div></div><div></div></div><div>8%</div><div></div><div>87%</div></div>
3	L	330	<div><div><div></div><div></div><div></div></div><div>5%8%</div><div>87%</div></div>
3	M	330	<div><div><div></div><div></div><div></div></div><div>8%5%</div><div>87%</div></div>
3	N	330	<div><div><div></div><div></div><div></div></div><div>5%8%</div><div>87%</div></div>
3	O	330	<div><div><div></div><div></div><div></div></div><div>8%5%</div><div>87%</div></div>
3	P	330	<div><div><div></div><div></div><div></div></div><div>5%8%</div><div>87%</div></div>
3	Q	330	<div><div><div></div><div></div><div></div></div><div>8%</div><div></div><div>87%</div></div>
3	R	330	<div><div><div></div><div></div><div></div></div><div>5%8%</div><div>87%</div></div>
3	S	330	<div><div><div></div><div></div><div></div></div><div>8%</div><div></div><div>87%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18838 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 Vacuolar protein sorting-associated protein 4,Protein hcp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	314	Total	C	N	O	S	0	0
			2427	1530	414	474	9		
1	B	322	Total	C	N	O	S	0	0
			2491	1568	427	487	9		
1	C	322	Total	C	N	O	S	0	0
			2491	1568	427	487	9		
1	D	322	Total	C	N	O	S	0	0
			2491	1568	427	487	9		
1	E	304	Total	C	N	O	S	0	0
			2360	1489	401	461	9		
1	F	308	Total	C	N	O	S	0	0
			2387	1507	405	466	9		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	GLY	-	expression tag	UNP P52917
A	438	GLY	-	linker	UNP P52917
A	439	GLY	-	linker	UNP P52917
A	440	GLY	-	linker	UNP P52917
A	441	GLY	-	linker	UNP P52917
A	442	SER	-	linker	UNP P52917
A	443	GLY	-	linker	UNP P52917
A	444	GLY	-	linker	UNP P52917
A	445	GLY	-	linker	UNP P52917
A	446	GLY	-	linker	UNP P52917
A	447	SER	-	linker	UNP P52917
A	448	GLY	-	linker	UNP P52917
A	449	GLY	-	linker	UNP P52917
A	450	GLY	-	linker	UNP P52917
A	451	GLY	-	linker	UNP P52917
A	452	SER	-	linker	UNP P52917
A	453	GLY	-	linker	UNP P52917
A	454	GLY	-	linker	UNP P52917

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Chain	Residue	Modelled	Actual	Comment	Reference
A	455	GLY	-	linker	UNP P52917
A	618	GLY	-	expression tag	UNP Q9I747
B	100	GLY	-	expression tag	UNP P52917
B	438	GLY	-	linker	UNP P52917
B	439	GLY	-	linker	UNP P52917
B	440	GLY	-	linker	UNP P52917
B	441	GLY	-	linker	UNP P52917
B	442	SER	-	linker	UNP P52917
B	443	GLY	-	linker	UNP P52917
B	444	GLY	-	linker	UNP P52917
B	445	GLY	-	linker	UNP P52917
B	446	GLY	-	linker	UNP P52917
B	447	SER	-	linker	UNP P52917
B	448	GLY	-	linker	UNP P52917
B	449	GLY	-	linker	UNP P52917
B	450	GLY	-	linker	UNP P52917
B	451	GLY	-	linker	UNP P52917
B	452	SER	-	linker	UNP P52917
B	453	GLY	-	linker	UNP P52917
B	454	GLY	-	linker	UNP P52917
B	455	GLY	-	linker	UNP P52917
B	618	GLY	-	expression tag	UNP Q9I747
C	100	GLY	-	expression tag	UNP P52917
C	438	GLY	-	linker	UNP P52917
C	439	GLY	-	linker	UNP P52917
C	440	GLY	-	linker	UNP P52917
C	441	GLY	-	linker	UNP P52917
C	442	SER	-	linker	UNP P52917
C	443	GLY	-	linker	UNP P52917
C	444	GLY	-	linker	UNP P52917
C	445	GLY	-	linker	UNP P52917
C	446	GLY	-	linker	UNP P52917
C	447	SER	-	linker	UNP P52917
C	448	GLY	-	linker	UNP P52917
C	449	GLY	-	linker	UNP P52917
C	450	GLY	-	linker	UNP P52917
C	451	GLY	-	linker	UNP P52917
C	452	SER	-	linker	UNP P52917
C	453	GLY	-	linker	UNP P52917
C	454	GLY	-	linker	UNP P52917
C	455	GLY	-	linker	UNP P52917
C	618	GLY	-	expression tag	UNP Q9I747

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Chain	Residue	Modelled	Actual	Comment	Reference
D	100	GLY	-	expression tag	UNP P52917
D	438	GLY	-	linker	UNP P52917
D	439	GLY	-	linker	UNP P52917
D	440	GLY	-	linker	UNP P52917
D	441	GLY	-	linker	UNP P52917
D	442	SER	-	linker	UNP P52917
D	443	GLY	-	linker	UNP P52917
D	444	GLY	-	linker	UNP P52917
D	445	GLY	-	linker	UNP P52917
D	446	GLY	-	linker	UNP P52917
D	447	SER	-	linker	UNP P52917
D	448	GLY	-	linker	UNP P52917
D	449	GLY	-	linker	UNP P52917
D	450	GLY	-	linker	UNP P52917
D	451	GLY	-	linker	UNP P52917
D	452	SER	-	linker	UNP P52917
D	453	GLY	-	linker	UNP P52917
D	454	GLY	-	linker	UNP P52917
D	455	GLY	-	linker	UNP P52917
D	618	GLY	-	expression tag	UNP Q9I747
E	100	GLY	-	expression tag	UNP P52917
E	438	GLY	-	linker	UNP P52917
E	439	GLY	-	linker	UNP P52917
E	440	GLY	-	linker	UNP P52917
E	441	GLY	-	linker	UNP P52917
E	442	SER	-	linker	UNP P52917
E	443	GLY	-	linker	UNP P52917
E	444	GLY	-	linker	UNP P52917
E	445	GLY	-	linker	UNP P52917
E	446	GLY	-	linker	UNP P52917
E	447	SER	-	linker	UNP P52917
E	448	GLY	-	linker	UNP P52917
E	449	GLY	-	linker	UNP P52917
E	450	GLY	-	linker	UNP P52917
E	451	GLY	-	linker	UNP P52917
E	452	SER	-	linker	UNP P52917
E	453	GLY	-	linker	UNP P52917
E	454	GLY	-	linker	UNP P52917
E	455	GLY	-	linker	UNP P52917
E	618	GLY	-	expression tag	UNP Q9I747
F	100	GLY	-	expression tag	UNP P52917
F	438	GLY	-	linker	UNP P52917

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Chain	Residue	Modelled	Actual	Comment	Reference
F	439	GLY	-	linker	UNP P52917
F	440	GLY	-	linker	UNP P52917
F	441	GLY	-	linker	UNP P52917
F	442	SER	-	linker	UNP P52917
F	443	GLY	-	linker	UNP P52917
F	444	GLY	-	linker	UNP P52917
F	445	GLY	-	linker	UNP P52917
F	446	GLY	-	linker	UNP P52917
F	447	SER	-	linker	UNP P52917
F	448	GLY	-	linker	UNP P52917
F	449	GLY	-	linker	UNP P52917
F	450	GLY	-	linker	UNP P52917
F	451	GLY	-	linker	UNP P52917
F	452	SER	-	linker	UNP P52917
F	453	GLY	-	linker	UNP P52917
F	454	GLY	-	linker	UNP P52917
F	455	GLY	-	linker	UNP P52917
F	618	GLY	-	expression tag	UNP Q9I747

- Molecule 2 is a protein called ACE-ASP-GLU-ILE-VAL-ASN-LYS-VAL-LEU-NH2.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	10	Total	C	N	O	1	1
			68	43	11	14		

- Molecule 3 is a protein called Vacuolar protein sorting-associated protein VTA1.

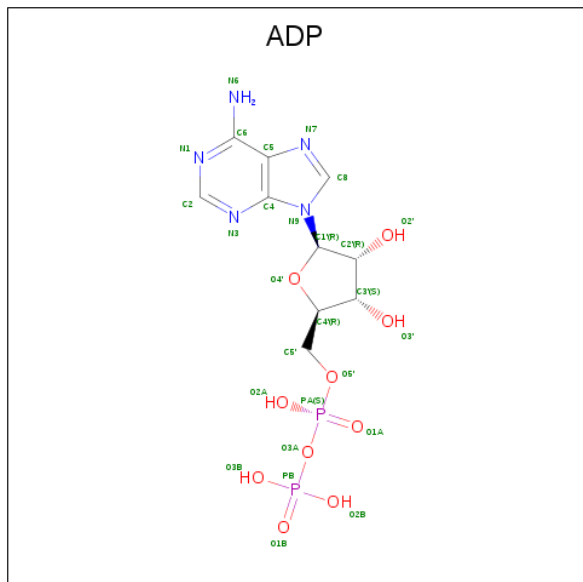
Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	42	Total	C	N	O	0	0
			331	209	54	68		
3	I	42	Total	C	N	O	0	0
			331	209	54	68		
3	J	42	Total	C	N	O	0	0
			331	209	54	68		
3	K	42	Total	C	N	O	0	0
			331	209	54	68		
3	L	42	Total	C	N	O	0	0
			331	209	54	68		
3	M	42	Total	C	N	O	0	0
			331	209	54	68		
3	N	42	Total	C	N	O	0	0
			331	209	54	68		

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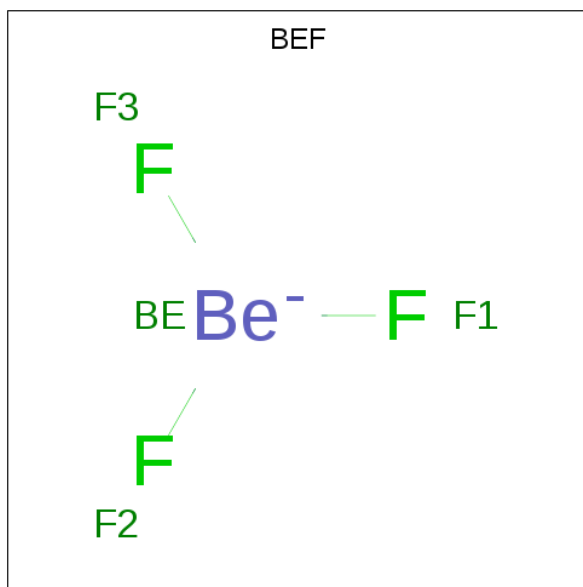
Mol	Chain	Residues	Atoms				AltConf	Trace
3	O	42	Total	C	N	O	0	0
			331	209	54	68		
3	P	42	Total	C	N	O	0	0
			331	209	54	68		
3	Q	42	Total	C	N	O	0	0
			331	209	54	68		
3	R	42	Total	C	N	O	0	0
			331	209	54	68		
3	S	42	Total	C	N	O	0	0
			331	209	54	68		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	Be	F	0
			4	1	3	
5	B	1	Total	Be	F	0
			4	1	3	
5	C	1	Total	Be	F	0
			4	1	3	

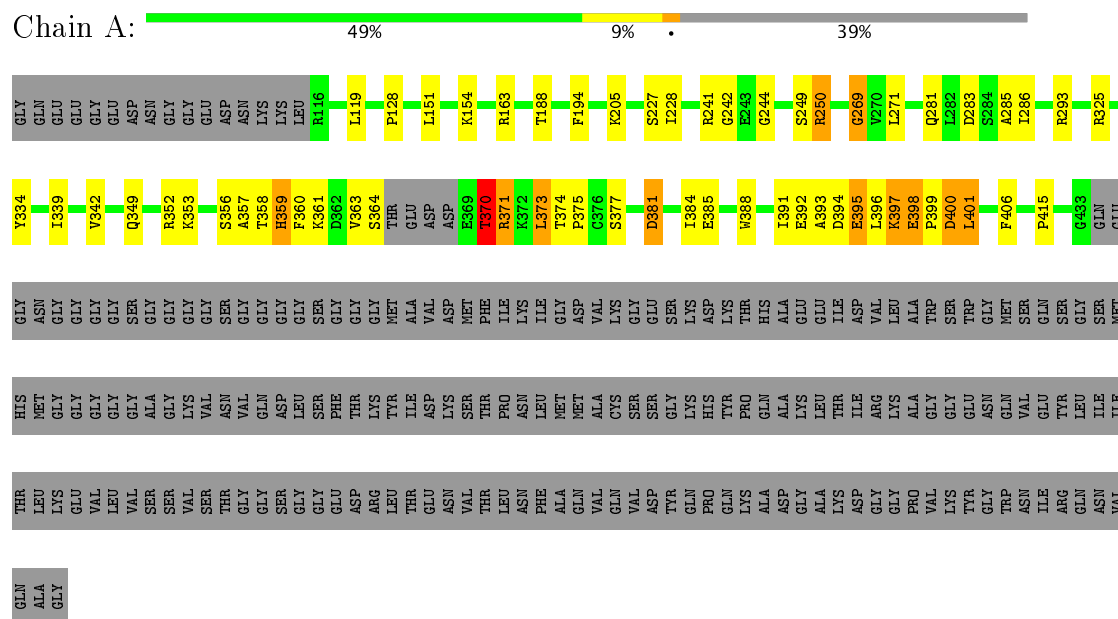
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Mg	0
			1	1	
6	A	1	Total	Mg	0
			1	1	
6	D	1	Total	Mg	0
			1	1	
6	C	1	Total	Mg	0
			1	1	

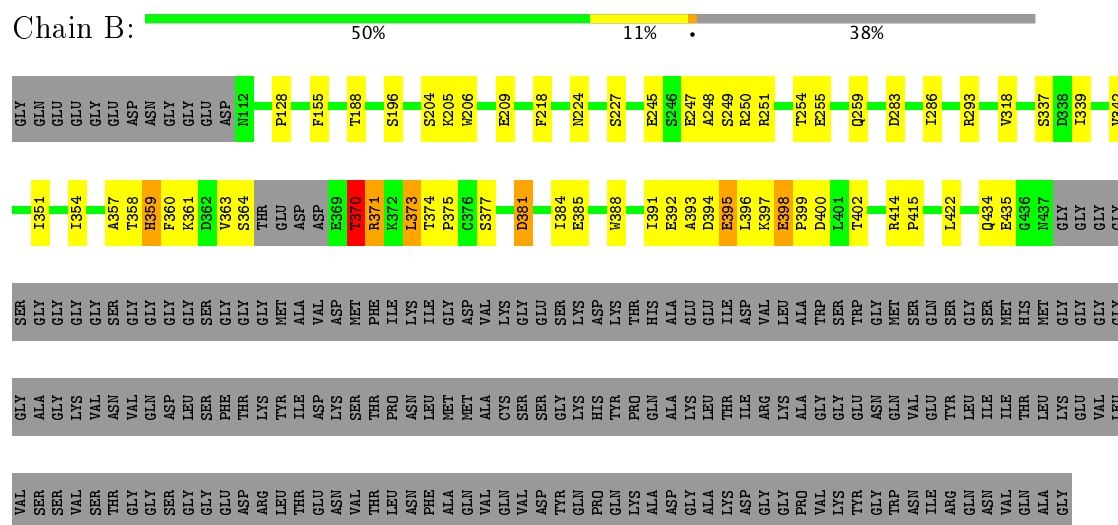
3 Residue-property plots

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: Vacuolar protein sorting-associated protein 4, Protein hcp1

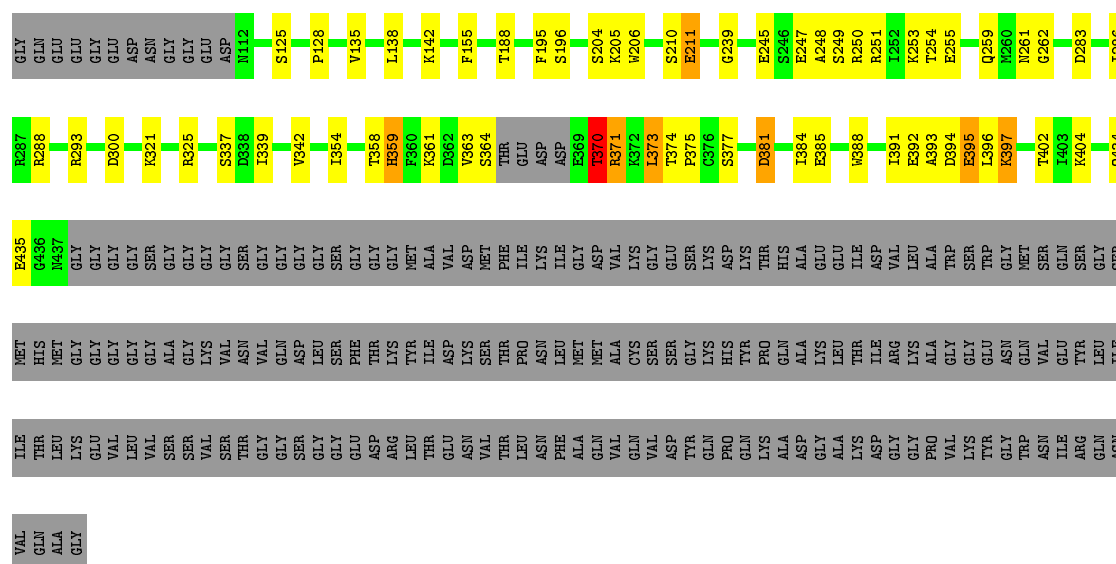


- Molecule 1: Vacuolar protein sorting-associated protein 4, Protein hcp1



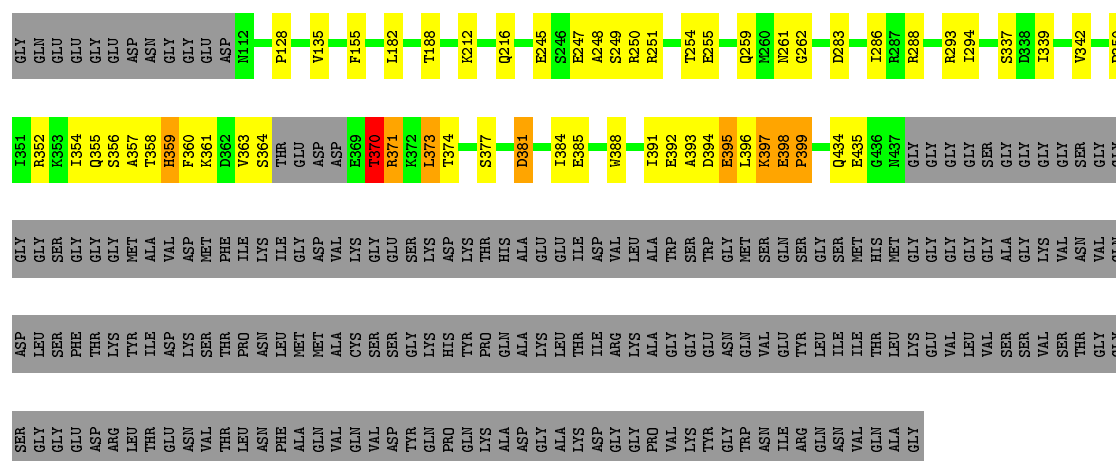
- Molecule 1: Vacuolar protein sorting-associated protein 4, Protein hcp1

Chain C:  50% 11% . 38%



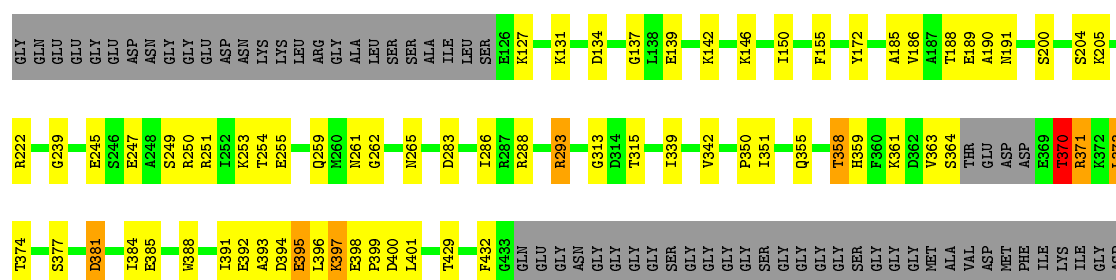
- Molecule 1: Vacuolar protein sorting-associated protein 4. Protein hcp1

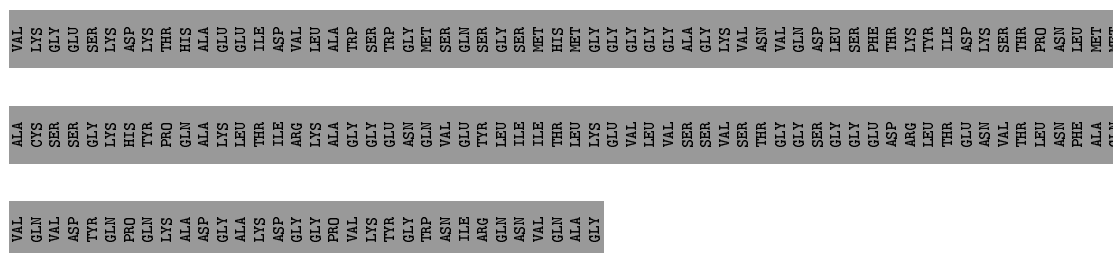
Chain D:  51% 9% 1% 38%



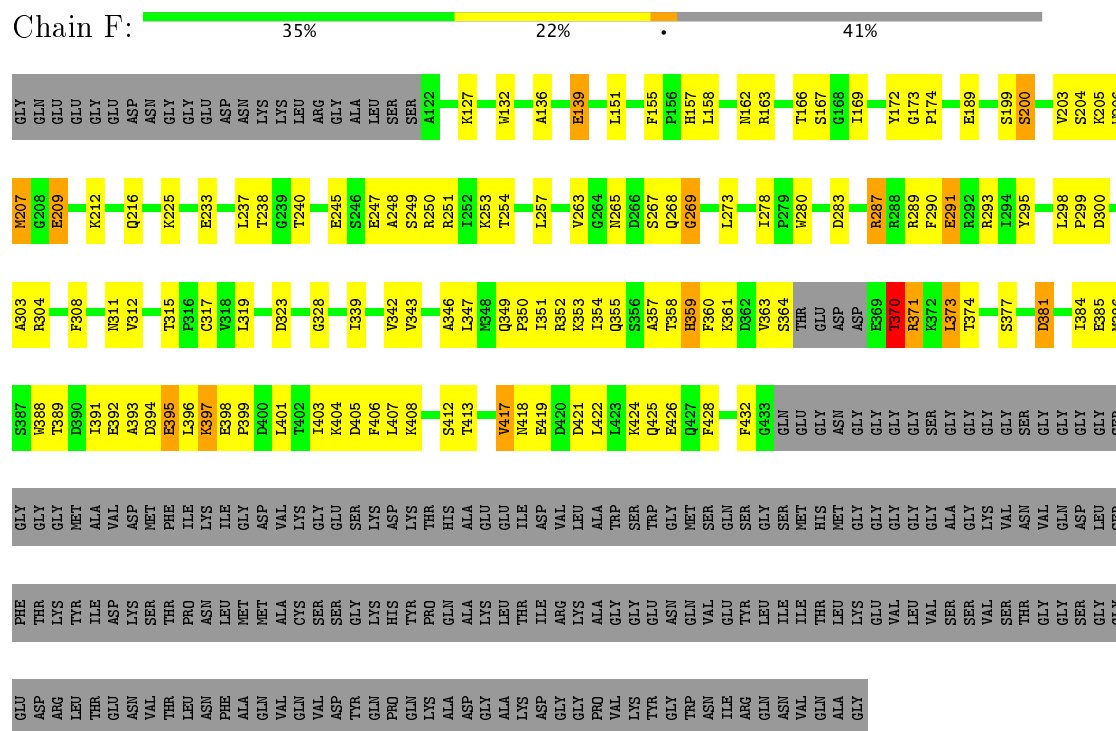
- Molecule 1: Vacuolar protein sorting-associated protein 4, Protein hcp1

Chain E: 45% 12% 41%

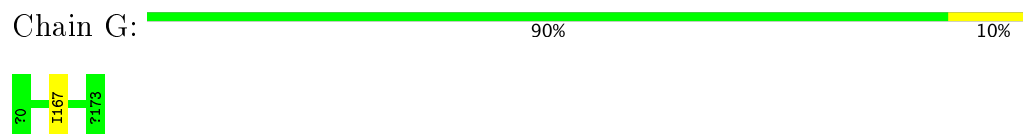




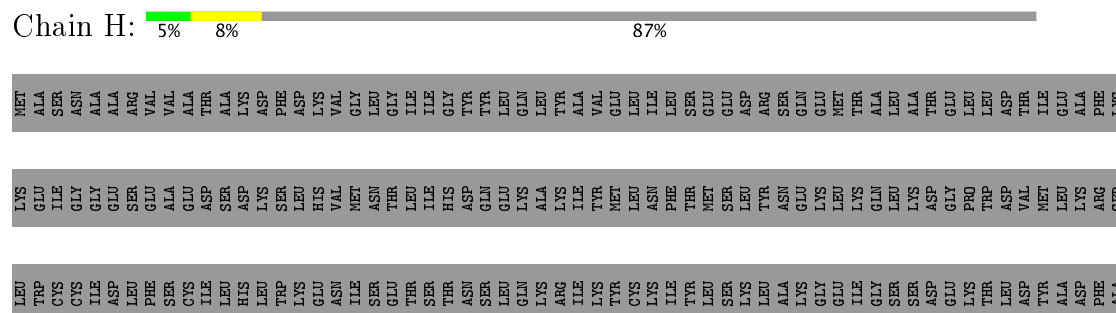
- Molecule 1: Vacuolar protein sorting-associated protein 4, Protein hcp1

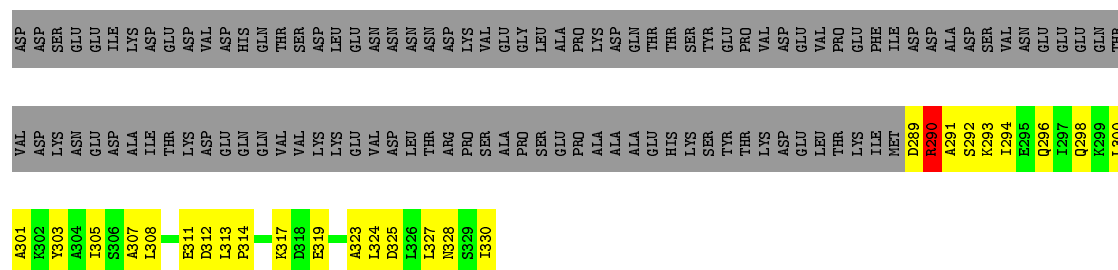


- Molecule 2: ACE-ASP-GLU-ILE-VAL-ASN-LYS-VAL-LEU-NH2

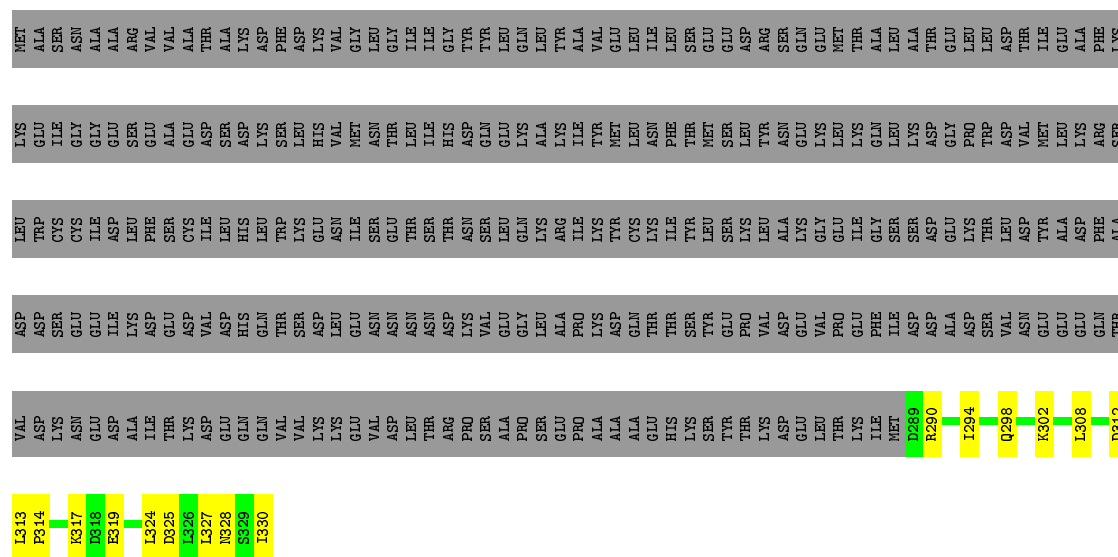


- Molecule 3: Vacuolar protein sorting-associated protein VTA1

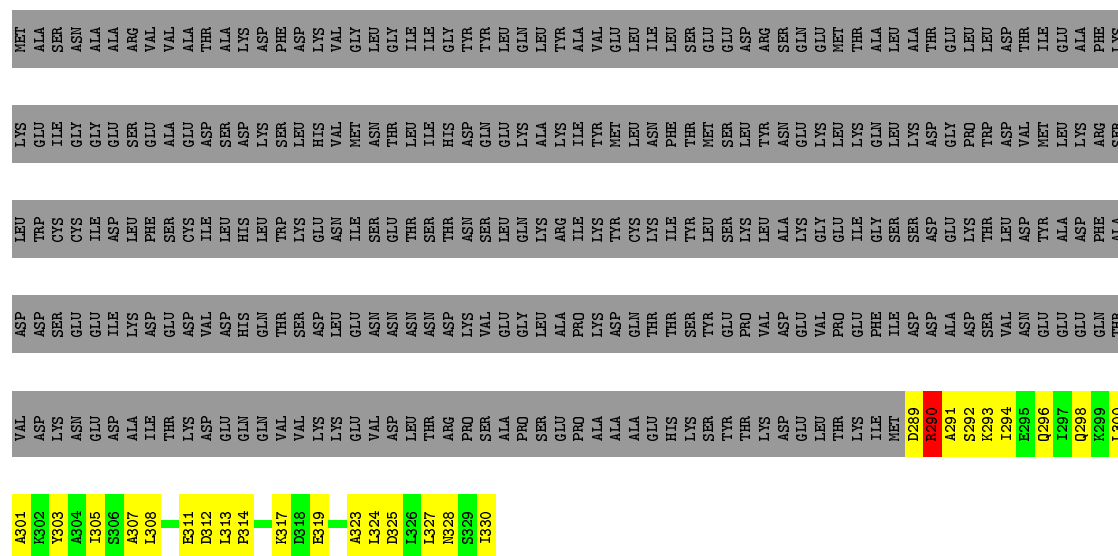




- Molecule 3: Vacuolar protein sorting-associated protein VTA1



- Molecule 3: Vacuolar protein sorting-associated protein VTA1



- Molecule 3: Vacuolar protein sorting-associated protein VTA1

Chain K: 8% . 87%

L313	VAL	ASP	LEU	LVS	MET
P314	ASP	ASP	TPR	GLU	ALA
K317	LVS	SER	CYS	ILE	ALA
D318	ASN	GLU	CYS	GLY	ASN
E319	ASP	ILE	ASP	GLU	ALA
L324	ALA	LVS	LEU	SER	ARG
D325	THR	ASP	PHE	GLU	VAL
L326	LVS	ASP	CYS	GLU	ALA
L327	ASP	VAL	ILE	ASP	THR
N328	GLU	ASP	LEU	SER	ALA
I330	GLN	HIS	LEU	ASP	LVS
	VAL	GLN	LEU	VAL	VAL
	GLU	GLU	ILE	MET	GLY
	VAL	ASN	SER	ASN	LEU
	ASP	ASN	GLU	THR	GLY
	LEU	ASN	THR	ILE	ILE
	THR	ASN	SER	ILE	ILE
	ARG	ASP	THR	HIS	GLY
	P324	LVS	ASN	ASP	TYR
	P325	LVS	ASN	ASP	TYR
	SER	VAL	SER	GLN	LEU
	P326	ALA	GLU	LEU	LEU
	P327	GLY	GLN	LVS	GLN
	SER	LEU	LVS	ALA	LEU
	GLU	ALA	ARG	LVS	ILE
	P328	P329	ILE	ILE	LEU
	ALA	LVS	LVS	TYR	LEU
	ALA	ASP	THR	PHE	SER
	ALA	GLN	THR	ASN	ARG
	GLU	THR	ILE	TYR	SER
	ALA	GLU	LEU	GLU	GLU
	ALA	GLU	LVS	LEU	ASP
	ALA	VAL	ALA	TYR	ARG
	LEU	VAL	LVS	GLU	SER
	THR	P330	GLY	LVS	GLN
	LVS	PHE	GLY	GLN	ALA
	ILE	ILE	SER	LEU	LEU
	MET	ASP	SER	LVS	LEU
D289	D289	ASP	SER	ASP	ASP
R290	R290	ALA	GLU	GLY	THR
I294	I294	ASP	THR	TPR	LEU
Q298	Q298	VAL	LEU	ASP	ASP
L308	L308	ASN	ASP	VAL	THR
N309	N309	GLU	TYR	MET	ILE
Y310	Y310	GLU	ALA	LEU	GLU
E311	E311	GLN	PHE	LVS	ALA
D312	D312	THR	ALA	SER	PHE

- Molecule 3: Vacuolar protein sorting-associated protein VTA1

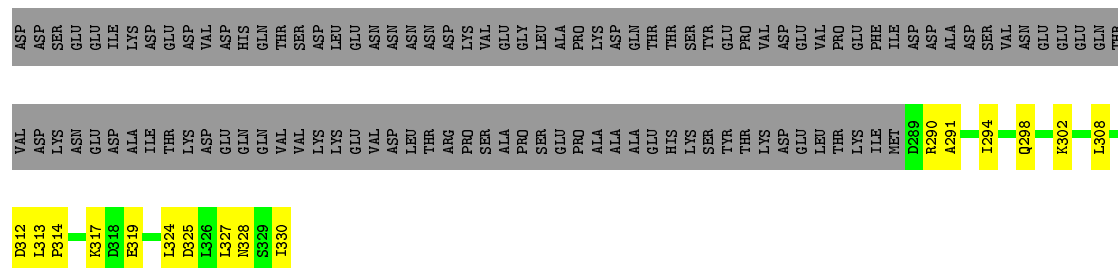
Chain L:  5% 8% 87%

A301	VAL	ASP	LEU	LVS	MET
F302	ASP	ASP	TRP	GLU	ALA
Y303	LVS	SER	CYS	ILE	SER
A304	ASN	GLU	CYS	GLY	ASN
I305	GLU	GLU	ILE	GLY	ALA
S306	ASP	ILE	ASP	GLU	ALA
A307	ALA	LVS	LEU	SER	ARG
L308	ILE	ASP	PHE	GLU	VAL
	THR	GLU	CYS	ALA	VAL
E311	LVS	ASP	CYS	GLU	ALA
D312	ASP	VAL	ILE	ASP	THR
L313	GLU	ASP	LEU	SER	ALA
P314	GLN	GLN	HIS	ASP	LVS
	VAL	GLN	TRP	LVS	ASP
F317	VAL	SER	TRP	SER	PHE
D318	VAL	SER	LVS	LEU	ASP
E319	LVS	ASP	GLU	HIS	LVS
	LVS	LEU	ASN	VAL	VAL
A323	GLU	GLU	ILE	MET	GLY
L324	VAL	ASN	SER	ASN	LEU
D325	VAL	ASN	GLU	THR	GLY
L326	LEU	ASN	THR	LEU	ILE
L327	THR	ASN	SER	ILE	ILE
N328	ARG	ASP	THR	HIS	GLY
S329	PRO	LVS	ASN	ASP	TYR
I330	SER	VAL	SER	GLN	TYR
	PRO	GLY	LEU	LEU	GLN
	SER	LEU	LVS	ALA	LEU
	GLU	ALA	ARG	LVS	TYR
	PRO	PRO	ILE	ILE	ALA
	ALA	ASP	LVS	TYR	VAL
	ALA	ASP	CYS	MET	GLU
	GLU	GLN	LVS	LEU	LEU
	GLU	THR	ILE	ASN	ILE
	HIS	THR	TYR	PHE	LEU
	LVS	SER	TYR	THR	SER
	THR	GLU	SER	SER	GLU
	THR	PRO	LVS	LEU	ASP
	LVS	VAL	LEU	TYR	ARG
	ASP	ASP	ALA	ASN	SER
	GLU	GLU	LVS	GLU	GLN
	LEU	VAL	GLY	LVS	GLU
	THR	PRO	GLU	LEU	MET
	LVS	GLU	ILE	LVS	THR
	ILE	PHE	GLY	GLN	ALA
	MET	ILE	SER	LEU	LEU
		ASP	SER	LVS	ALA
D289	ASP	ASP	SER	LVS	ALA
R290	ASP	ASP	ASP	GLY	THR
A291	ALA	GLU	GLU	ASP	GLU
S292	ASP	LVS	LVS	PRO	LEU
K293	SER	THR	THR	TRP	LEU
I294	VAL	LEU	LEU	ASP	ASP
E295	ASN	ASN	LEU	VAL	THR
Q296	GLU	GLU	TYR	MET	ILE
I297	GLU	GLU	ALA	LEU	GLU
Q298	GLU	GLU	ASP	LVS	ALA
K299	GLN	PHE	SER	ARG	PHE
L300	THR	ALA	ALA	SER	LVS

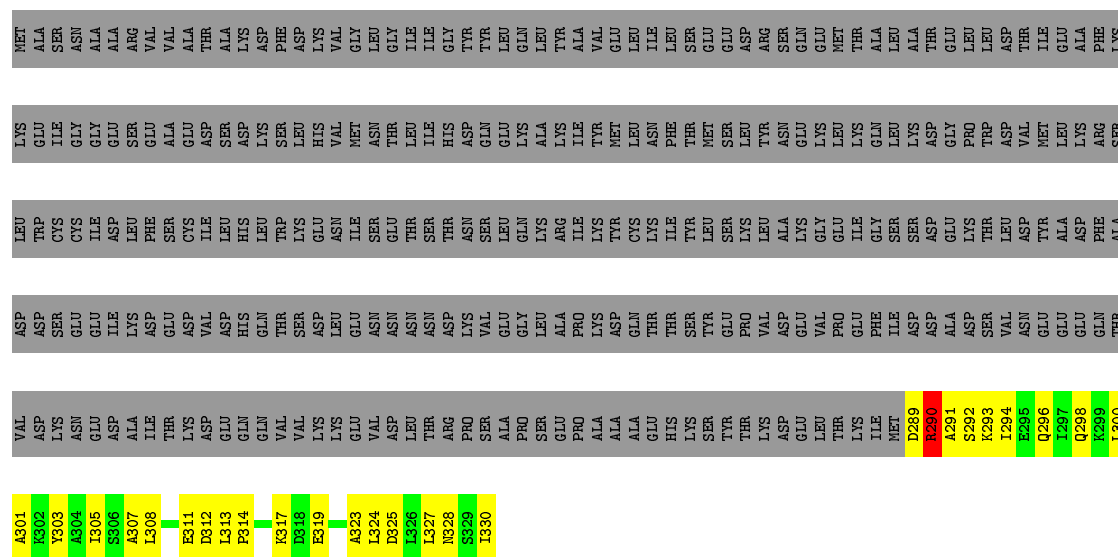
- Molecule 3: Vacuolar protein sorting-associated protein VTA1

Chain M:  8% 5% 87%

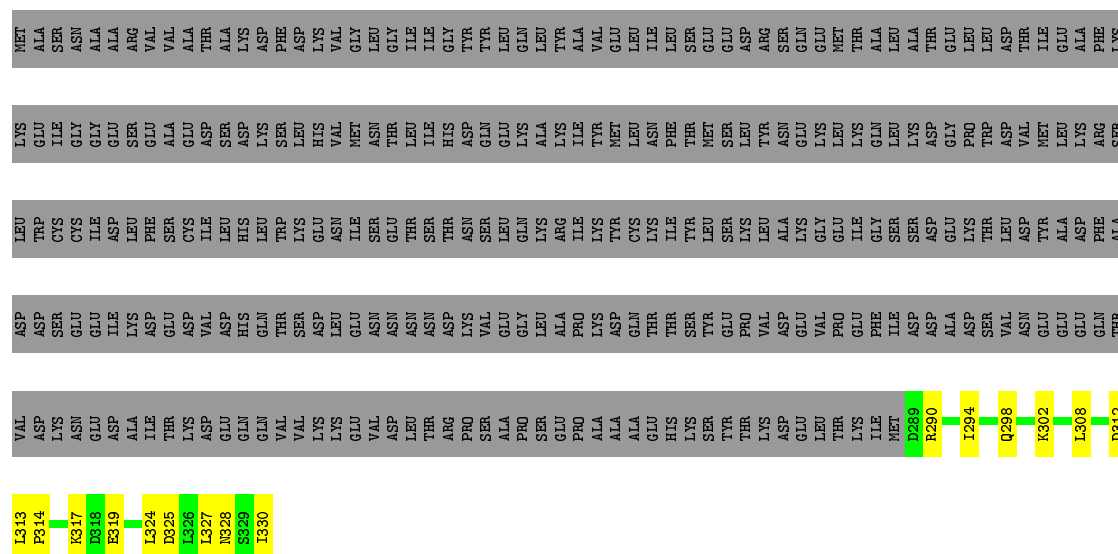
[illegible]



- Molecule 3: Vacuolar protein sorting-associated protein VTA1



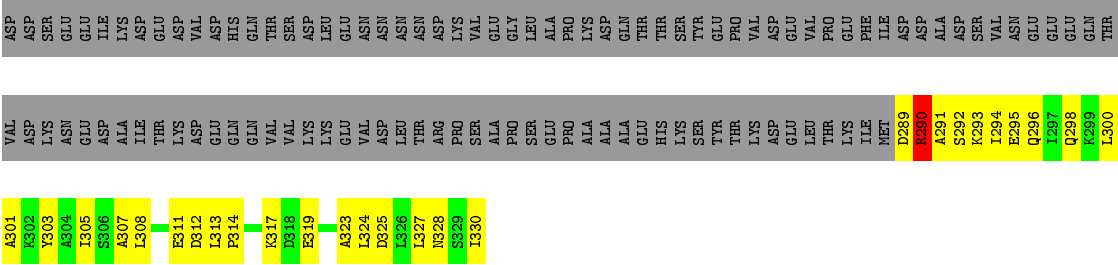
- Molecule 3: Vacuolar protein sorting-associated protein VTA1



- Molecule 3: Vacuolar protein sorting-associated protein VTA1

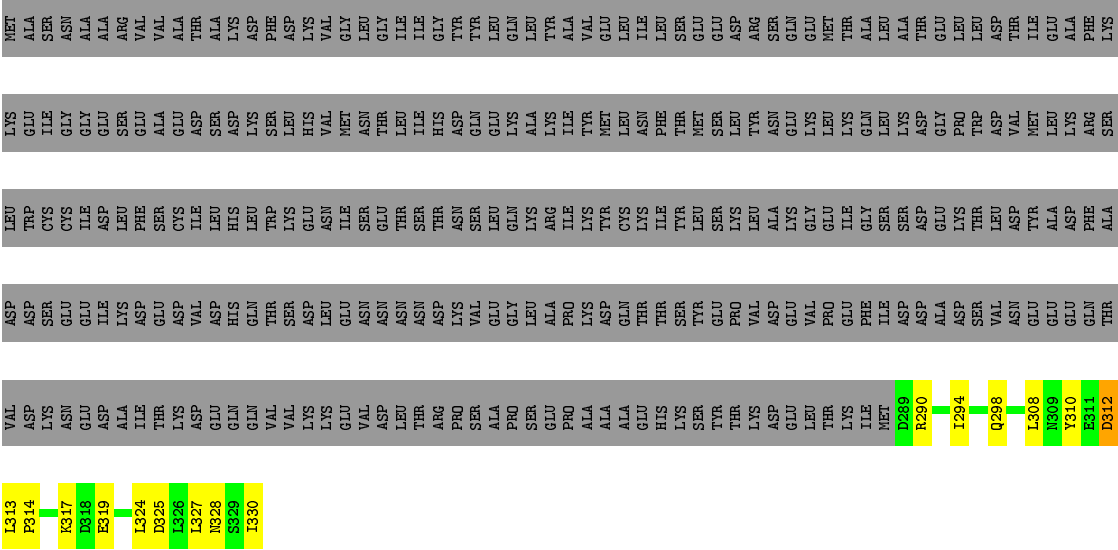
A301	VAL	ASP	LEU	LVS	MET
	ASP	ASP	TRP	GLU	ALA
I305	LVS	SER	CYS	ILE	SER
S306	ASN	GLU	CYS	GLY	ASN
A307	GLU	GLU	ILE	GLY	ALA
L308	ASP	ILE	ASP	GLU	ALA
	ALA	LVS	LEU	SER	ARG
E311	ILE	ASP	PHE	GLU	VAL
D312	THR	GLU	SER	ALA	VAL
L313	LVS	ASP	CYS	GLU	ALA
P314	ASP	VAL	ILE	ASP	THR
	GLU	ASP	LEU	SER	ALA
F317	GLN	HIS	HIS	ASP	LVS
D318	GLN	GLN	THR	LVS	ASP
E319	VAL	THR	TRP	SER	PHE
	VAL	SER	LVS	LEU	ASP
A323	LVS	ASP	GLU	HIS	LVS
L324	LVS	LEU	ASN	VAL	VAL
D325	VAL	GLU	ILE	MET	GLY
L326	GLU	ASN	SER	ASN	LEU
L327	ASP	ASN	GLU	THR	GLY
N328	LEU	ASN	THR	LEU	ILE
S329	THR	ASN	SER	ILE	ILE
I330	ARG	ASP	THR	HIS	GLY
	PRO	LVS	ASN	ASP	TYR
	SER	VAL	LEU	GLN	TYR
	ALA	GLU	SER	GLU	LEU
	PRO	GLY	GLN	LVS	GLN
	SER	LEU	LVS	ALA	LEU
	GLU	ALA	ARG	LVS	ILE
	PRO	PRO	ILE	ILE	LEU
	ALA	LVS	THR	ASN	LEU
	ALA	GLN	LVS	ASN	SER
	GLU	THR	ILE	THR	GLU
	LVS	SER	THR	MET	GLU
	HIS	THR	LEU	SER	ASP
	LVS	GLU	LVS	THR	ARG
	THR	THR	LEU	TYR	SER
	ASP	VAL	ALA	ASN	SER
	GLU	GLU	LVS	GLU	GLN
	LEU	VAL	GLY	LVS	GLU
	THR	PRO	GLU	LEU	MET
	LVS	PHE	ILE	LVS	THR
	ILE	THR	GLY	GLN	ALA
	MET	ILE	SER	LEU	LEU
D289	ASP	ASP	SER	LVS	ALA
E290	ASP	ASP	ASP	GLY	THR
A291	ALA	GLU	GLU	ASP	ALA
S292	ASP	LVS	LVS	GLY	GLU
K293	SER	THR	THR	THR	THR
I294	VAL	LEU	LEU	ASP	ASP
E295	ASN	VAL	VAL	VAL	THR
Q296	GLU	GLU	TYR	MET	ILE
I297	GLU	ALA	ALA	LEU	GLU
Q298	GLN	ASP	ASP	LVS	ALA
K299	THR	PHE	THR	SER	PHE
L300	GLN	ALA	ALA	ALA	LVS

[illegible][illegible]



● Molecule 3: Vacuolar protein sorting-associated protein VTA1

Chain S: 8% . 87%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	82225	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.55	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BEF, ACE, ADP, NH2

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	0/2468	0.81	2/3334 (0.1%)
1	B	0.78	0/2532	0.79	0/3418
1	C	0.79	1/2532 (0.0%)	0.83	2/3418 (0.1%)
1	D	0.75	0/2532	0.78	0/3418
1	E	0.70	0/2401	0.79	0/3244
1	F	0.59	0/2428	0.70	2/3281 (0.1%)
2	G	1.02	0/64	1.07	0/86
3	H	0.53	0/333	0.75	0/447
3	I	0.54	0/333	0.69	0/447
3	J	0.53	0/333	0.75	0/447
3	K	0.54	0/333	0.69	0/447
3	L	0.52	0/333	0.75	0/447
3	M	0.54	0/333	0.70	0/447
3	N	0.53	0/333	0.75	0/447
3	O	0.54	0/333	0.70	0/447
3	P	0.52	0/333	0.74	0/447
3	Q	0.54	0/333	0.69	0/447
3	R	0.53	0/333	0.75	0/447
3	S	0.54	0/333	0.69	0/447
All	All	0.69	1/18953 (0.0%)	0.77	6/25563 (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
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	211	GLU	CG-CD	-5.85	1.43	1.51

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	ARG	NE-CZ-NH1	-6.81	116.89	120.30
1	C	138	LEU	CB-CG-CD2	-6.21	100.45	111.00
1	A	119	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	F	269	GLY	N-CA-C	5.18	126.06	113.10
1	F	287	ARG	NE-CZ-NH1	5.16	122.88	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	GLY	Peptide
1	B	205	LYS	Peptide
1	C	125	SER	Mainchain

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	2427	0	2449	107	0
1	B	2491	0	2516	71	0
1	C	2491	0	2516	86	0
1	D	2491	0	2516	78	0
1	E	2360	0	2377	124	0
1	F	2387	0	2409	340	0
2	G	68	0	71	1	0
3	H	331	0	344	33	0
3	I	331	0	344	17	0
3	J	331	0	344	33	0
3	K	331	0	344	22	0
3	L	331	0	344	34	0
3	M	331	0	344	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	331	0	344	34	0
3	O	331	0	344	19	0
3	P	331	0	344	33	0
3	Q	331	0	344	18	0
3	R	331	0	344	36	0
3	S	331	0	344	29	0
4	A	27	0	12	1	0
4	B	27	0	12	1	0
4	C	27	0	12	1	0
4	D	27	0	12	0	0
4	E	27	0	12	0	0
5	A	4	0	0	1	0
5	B	4	0	0	1	0
5	C	4	0	0	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
All	All	18838	0	19042	904	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 24.

The worst 5 of 904 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:F:172:TYR:CZ	1:F:428:PHE:CD2	1.78	1.63
1:F:172:TYR:CZ	1:F:428:PHE:HD2	0.93	1.57
1:F:295:TYR:CE1	1:F:425:GLN:HB3	1.37	1.54
1:F:199:SER:HB3	1:F:237:LEU:CG	1.39	1.53
1:E:388:TRP:CZ3	1:F:151:LEU:CD1	1.90	1.52

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	310/519 (60%)	274 (88%)	31 (10%)	5 (2%)	11	50
1	B	318/519 (61%)	284 (89%)	29 (9%)	5 (2%)	11	50
1	C	318/519 (61%)	280 (88%)	33 (10%)	5 (2%)	11	50
1	D	318/519 (61%)	279 (88%)	33 (10%)	6 (2%)	9	46
1	E	300/519 (58%)	260 (87%)	36 (12%)	4 (1%)	14	55
1	F	304/519 (59%)	277 (91%)	20 (7%)	7 (2%)	7	40
2	G	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
3	H	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	19
3	I	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	6	38
3	J	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	19
3	K	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	6	38
3	L	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	19
3	M	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	6	38
3	N	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	19
3	O	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	6	38
3	P	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	19
3	Q	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	6	38
3	R	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	19
3	S	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	6	38
All	All	2356/7084 (33%)	2050 (87%)	256 (11%)	50 (2%)	12	42

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	359	HIS
1	A	371	ARG
1	A	395	GLU
1	B	371	ARG
1	B	395	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	266/418 (64%)	258 (97%)	8 (3%)	46	79
1	B	273/418 (65%)	269 (98%)	4 (2%)	70	90
1	C	273/418 (65%)	269 (98%)	4 (2%)	70	90
1	D	273/418 (65%)	268 (98%)	5 (2%)	64	87
1	E	259/418 (62%)	254 (98%)	5 (2%)	62	86
1	F	262/418 (63%)	251 (96%)	11 (4%)	34	72
2	G	8/8 (100%)	8 (100%)	0	100	100
3	H	36/294 (12%)	34 (94%)	2 (6%)	25	64
3	I	36/294 (12%)	35 (97%)	1 (3%)	49	81
3	J	36/294 (12%)	34 (94%)	2 (6%)	25	64
3	K	36/294 (12%)	35 (97%)	1 (3%)	49	81
3	L	36/294 (12%)	34 (94%)	2 (6%)	25	64
3	M	36/294 (12%)	35 (97%)	1 (3%)	49	81
3	N	36/294 (12%)	34 (94%)	2 (6%)	25	64
3	O	36/294 (12%)	35 (97%)	1 (3%)	49	81
3	P	36/294 (12%)	34 (94%)	2 (6%)	25	64
3	Q	36/294 (12%)	35 (97%)	1 (3%)	49	81
3	R	36/294 (12%)	34 (94%)	2 (6%)	25	64
3	S	36/294 (12%)	35 (97%)	1 (3%)	49	81
All	All	2046/6044 (34%)	1991 (97%)	55 (3%)	54	82

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	373	LEU
1	F	278	ILE
3	P	319	GLU
1	E	397	LYS

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Mol	Chain	Res	Type
1	F	139	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	355	GLN
3	I	298	GLN
3	R	296	GLN
1	F	425	GLN
3	H	296	GLN

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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\# Z > 2$
4	ADP	A	701	5,6	25,29,29	1.40	3 (12%)	24,45,45	1.68	6 (25%)
5	BEF	A	702	4	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ADP	B	701	5,6	25,29,29	1.56	4 (16%)	24,45,45	1.58	4 (16%)
5	BEF	B	702	4	0,3,3	0.00	-	0,3,3	0.00	-
4	ADP	C	701	5,6	25,29,29	1.58	5 (20%)	24,45,45	1.78	7 (29%)
5	BEF	C	702	4	0,3,3	0.00	-	0,3,3	0.00	-
4	ADP	D	701	6	25,29,29	1.16	2 (8%)	24,45,45	1.95	7 (29%)
4	ADP	E	701	-	25,29,29	0.91	2 (8%)	24,45,45	1.78	2 (8%)

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
4	ADP	A	701	5,6	-	0/12/32/32	0/3/3/3
5	BEF	A	702	4	-	0/0/0/0	0/0/0/0
4	ADP	B	701	5,6	-	0/12/32/32	0/3/3/3
5	BEF	B	702	4	-	0/0/0/0	0/0/0/0
4	ADP	C	701	5,6	-	0/12/32/32	0/3/3/3
5	BEF	C	702	4	-	0/0/0/0	0/0/0/0
4	ADP	D	701	6	-	0/12/32/32	0/3/3/3
4	ADP	E	701	-	-	0/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	701	ADP	PB-O3A	-4.33	1.53	1.60
4	C	701	ADP	PB-O3A	-4.08	1.53	1.60
4	A	701	ADP	PB-O3A	-3.53	1.54	1.60
4	C	701	ADP	C8-N7	-3.03	1.29	1.34
4	B	701	ADP	C8-N7	-2.73	1.29	1.34

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	701	ADP	N3-C2-N1	-6.65	123.07	128.86
4	D	701	ADP	N3-C2-N1	-5.97	123.66	128.86
4	B	701	ADP	O3B-PB-O1B	-4.13	94.35	110.50
4	C	701	ADP	C4'-O4'-C1'	-4.07	105.44	109.77
4	A	701	ADP	C2'-C3'-C4'	-3.99	94.84	102.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	ADP	1	0
5	A	702	BEF	1	0
4	B	701	ADP	1	0
5	B	702	BEF	1	0
4	C	701	ADP	1	0
5	C	702	BEF	1	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.