



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 16, 2018 – 10:00 am GMT

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 : 2017-08-16  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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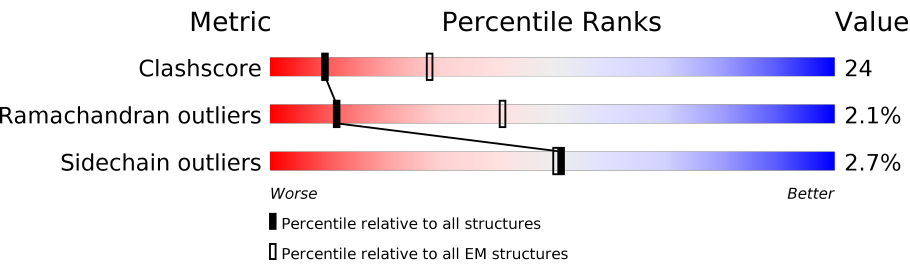
MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

# 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 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	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531

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	519	<div><div>49%</div><div>9%</div><div>.</div><div>39%</div></div>
1	B	519	<div><div>50%</div><div>11%</div><div>.</div><div>38%</div></div>
1	C	519	<div><div>50%</div><div>11%</div><div>.</div><div>38%</div></div>
1	D	519	<div><div>51%</div><div>9%</div><div>.</div><div>38%</div></div>
1	E	519	<div><div>45%</div><div>12%</div><div>.</div><div>41%</div></div>
1	F	519	<div><div>35%</div><div>22%</div><div>.</div><div>41%</div></div>
2	G	10	<div><div>90%</div><div>10%</div></div>
3	H	330	<div><div>5%</div><div>8%</div><div>87%</div></div>
3	I	330	<div><div>8%</div><div>5%</div><div>87%</div></div>

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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.

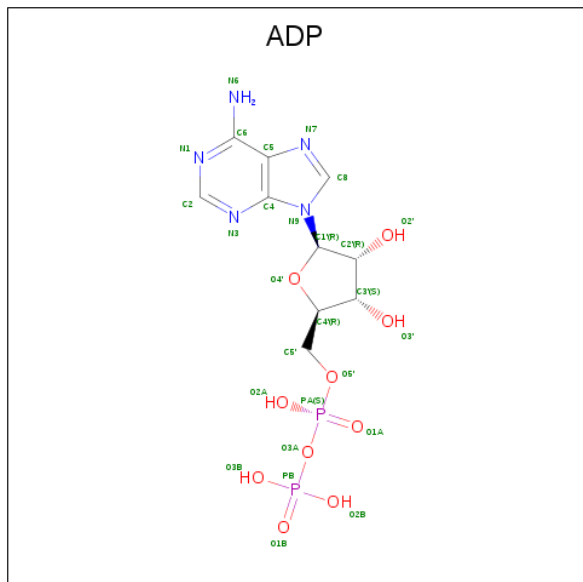
Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	42	Total	C	N	O	0	0
			331	209	54	68		
3	I	42	Total	C	N	O	0	0
			331	209	54	68		
3	J	42	Total	C	N	O	0	0
			331	209	54	68		
3	K	42	Total	C	N	O	0	0
			331	209	54	68		
3	L	42	Total	C	N	O	0	0
			331	209	54	68		
3	M	42	Total	C	N	O	0	0
			331	209	54	68		
3	N	42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

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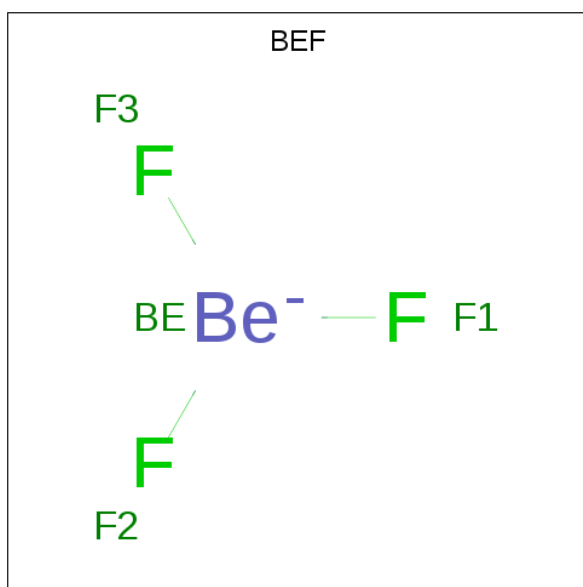
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Mol	Chain	Residues	Atoms				AltConf	Trace
3	O	42	Total	C	N	O	0	0
			331	209	54	68		
3	P	42	Total	C	N	O	0	0
			331	209	54	68		
3	Q	42	Total	C	N	O	0	0
			331	209	54	68		
3	R	42	Total	C	N	O	0	0
			331	209	54	68		
3	S	42	Total	C	N	O	0	0
			331	209	54	68		

- 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
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	

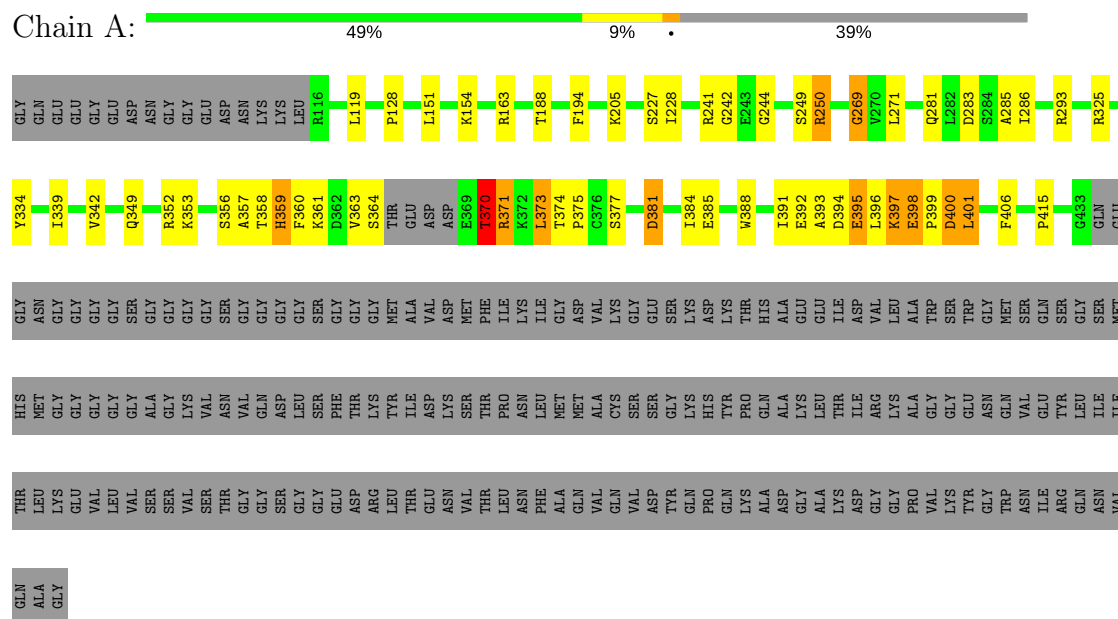
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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	

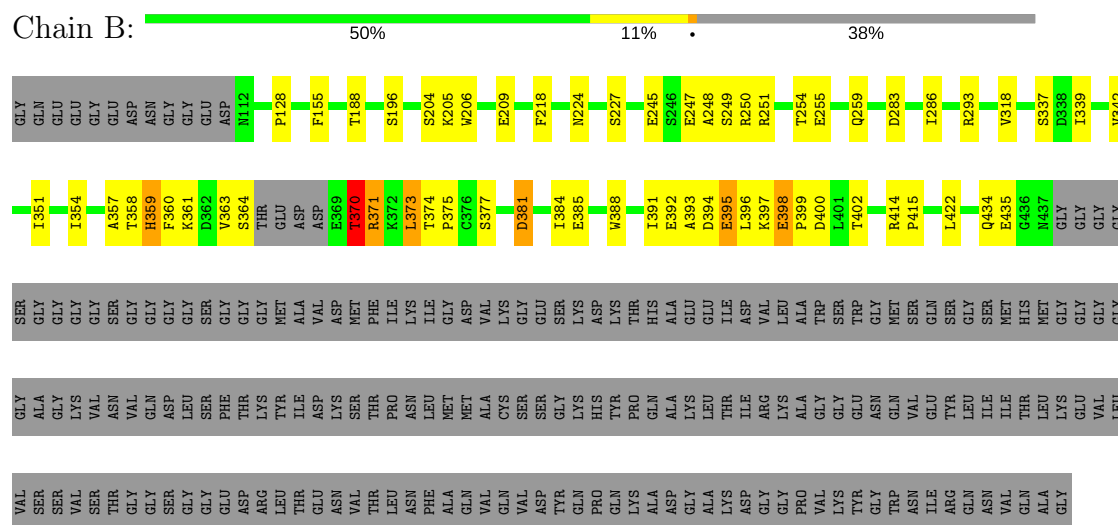
### 3 Residue-property plots

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

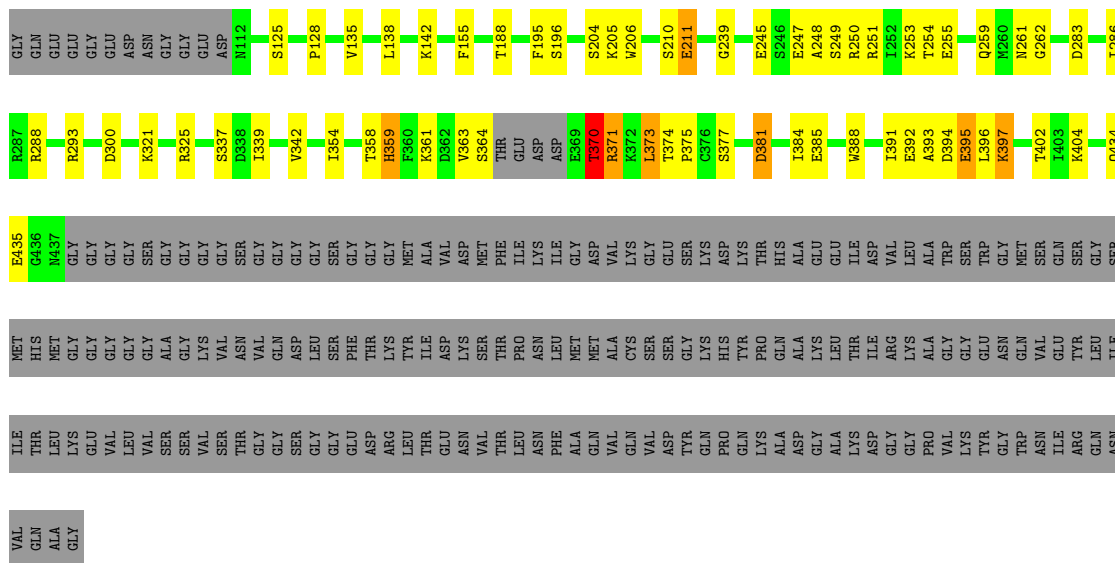


- Molecule 1: Vacuolar protein sorting-associated protein 4, Protein hcp1



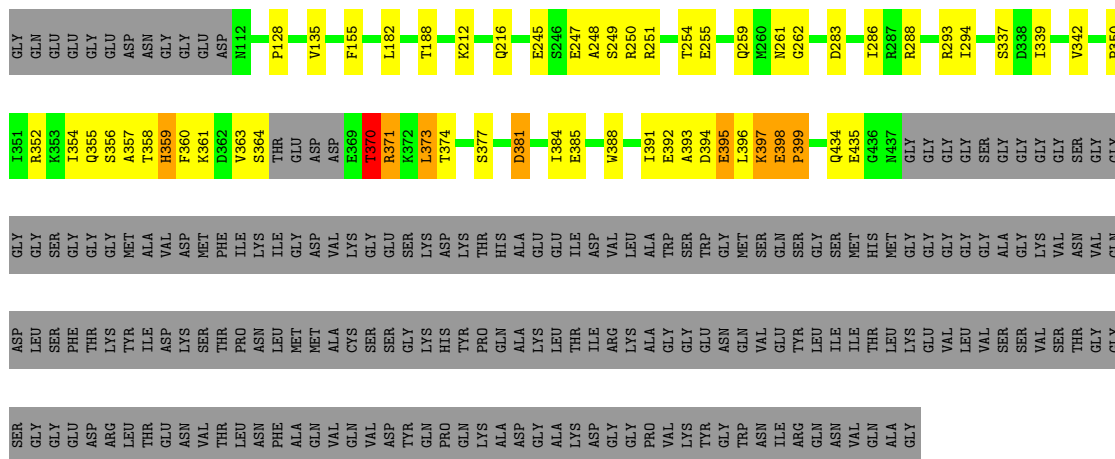
- Molecule 1: Vacuolar protein sorting-associated protein 4, Protein hcp1

Chain C:



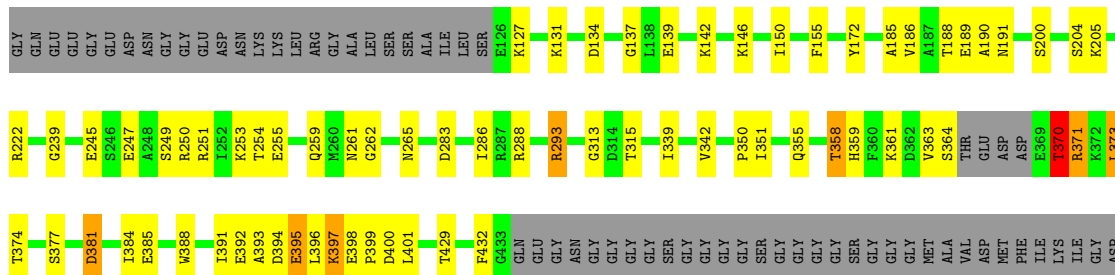
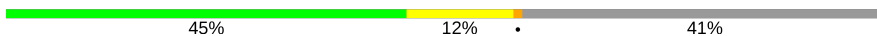
- Molecule 1: Vacuolar protein sorting-associated protein 4, Protein hcp1

Chain D:



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

Chain E:



VAL	LYS	GLY	GLU	SER	LYS	ASP	LYS	THR	HIS	ALA	GLU	GLU	ILE	ASP	VAL	LEU	ALA	TRP	SER	SER	TRP	GLY	MET	SER	GLN	SER	GLY	MET	HIS	MET	GLY	GLY	GLY	GLY	GLY	ALA	LYS	ASN	VAL	ASN	VAL	GLN	ASP	LEU	SER	PHI	THR	LYS	TYR	ILE	ILE	ASP	LYS	SER	LYS	THR	PRO	ASN	LEU	ASP	MET	...
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ALA CYS SER SER GLY LYS HIS TYR PRO GLN ALA LYS LYS LEU THR ILE ARG LYS ALA GLY GLU ASN GLN VAL GLU TYR LEU LEU ILE ILE THR LEU LYS GLU VAL LEU VAL SER SER VAL SER SER THR GLY GLY SER SER GLY GLU ASP ARG LEU THR THR LEU ASN VAL THR LEU ASN PHE ALA

VAL	GLN	VAL	ASP	TYR	GLN	PRO	GLN	LYS	ALA	ASP	GLY	ALA	LYS	ASP	GLY	GLY	PRO	VAL	LYS	TYR	GLY	TRP	ASN	ILE	ARG	GLN	ASN	VAL	GLN	ALA	GLY
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- Molecule 1: Vacuolar protein sorting-associated protein 4, Protein hcp1

Chain F:  35% 22% 1% 41%

GLY	GLN	GLU	GLY	GLU	ASP	ASN	GLY	GLY	GLU	ASP	ASN	LYS	LYS	ARG	LEU	GLY	ALA	LEU	SER	SER	<b>A122</b>	<b>K127</b>	<b>W132</b>	<b>A136</b>	<b>E139</b>	<b>L151</b>	<b>F155</b>	<b>F156</b>	<b>H157</b>	<b>L158</b>	<b>L162</b>	<b>L163</b>	<b>T166</b>	<b>S167</b>	<b>G168</b>	<b>L169</b>	<b>Y172</b>	<b>G173</b>	<b>P174</b>	<b>E189</b>	<b>S199</b>	<b>S200</b>	<b>V203</b>	<b>S204</b>	<b>K205</b>
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Q207 Q208 Q209 Q210 Q211 Q212 Q213 Q214 Q215 Q216 Q217 Q218 Q219 Q220 Q221 Q222 Q223 Q224 Q225 Q226 Q227 Q228 Q229 Q230 Q231 Q232 Q233 Q234 Q235 Q236 Q237 Q238 Q239 Q240 Q241 Q242 Q243 Q244 Q245 Q246 Q247 Q248 Q249 Q250 Q251 Q252 Q253 Q254 Q255 Q256 Q257 Q258 Q259 Q260 Q261 Q262 Q263 Q264 Q265 Q266 Q267 Q268 Q269 Q270 Q271 Q272 Q273 Q274 Q275 Q276 Q277 Q278 Q279 Q280 Q281 Q282 Q283 Q284 Q285 Q286 Q287 Q288 Q289 Q290 Q291 Q292 Q293 Q294 Q295 Q296 Q297 Q298 Q299 Q300

A303	R304	F308	N311	V312	T315	P316	G317	F318	L319	D323	G328	I339	V342	V343	A346	L347	M348	Q349	P350	I351	R352	K353	L354	P355	G356	A357	R358	H359	F360	K361	L362	G363	S364	THR	GLU	ASP	ASP	E369	<b>F370</b>	R371	<b>K372</b>	<b>L373</b>	T374	<b>S377</b>	D381	I384	E385
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3387	K388	K389	K390	K391	K392	K393	K394	K395	K396	K397	K398	K399	K400	K401	K402	K403	K404	K405	K406	K407	K408	K409	K410	K411	K412	K413	K414	K415	K416	K417	K418	K419	K420	K421	K422	K423	K424	K425	K426	K427	K428	K429	K430	K431	K432	K433	K434	K435	K436	K437	K438	K439	K440	K441	K442	K443	K444	K445	K446	K447	K448	K449	K450	K451	K452	K453	K454	K455	K456	K457	K458	K459	K460	K461	K462	K463	K464	K465	K466	K467	K468	K469	K470	K471	K472	K473	K474	K475	K476	K477	K478	K479	K480	K481	K482	K483	K484	K485	K486	K487	K488	K489	K490	K491	K492	K493	K494	K495	K496	K497	K498	K499	K500	K501	K502	K503	K504	K505	K506	K507	K508	K509	K510	K511	K512	K513	K514	K515	K516	K517	K518	K519	K520	K521	K522	K523	K524	K525	K526	K527	K528	K529	K530	K531	K532	K533	K534	K535	K536	K537	K538	K539	K540	K541	K542	K543	K544	K545	K546	K547	K548	K549	K550	K551	K552	K553	K554	K555	K556	K557	K558	K559	K560	K561	K562	K563	K564	K565	K566	K567	K568	K569	K570	K571	K572	K573	K574	K575	K576	K577	K578	K579	K580	K581	K582	K583	K584	K585	K586	K587	K588	K589	K590	K591	K592	K593	K594	K595	K596	K597	K598	K599	K600	K601	K602	K603	K604	K605	K606	K607	K608	K609	K610	K611	K612	K613	K614	K615	K616	K617	K618	K619	K620	K621	K622	K623	K624	K625	K626	K627	K628	K629	K630	K631	K632	K633	K634	K635	K636	K637	K638	K639	K640	K641	K642	K643	K644	K645	K646	K647	K648	K649	K650	K651	K652	K653	K654	K655	K656	K657	K658	K659	K660	K661	K662	K663	K664	K665	K666	K667	K668	K669	K670	K671	K672	K673	K674	K675	K676	K677	K678	K679	K680	K681	K682	K683	K684	K685	K686	K687	K688	K689	K690	K691	K692	K693	K694	K695	K696	K697	K698	K699	K700	K701	K702	K703	K704	K705	K706	K707	K708	K709	K710	K711	K712	K713	K714	K715	K716	K717	K718	K719	K720	K721	K722	K723	K724	K725	K726	K727	K728	K729	K730	K731	K732	K733	K734	K735	K736	K737	K738	K739	K740	K741	K742	K743	K744	K745	K746	K747	K748	K749	K750	K751	K752	K753	K754	K755	K756	K757	K758	K759	K760	K761	K762	K763	K764	K765	K766	K767	K768	K769	K770	K771	K772	K773	K774	K775	K776	K777	K778	K779	K780	K781	K782	K783	K784	K785	K786	K787	K788	K789	K790	K791	K792	K793	K794	K795	K796	K797	K798	K799	K800	K801	K802	K803	K804	K805	K806	K807	K808	K809	K810	K811	K812	K813	K814	K815	K816	K817	K818	K819	K820	K821	K822	K823	K824	K825	K826	K827	K828	K829	K830	K831	K832	K833	K834	K835	K836	K837	K838	K839	K840	K841	K842	K843	K844	K845	K846	K847	K848	K849	K850	K851	K852	K853	K854	K855	K856	K857	K858	K859	K860	K861	K862	K863	K864	K865	K866	K867	K868	K869	K870	K871	K872	K873	K874	K875	K876	K877	K878	K879	K880	K881	K882	K883	K884	K885	K886	K887	K888	K889	K890	K891	K892	K893	K894	K895	K896	K897	K898	K899	K900	K901	K902	K903	K904	K905	K906	K907	K908	K909	K910	K911	K912	K913	K914	K915	K916	K917	K918	K919	K920	K921	K922	K923	K924	K925	K926	K927	K928	K929	K930	K931	K932	K933	K934	K935	K936	K937	K938	K939	K940	K941	K942	K943	K944	K945	K946	K947	K948	K949	K950	K951	K952	K953	K954	K955	K956	K957	K958	K959	K960	K961	K962	K963	K964	K965	K966	K967	K968	K969	K970	K971	K972	K973	K974	K975	K976	K977	K978	K979	K980	K981	K982	K983	K984	K985	K986	K987	K988	K989	K990	K991	K992	K993	K994	K995	K996	K997	K998	K999	K1000
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GLY	GLY	GLY	GLY	ALA	VAL	ASP	MET	PHE	ILE	LYS	LYE	GLY	GLY	GLU	SER	LYS	ASP	THR	HIS	ALA	GLU	GLU	ILE	ASP	VAL	LEU	ALA	TRP	TRP	TRP	GLY	MET	SER	SER	SER	SER	MET	HIS	MET	MET	GLY	GLY	GLY	GLY	LYS	VAL	VAL	ASN	VAL	GLN	ASP	GLN	LEU
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PHE THR LYS TYR ILE ASP SER LYS PRO ASN LEU MET ALA CYS SVS SER GLY HIS TYR PRO GLN ALA LYS LEU THR ILE ARG LYS ALA GLY GLY GLN VAL GLU ASN GLN VAL GLU TYR LEU ILE THR LER LEU LYS VAL GLU VAL SER SER VAL SER THR GLY GLY SER GLY

GLU	ASP	ARG	LEU	THR	GLU	ASN	ASN	VAL	THR	LEU	ASN	PHE	ALA	GLN	GLN	VAL	VAL	ASP	TYR	PRO	GLN	LYS	ALA	ASP	GLY	LYS	ASP	GLY	GLY	GLY	PRO	VAL	LYS	TYR	GLY	GLY	TRP	ASN	ILE	ARG	GLN	ASN	VAL	VAL	GLN	ALA	GLY
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- Molecule 2: ACE-ASP-GLU-ILE-VAL-ASN-LYS-VAL-LEU-NH2

Chain G:  90% 10%

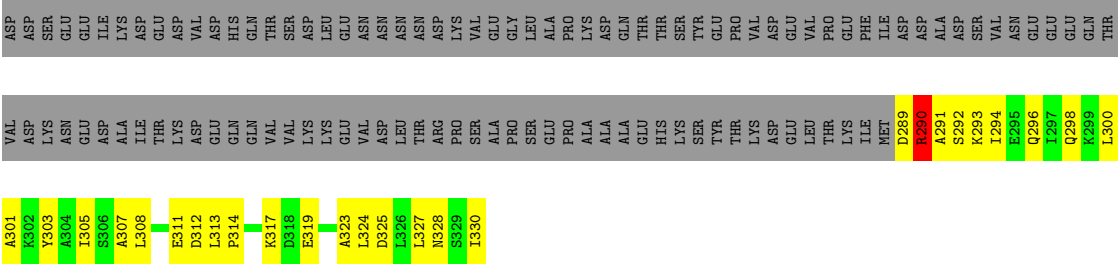
- Molecule 3: Vacuolar protein sorting-associated protein VTA1

Chain H:  5% 8% 87%

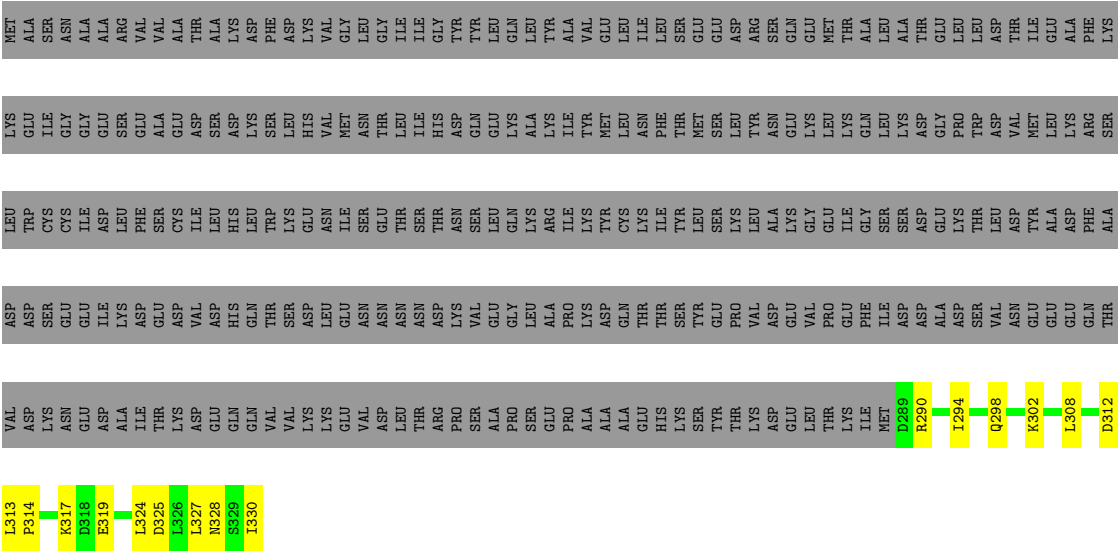
MET	ALA	SER	ASN	ALA	ALA	ARG	VAL	VAL	ALA	ALA	ALA	ALA	ALA	LYS	LYS	VAL	GLY	LEU	GLY	ILE	ILE	GLY	TYR	TYR	LEU	LEU	GLN	LEU	LEU	TYR	ALA	VAL	GLU	LEU	ILE	LEU	SER	GLU	GLU	GLU	ASP	ARG	SER	GLN	GLN	MET	THR	THR	ALA	ALA	ALA	ALA	THR	GLU	GLU	LEU	LEU	ASP	THR	ILE	ILE	ALA	ALA	PHE
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LYS GLU GLU ILE GLY GLY GLU SER GLU GLU ALA GLU ASP SER ASP LYS SER SER LEU HIS VAL MET ASN THR LEU ILE HIS ASP GLN GLU LYS LYS LYS ALA LYS ILE TYR MET MET LEU MET LEU TYR ASN GLU LYS LEU LEU LYS GLN LEU LYS ASP ASP VAL MET MET LEU LYS ARG

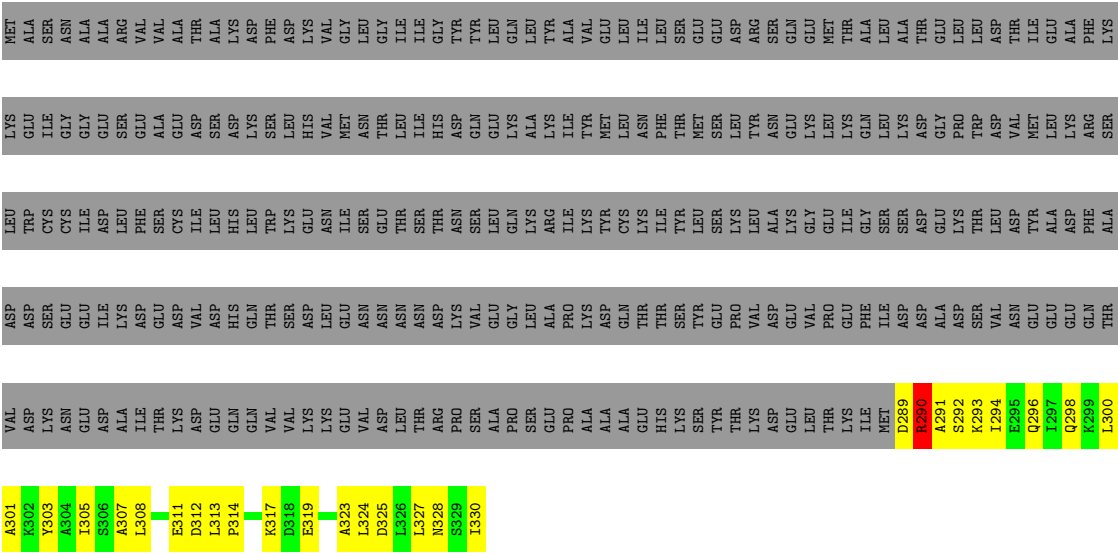
LEU TRP CYS CYS ILE ASP LEU LEU HIS LEU TRP LEU TRP GLU GLY ASN ILE SER SER GLU THR SER SER ASN SER LEU SER LEU GLN LYS ARG ILE LYS TYR CYS TYR LYS TYR ILE ILE TYR TYR LEU SER SER LYS LEU LEU ALA LYS GLY GLU ILE GLY SER SER ASP ASP GLU LYS THR LEU ASP TYR ALA ASP PHE



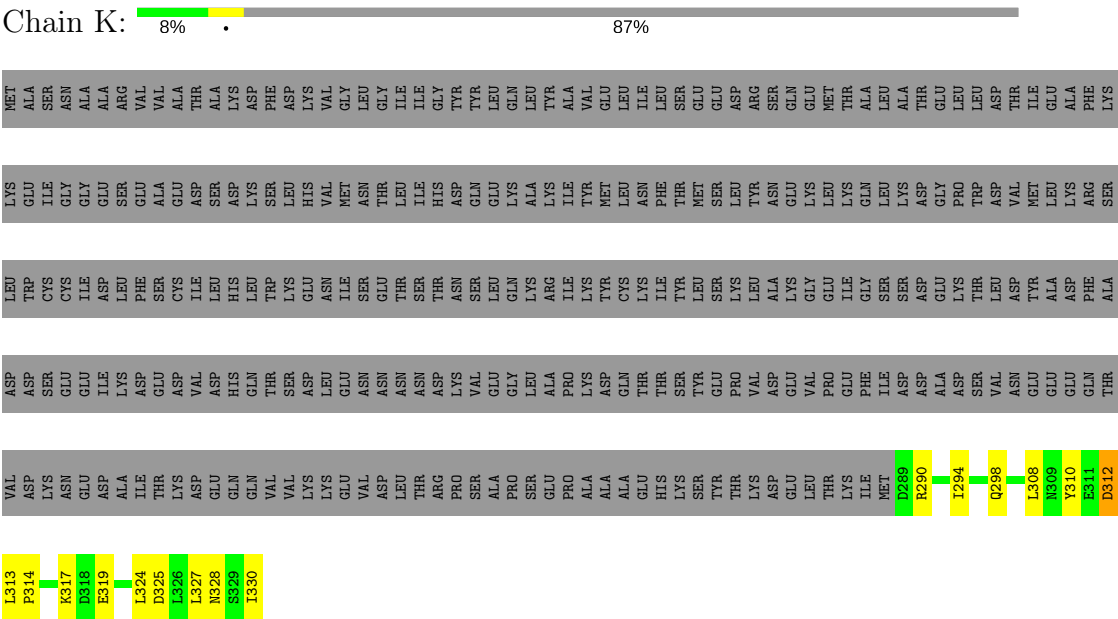
• Molecule 3: Vacuolar protein sorting-associated protein VTA1



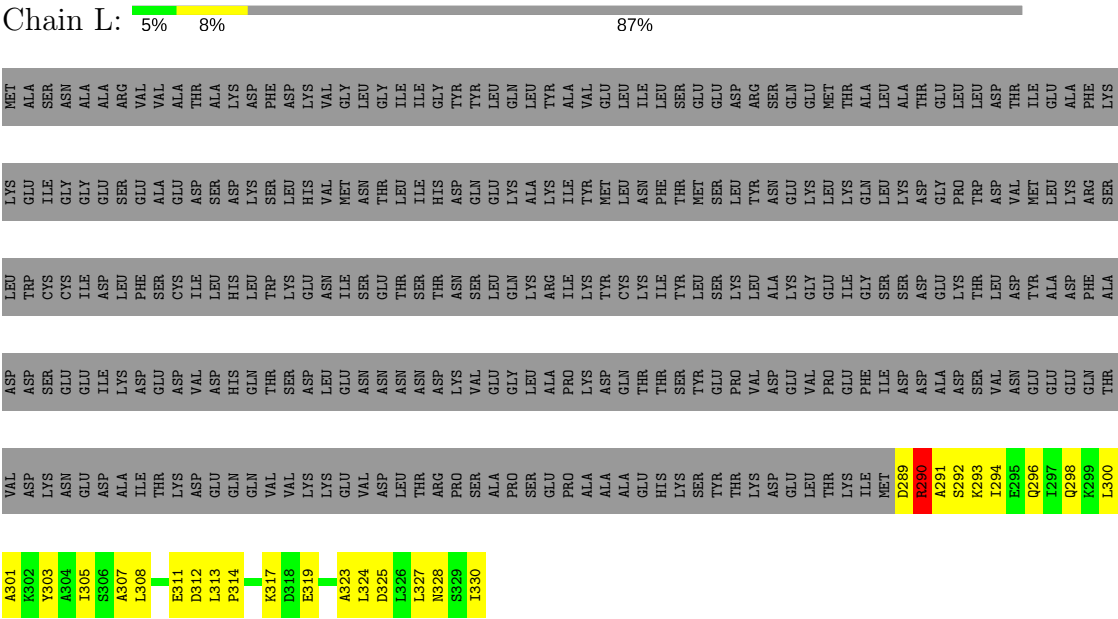
• Molecule 3: Vacuolar protein sorting-associated protein VTA1



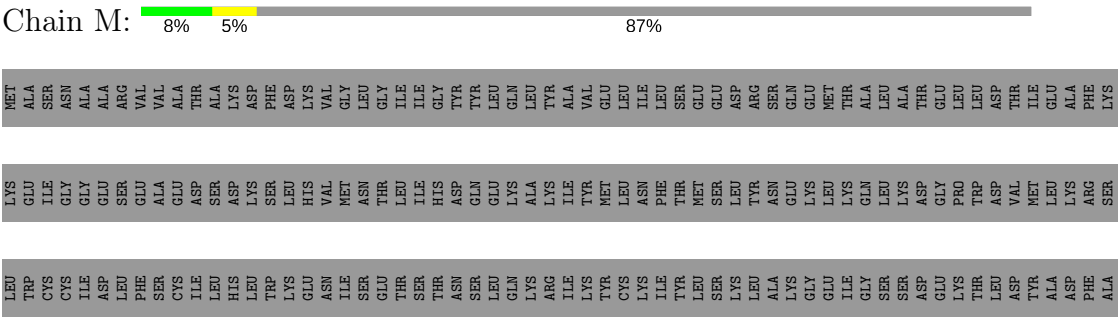
• Molecule 3: Vacuolar protein sorting-associated protein VTA1

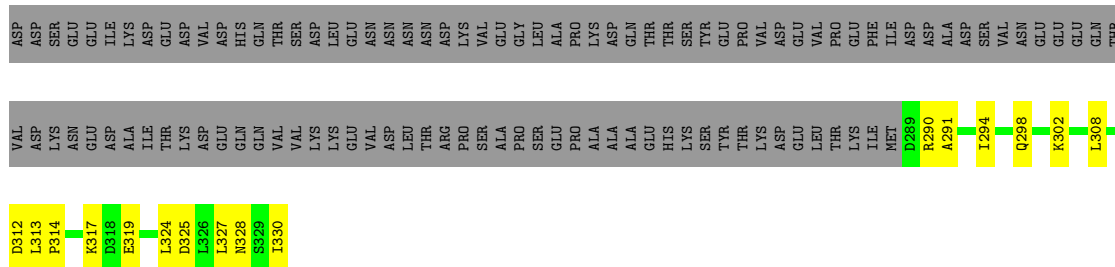


• Molecule 3: Vacuolar protein sorting-associated protein VTA1

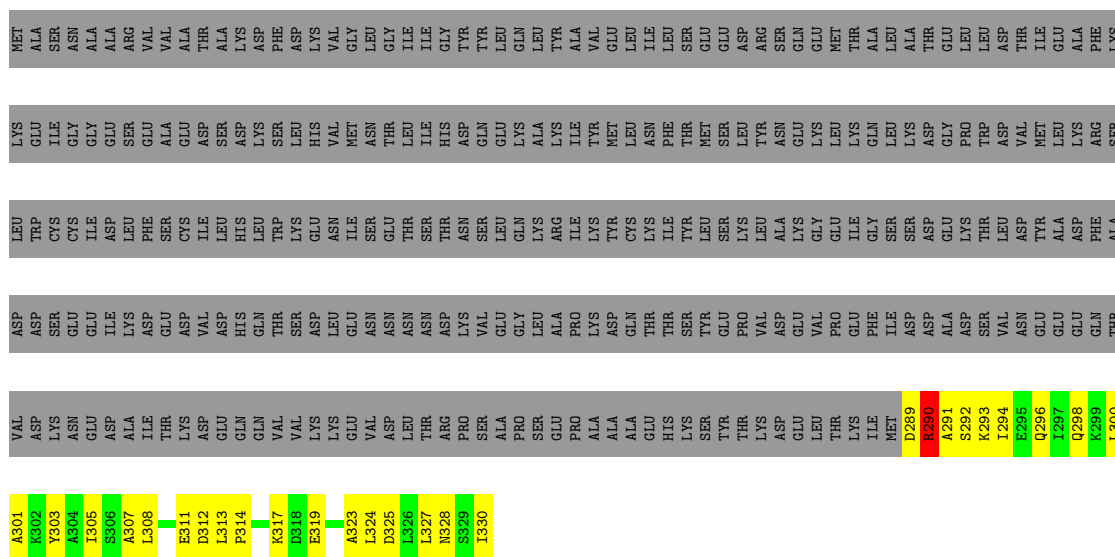


• Molecule 3: Vacuolar protein sorting-associated protein VTA1

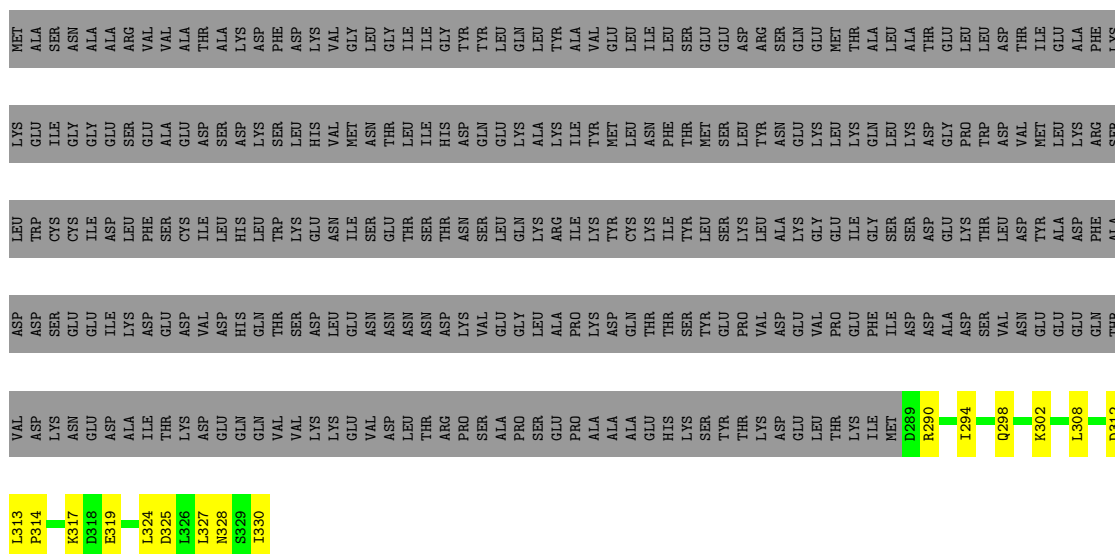




- Molecule 3: Vacuolar protein sorting-associated protein VTA1



- Molecule 3: Vacuolar protein sorting-associated protein VTA1



- Molecule 3: Vacuolar protein sorting-associated protein VTA1

Chain P:  5% 8% 87%

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	ALA
L313	LVS	ASP	CYS	GLU	ALA
P314	ASP	VAL	ILE	ASP	THR
	GLU	ASP	LEU	SER	ALA
K317	GLN	HIS	HIS	ASP	LVS
D318	GLN	GLN	LEU	ASP	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	GLU	GLU	ILE	MET	GLY
L326	VAL	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	SER	GLN	TYR
	ALA	GLU	LEU	GLU	LEU
	PRO	GLY	GLN	LVS	GLN
	SER	LEU	LVS	ALA	LEU
	GLU	ALA	ARG	LVS	TYR
	PRO	PRO	ILE	ILE	ALA
	ALA	LVS	LYS	TYR	VAL
	ALA	ASP	TYR	MET	GLU
	ALA	GLN	CYS	LEU	LEU
	GLU	THR	LVS	ASN	ILE
	HIS	THR	ILE	PHE	LEU
	LVS	SER	TYR	THR	SER
	TYR	GLU	SER	MET	GLU
	THR	PRO	LVS	LEU	ASP
	LVS	VAL	LEU	TYR	ARG
	ASP	ASP	ALA	ASN	SER
	GLU	GLU	LYS	GLU	GLN
	LEU	VAL	GLY	LYS	GLU
	THR	PRO	GLU	LEU	MET
	LVS	GLU	ILE	LVS	THR
	ILE	PHE	GLY	GLN	ALA
	MET	ILE	SER	LEU	LEU
	D289	ASP	SER	LVS	ALA
	K290	ASP	ASP	ASP	THR
	A291	ALA	GLU	GLY	GLU
	S292	ASP	LVS	PRO	LEU
	K293	SER	THR	TRP	LEU
	I294	VAL	THR	ASP	ASP
	E295	ASN	ASP	VAL	THR
	Q296	GLU	TYR	MET	ILE
	I297	GLU	ALA	LEU	LEU
	Q298	GLU	ASP	LVS	ALA
	K299	GLN	PHE	ARG	PHE

- Molecule 3: Vacuolar protein sorting-associated protein VTA1

Chain Q:  8% . 87%

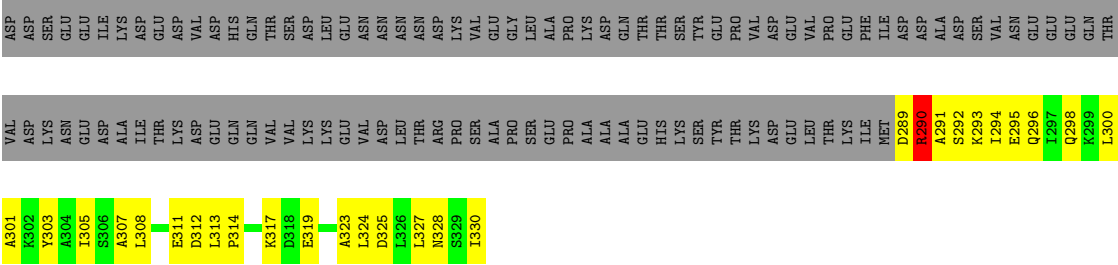
[illegible]

- Molecule 3: Vacuolar protein sorting-associated protein VTA1

Chain R:  5% 8% 87%

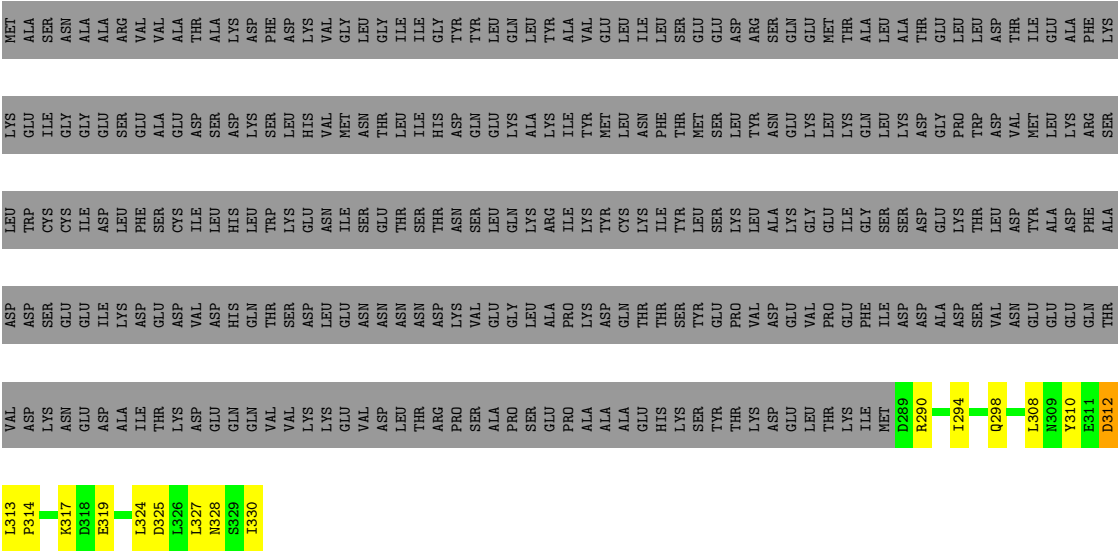
LEU	TRP	CYS	ILE	ASP	LEU	PHE	SER	CYS	ILE	LEU	HIS	ASN	GLU	SER	THR	SER	LEU	GLY	VAL	LYS	ASP	PHE	LYS	ASP	LYS	GLY	LEU	GLN	LEU	TYR	ALA	ILE	LYS	ASP	LEU	GLY	VAL	ARG	ASN	GLY	ILE	TRP	LEU
LYS	GLU	ILE	GLY	GLU	SER	ALA	GLU	ASP	SER	ASP	VAL	HIS	LEU	SER	ASP	GLN	ASP	GLN	TYR	GLY	THR	ASN	MET	VAL	VAL	LEU	GLY	LEU	GLN	TYR	ALA	ILE	LYS	ASP	LEU	GLY	VAL	ARG	ASN	GLY	ILE	TRP	LEU





● 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	47
1	B	318/519 (61%)	284 (89%)	29 (9%)	5 (2%)	11	47
1	C	318/519 (61%)	280 (88%)	33 (10%)	5 (2%)	11	47
1	D	318/519 (61%)	279 (88%)	33 (10%)	6 (2%)	9	43
1	E	300/519 (58%)	260 (87%)	36 (12%)	4 (1%)	13	52
1	F	304/519 (59%)	277 (91%)	20 (7%)	7 (2%)	7	38
2	G	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
3	H	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	18
3	I	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	6	36
3	J	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	18
3	K	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	6	36
3	L	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	18
3	M	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	6	36
3	N	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	18
3	O	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	6	36
3	P	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	18
3	Q	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	6	36
3	R	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	18
3	S	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	6	36
All	All	2356/7084 (33%)	2050 (87%)	256 (11%)	50 (2%)	12	40

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%)	44	76
1	B	273/418 (65%)	269 (98%)	4 (2%)	67	88
1	C	273/418 (65%)	269 (98%)	4 (2%)	67	88
1	D	273/418 (65%)	268 (98%)	5 (2%)	62	85
1	E	259/418 (62%)	254 (98%)	5 (2%)	60	84
1	F	262/418 (63%)	251 (96%)	11 (4%)	32	69
2	G	8/8 (100%)	8 (100%)	0	100	100
3	H	36/294 (12%)	34 (94%)	2 (6%)	23	61
3	I	36/294 (12%)	35 (97%)	1 (3%)	47	77
3	J	36/294 (12%)	34 (94%)	2 (6%)	23	61
3	K	36/294 (12%)	35 (97%)	1 (3%)	47	77
3	L	36/294 (12%)	34 (94%)	2 (6%)	23	61
3	M	36/294 (12%)	35 (97%)	1 (3%)	47	77
3	N	36/294 (12%)	34 (94%)	2 (6%)	23	61
3	O	36/294 (12%)	35 (97%)	1 (3%)	47	77
3	P	36/294 (12%)	34 (94%)	2 (6%)	23	61
3	Q	36/294 (12%)	35 (97%)	1 (3%)	47	77
3	R	36/294 (12%)	34 (94%)	2 (6%)	23	61
3	S	36/294 (12%)	35 (97%)	1 (3%)	47	77
All	All	2046/6044 (34%)	1991 (97%)	55 (3%)	51	78

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	1.42	3 (12%)	25,45,45	1.76	7 (28%)
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	1.64	4 (16%)	25,45,45	1.62	5 (20%)
5	BEF	B	702	4	0,3,3	0.00	-	0,3,3	0.00	-
4	ADP	C	701	5,6	25,29,29	1.68	6 (24%)	25,45,45	1.89	9 (36%)
5	BEF	C	702	4	0,3,3	0.00	-	0,3,3	0.00	-
4	ADP	D	701	6	25,29,29	1.23	2 (8%)	25,45,45	2.06	7 (28%)
4	ADP	E	701	-	25,29,29	1.04	2 (8%)	25,45,45	1.88	3 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	701	ADP	PB-O3A	-4.59	1.53	1.60
4	C	701	ADP	PB-O3A	-4.32	1.53	1.60
4	A	701	ADP	PB-O3A	-3.74	1.54	1.60
4	E	701	ADP	C8-N9	-3.24	1.33	1.36
4	D	701	ADP	C8-N9	-3.13	1.33	1.36

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	701	ADP	N3-C2-N1	-6.77	123.07	128.86
4	D	701	ADP	N3-C2-N1	-6.08	123.66	128.86
4	C	701	ADP	C4'-O4'-C1'	-4.21	105.44	109.83
4	B	701	ADP	O3B-PB-O1B	-4.16	94.35	110.60
4	D	701	ADP	PA-O3A-PB	-4.15	118.69	132.63

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.