wwPDB EM Validation Summary Report (i)

Nov 14, 2022 – 03:03 AM EST

PDB ID	:	6WM3
EMDB ID	:	EMD-21848
Title	:	Human V-ATPase in state 2 with SidK and ADP
Authors	:	Wang, L.; Wu, H.; Fu, T.M.
Deposited on	:	2020-04-20
Resolution	:	3.40 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

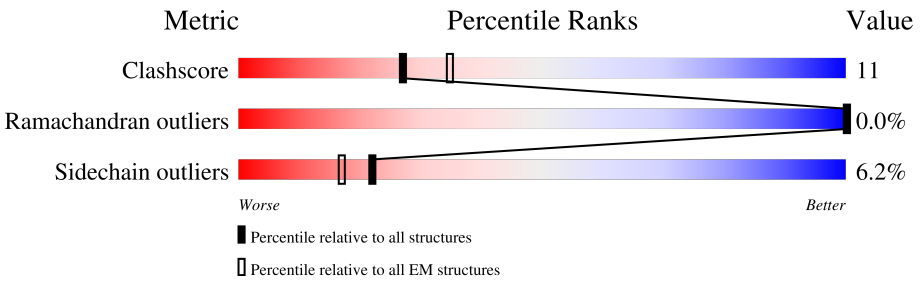
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.40 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	R	837	18% 51% 37% • 10%
2	O	382	28% 93% 5% •
3	H	226	5% 73% 27%
3	I	226	8% 71% 27% •
3	J	226	19% 70% 28% •
4	K	118	9% 58% 36% • •
4	L	118	24% 66% 30% • •
4	M	118	40% 59% 34% • •

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Mol	Chain	Length	Quality of chain
5	S	81	5% 69% 26% 5%
6	T	137	14% 45% 16% • 38%
7	U	470	27% 15% • 57%
8	V	350	9% 5% 86%
9	0	205	68% 29% •
10	1	155	75% 21% • •
10	2	155	65% 30% • •
10	3	155	68% 28% • •
10	4	155	65% 28% • •
10	5	155	69% 26% • •
10	6	155	65% 30% • •
10	7	155	68% 27% • •
10	8	155	65% 28% • •
10	9	155	65% 30% • •
11	Q	351	• 69% 29% •
12	A	617	• 73% 22% • •
12	B	617	75% 21% • •
12	C	617	• 76% 19% • •
13	D	511	• 74% 17% • 8%
13	E	511	5% 69% 21% • 8%
13	F	511	• 68% 21% • 8%
14	X	573	• 35% 11% • 53%
14	Y	573	25% 31% 14% • 54%
14	Z	573	7% 32% 13% • 54%
15	G	247	• 68% 17% • 14%

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Mol	Chain	Length	Quality of chain
16	N	119	13% 55% 34% 8%
17	P	483	81% 7% 12%

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 69755 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 V-type proton ATPase 116 kDa subunit a isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	R	753	6147	4016	1023	1068	40	0	0

- Molecule 2 is a protein called V-type proton ATPase subunit C 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	O	375	1864	1114	375	375	0	0

- Molecule 3 is a protein called V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J	225	1822	1143	322	347	10	0	0
3	I	225	1822	1143	322	347	10	0	0
3	H	225	1822	1143	322	347	10	0	0

- Molecule 4 is a protein called V-type proton ATPase subunit G 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	M	114	938	573	179	183	3	0	0
4	L	114	938	573	179	183	3	0	0
4	K	114	938	573	179	183	3	0	0

- Molecule 5 is a protein called V-type proton ATPase subunit e 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	S	77	631	436	97	93	5	0	0

- Molecule 6 is a protein called Ribonuclease kappa.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	T	85	658	434	102	115	7	0	0

- Molecule 7 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	U	204	1662	1086	267	299	10	0	0

- Molecule 8 is a protein called Renin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	V	49	411	280	57	71	3	0	0

- Molecule 9 is a protein called V-type proton ATPase 21 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	0	204	1498	990	238	259	11	0	0

- Molecule 10 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	1	150	1065	698	169	191	7	0	0
10	2	150	1065	698	169	191	7	0	0
10	3	150	1065	698	169	191	7	0	0
10	4	150	1065	698	169	191	7	0	0
10	5	150	1065	698	169	191	7	0	0
10	6	150	1065	698	169	191	7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	7	150	1065	698	169	191	7	0	0
10	8	150	1065	698	169	191	7	0	0
10	9	150	1065	698	169	191	7	0	0

- Molecule 11 is a protein called V-type proton ATPase subunit d 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	Q	351	2844	1834	463	532	15	0	0

- Molecule 12 is a protein called V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	C	600	4656	2952	786	890	28	0	0
12	A	600	4656	2952	786	890	28	0	0
12	B	600	4656	2952	786	890	28	0	0

- Molecule 13 is a protein called V-type proton ATPase subunit B, brain isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	F	468	3666	2325	625	696	20	0	0
13	D	468	3666	2325	625	696	20	0	0
13	E	468	3666	2325	625	696	20	0	0

- Molecule 14 is a protein called SidK.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	Z	262	2110	1339	353	408	10	0	0
14	X	267	2136	1355	359	411	11	0	0
14	Y	262	2111	1339	354	408	10	0	0

- Molecule 15 is a protein called V-type proton ATPase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	G	213	1717	1090	310	312	5	0	0

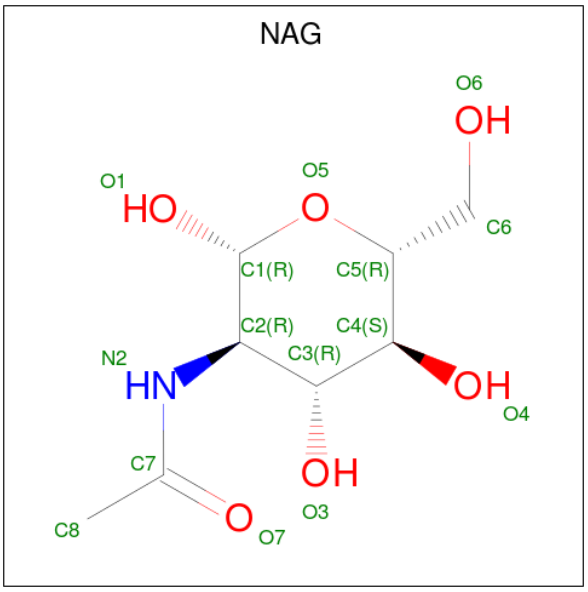
- Molecule 16 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	N	110	875	552	157	164	2	0	0

- Molecule 17 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	P	427	2121	1267	427	427	0	0

- Molecule 18 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
18	R	1	14	8	1	5	0
18	S	1	14	8	1	5	0
18	U	1	84	48	6	30	0

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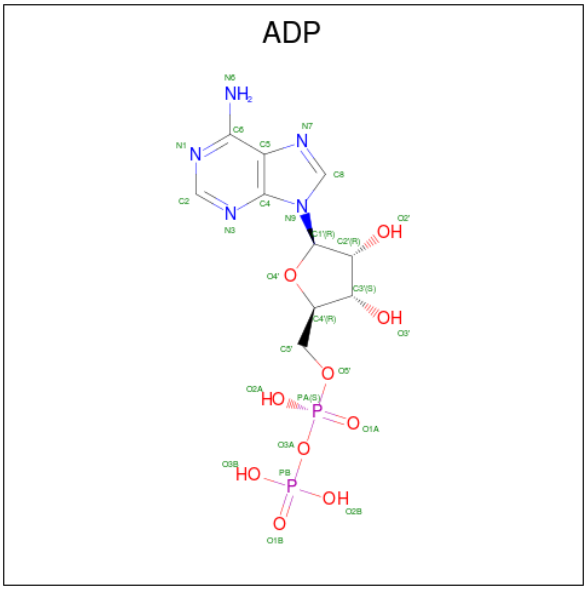
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
18	U	1	84	48	6	30	0
18	U	1	84	48	6	30	0
18	U	1	84	48	6	30	0
18	U	1	84	48	6	30	0
18	U	1	84	48	6	30	0

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



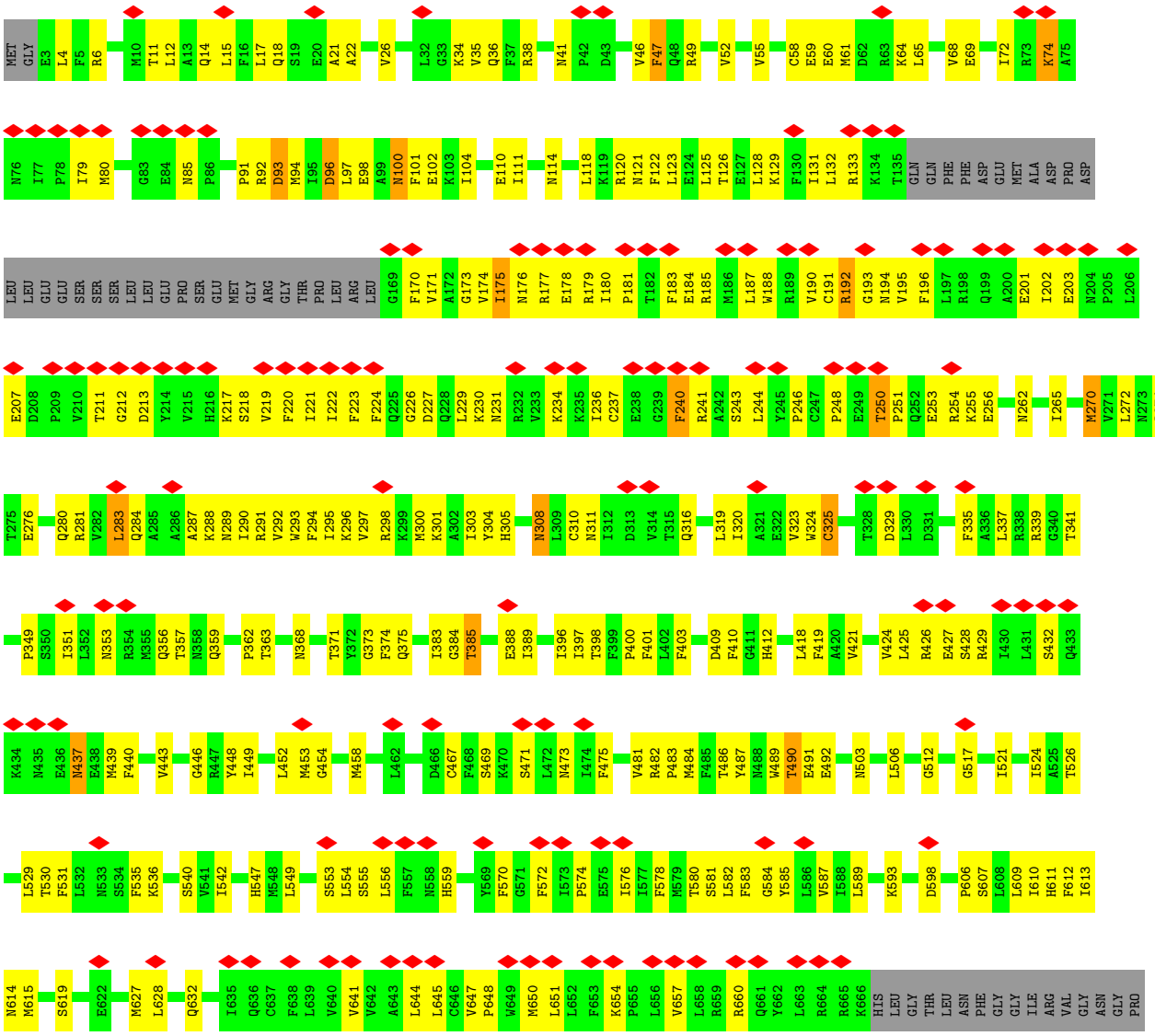
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
19	B	1	27	10	5	10	2	0

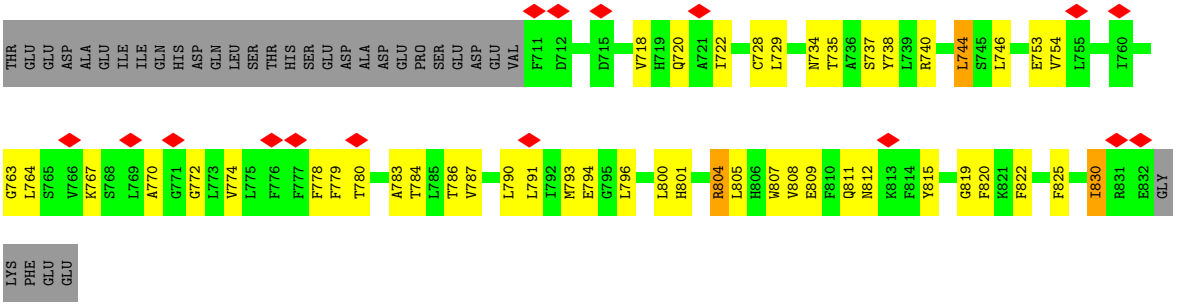
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: V-type proton ATPase 116 kDa subunit a isoform 1

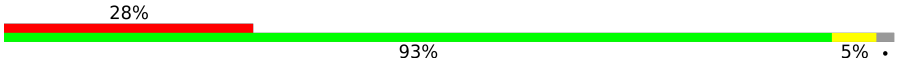
Chain R:

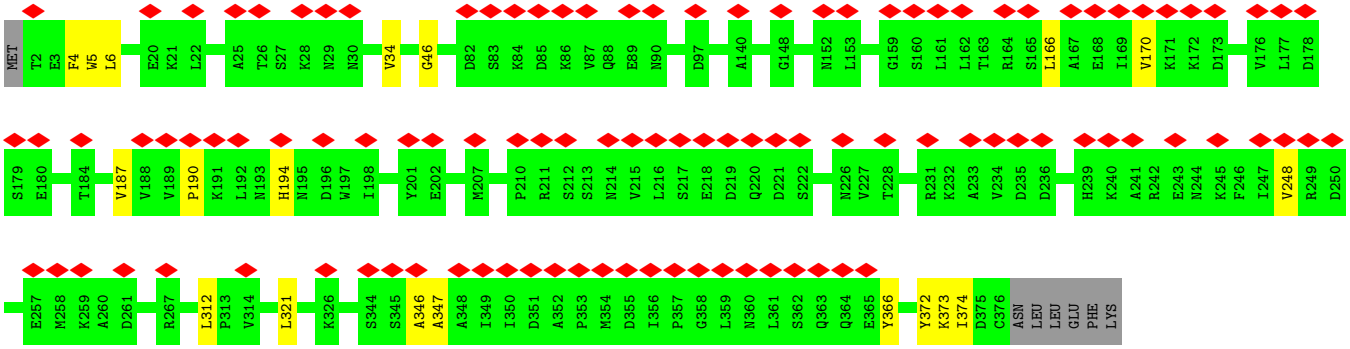




- Molecule 2: V-type proton ATPase subunit C 1

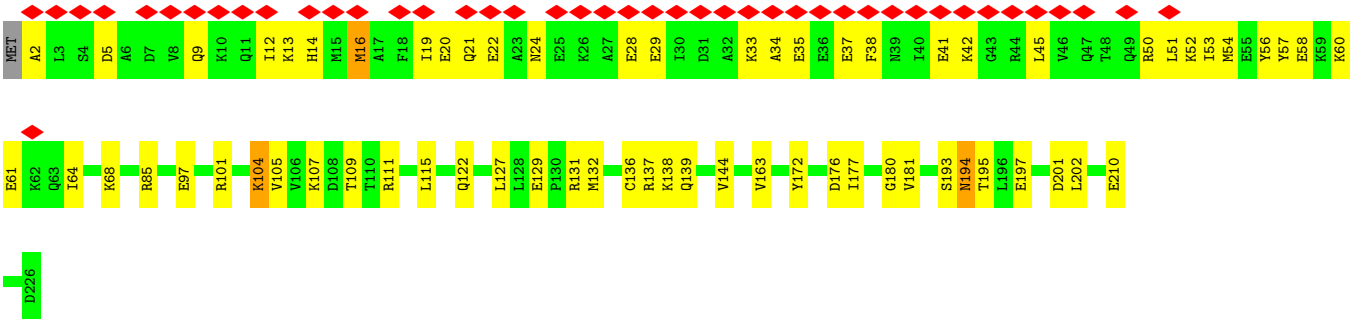
Chain O:





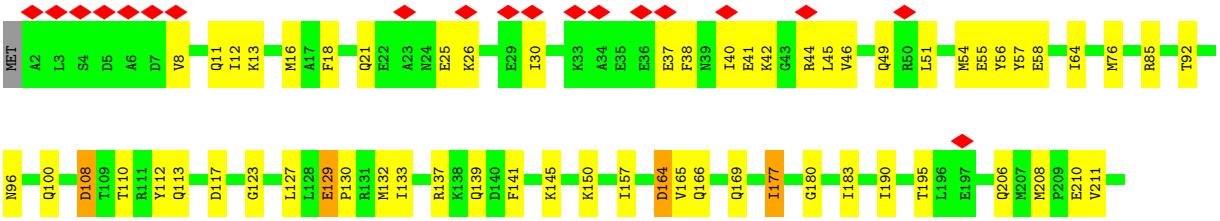
- Molecule 3: V-type proton ATPase subunit E 1

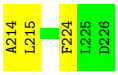
Chain J:



- Molecule 3: V-type proton ATPase subunit E 1

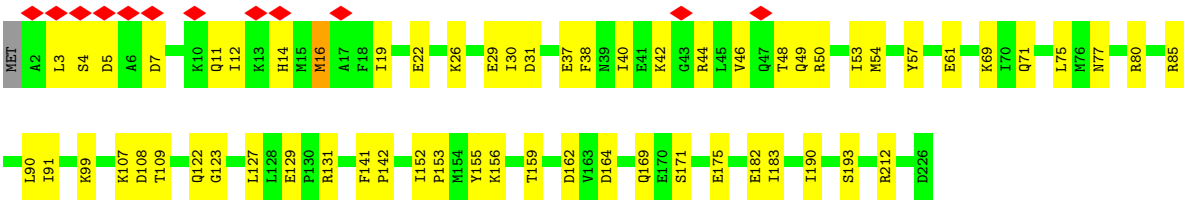
Chain I:





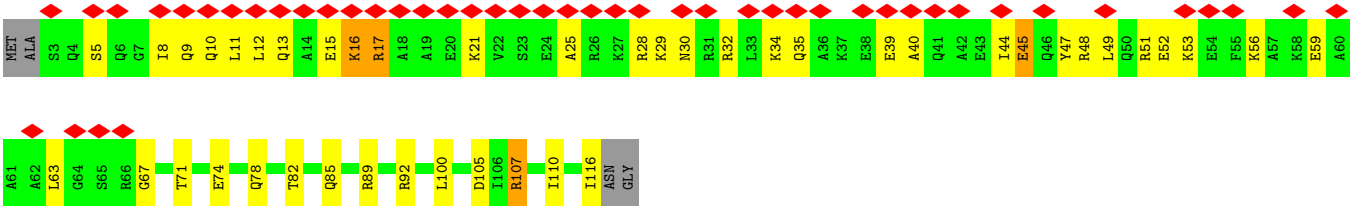
• Molecule 3: V-type proton ATPase subunit E 1

Chain H:



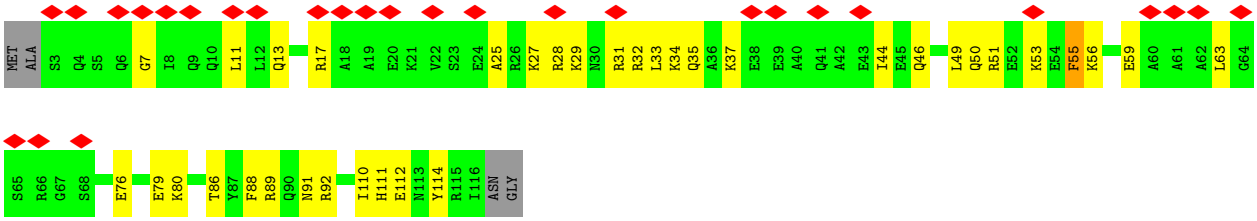
• Molecule 4: V-type proton ATPase subunit G 1

Chain M:



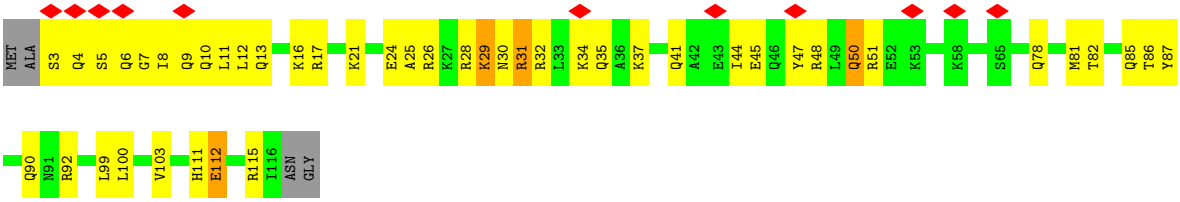
• Molecule 4: V-type proton ATPase subunit G 1

Chain L:



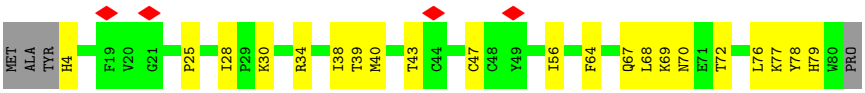
• Molecule 4: V-type proton ATPase subunit G 1

Chain K:



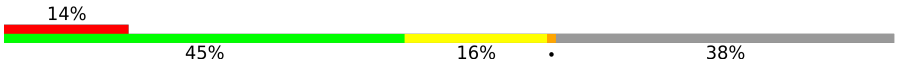
• Molecule 5: V-type proton ATPase subunit e 1

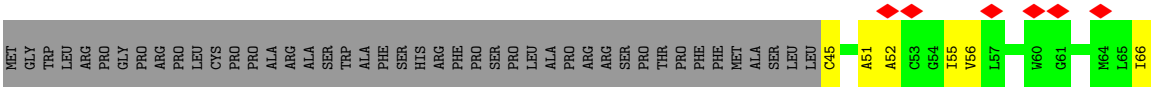
Chain S:

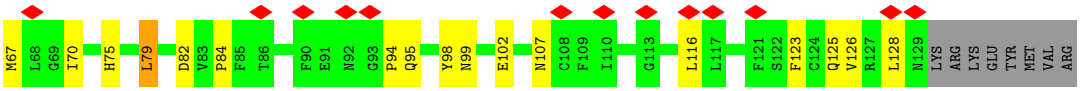


• Molecule 6: Ribonuclease kappa

Chain T:

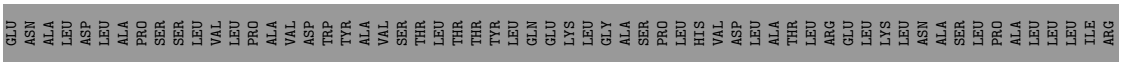


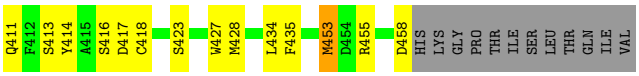




• Molecule 7: V-type proton ATPase subunit S1

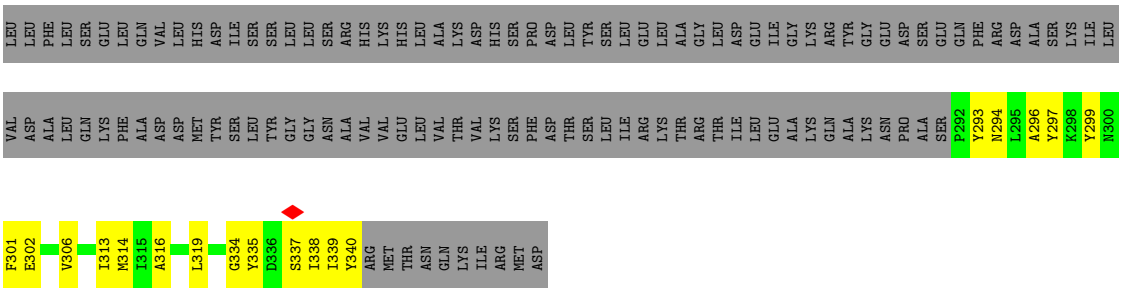
Chain U:





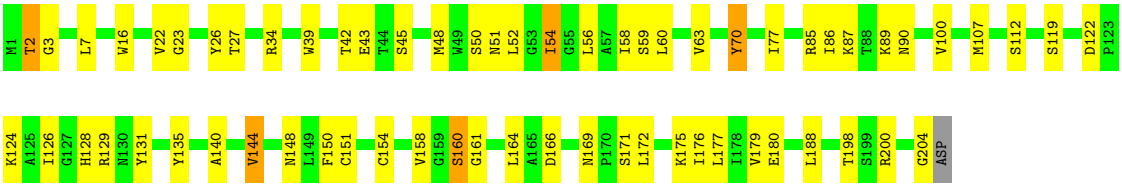
• Molecule 8: Renin receptor

Chain V:



• Molecule 9: V-type proton ATPase 21 kDa proteolipid subunit

Chain 0:

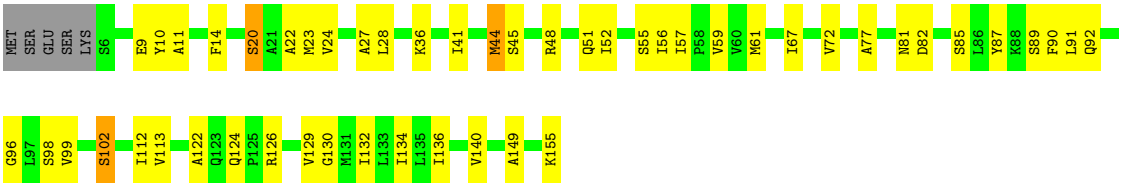


• Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit

Chain 1:

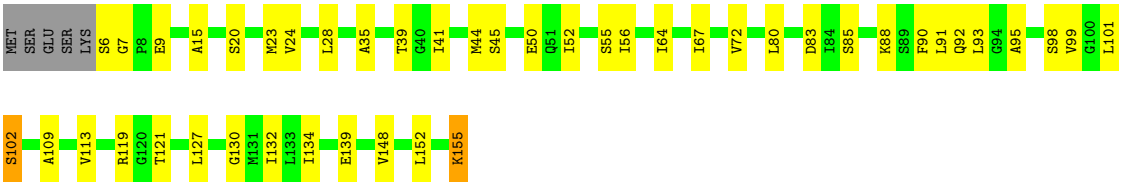
• Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit

Chain 2:



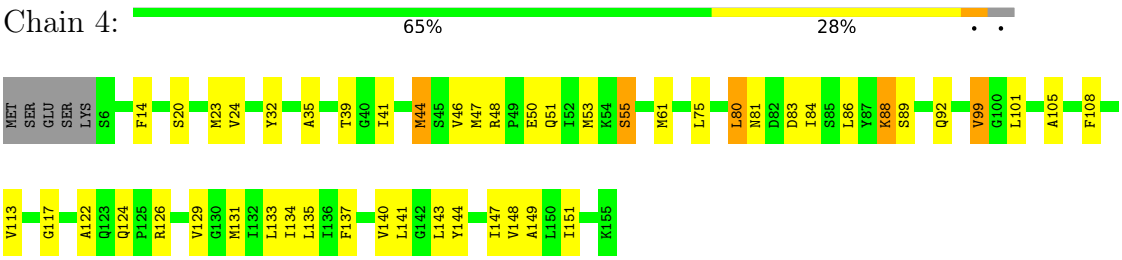
• Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit

Chain 3:



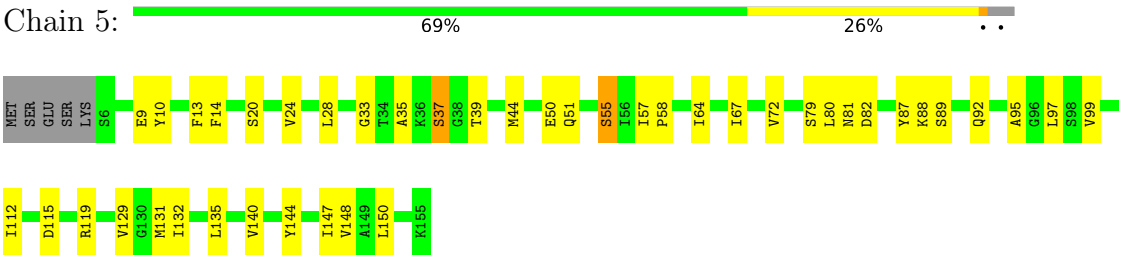
• Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit

Chain 4:



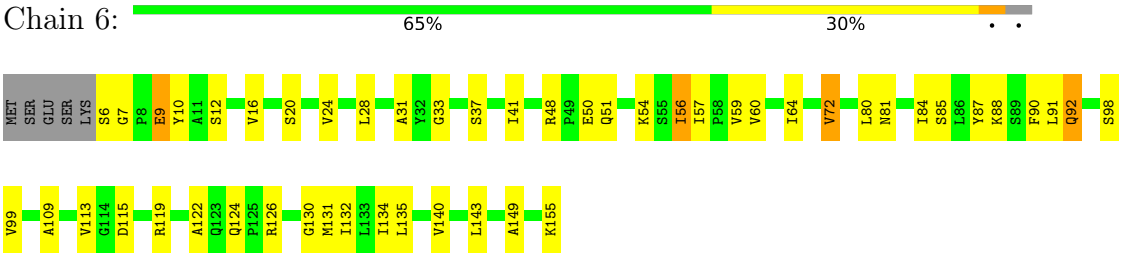
• Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit

Chain 5:



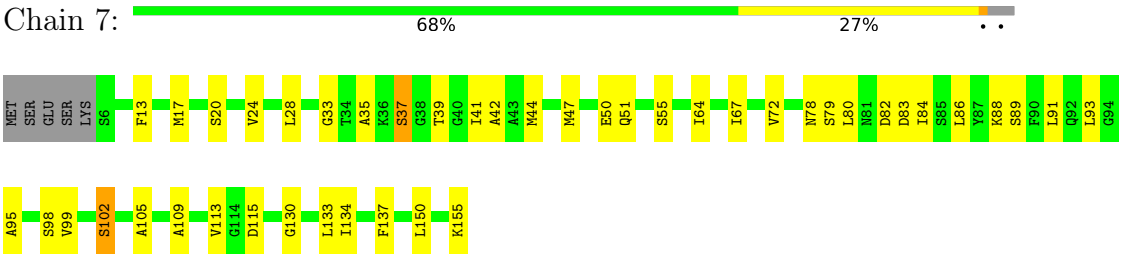
• Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit

Chain 6:



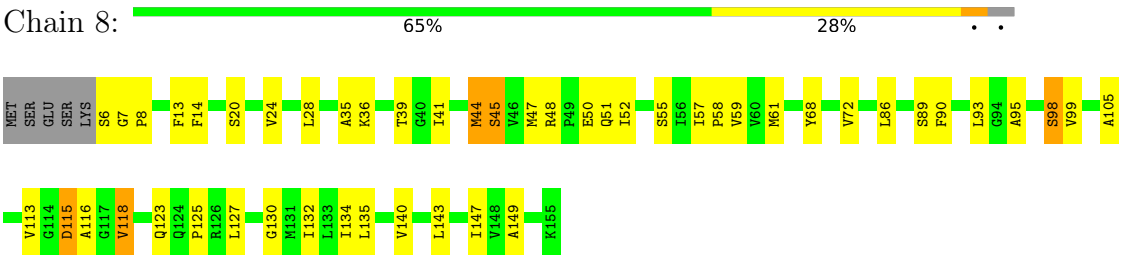
• Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit

Chain 7:



• Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit

Chain 8:



• Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit

Chain 9: 65% 30%

MET SER GLU SER LYS S6 E9 Y10 F13 F14 S20 A21 A22 M23 V24 L28 M44 S45 V46 M47 R48 P49 E50 Q51 I52 S55 V60 I67 V72 S79 L80 N81 D82 D83 I84 Y87 K88 S89 F90 L91 G96 L97 S98 V99 A105 I112

V113 G120 T121 A122 Q123 L127 F128 V129 G130 M131 I134 L135 I136 F137 V140 L143 L150 I151 K155

• Molecule 11: V-type proton ATPase subunit d 1

Chain Q: 69% 29%

M1 S2 F3 F4 P5 E6 L16 E17 G18 L19 V20 R21 L28 Y33 L36 V37 Q38 T41 L42 E43 D44 L49 T52 D53 Y54 F57 L58 T66 V67 S68 V69 D72 R73 M78 R83 H84 M85 L93 L97 D98 F99 I100 T101 Y104

N108 V109 I110 T114 G115 I122 L125 P131 L132 G133 E139 N142 I143 A144 Q145 T146 E149 L150 T158 P159 L160 A161 Q165 D166 S169 E170 Q171 N177 I178 E179 I180 I181 R182 Y189 C197 T198 L199 L200 G201 G202 T203 D217 F221 S227

F228 G229 T230 E231 R246 E250 G251 L252 L255 D259 Q263 A268 D269 Y270 Y271 Y274 L277 G280 P285 G286 D287 K288 R293 V299 L304 N308 Q309 F310 H311 F312 F315 L321 K322 E325 C326 R327 N328 E334 A337 I348

P349 I350 F351

• Molecule 12: V-type proton ATPase catalytic subunit A

Chain C: 76% 19%

MET ASP PHE SER LYS LEU PRO LYS ILE LEU ASP GLU ASP LYS GLU SER T17 F18 S25 D33 A38 V43 L50 V51 I55 I64 Q65 V66 Y67 E68 S74 V75 K84 S87 G91 D100 S111 I118 S128 I131 K132 W133 D134

D151 I152 K163 M167 T175 V176 T177 Y185 L194 E195 F196 E197 G198 E201 V206 Q207 V208 T229 G230 Q231 R232 V233 L234 T246 A247 I248 P249 G250 A251 F252 Q261 S262 L263 S264 S267 N268 C277 R280 E283 V298 D299 M306 K307 R308

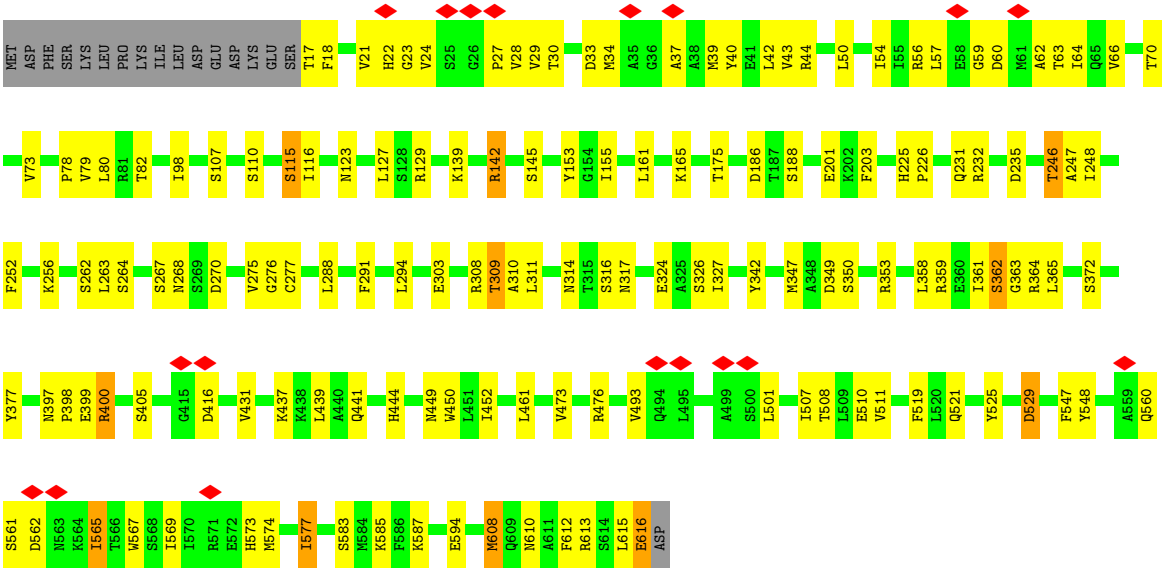
T309 N314 A321 A322 R323 E324 R338 Y342 S350 R353 W354 A357 I361 S362 L365 S372 A376 L382 A389 G390 R391 V392 K393 N397 P398 E399 R400 E401 G402 S403 V404 S405 I406 V407 G408 A409 V410 G414 G415 D416 D419 A424

I428 V431 D436 K437 R442 S447 V448 S453 R459 D466 T470 R476 T477 K478 A479 K480 Q484 L495 E503 I507 E510 V511 D529 C532 K536 M540 Y648 R553 A554 V555 E556 A559 Q560 S561 D562 N563 K564 I565 T566

W567 E572 D576 I577 K580 E594 K598 N610 A611 F612 R613 S614 L615 E616 ASP

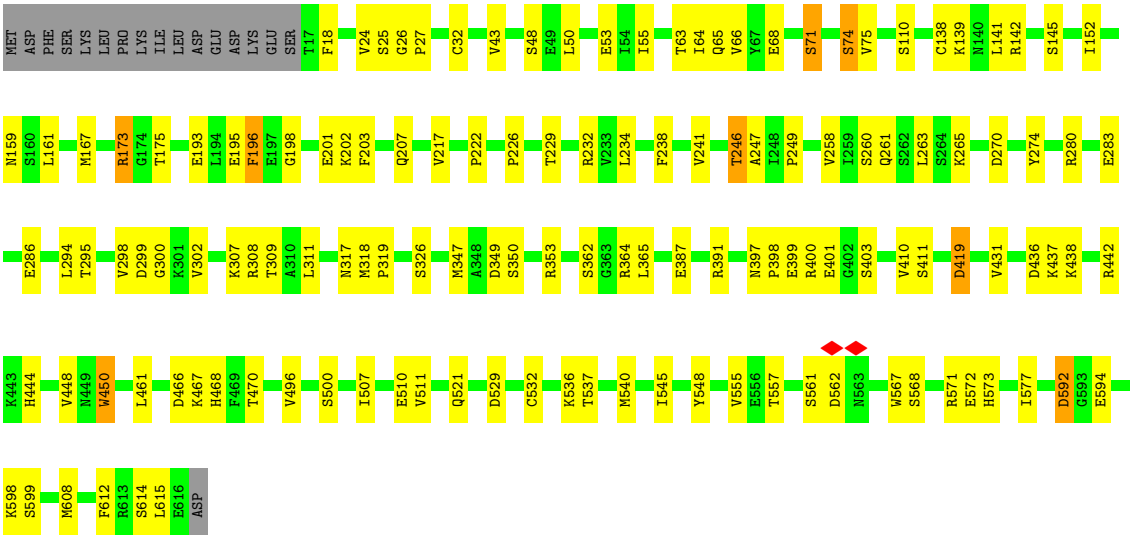
• Molecule 12: V-type proton ATPase catalytic subunit A

Chain A: 73% 22%



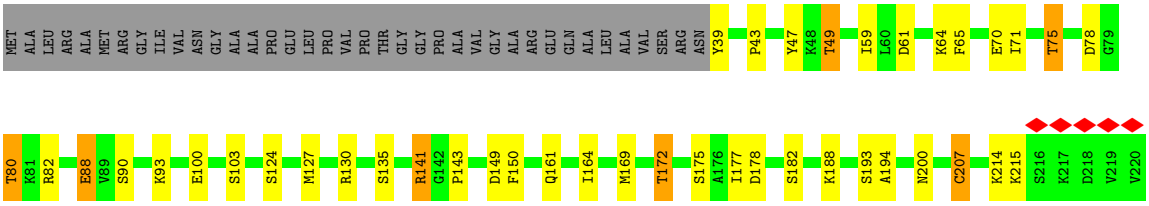
- Molecule 12: V-type proton ATPase catalytic subunit A

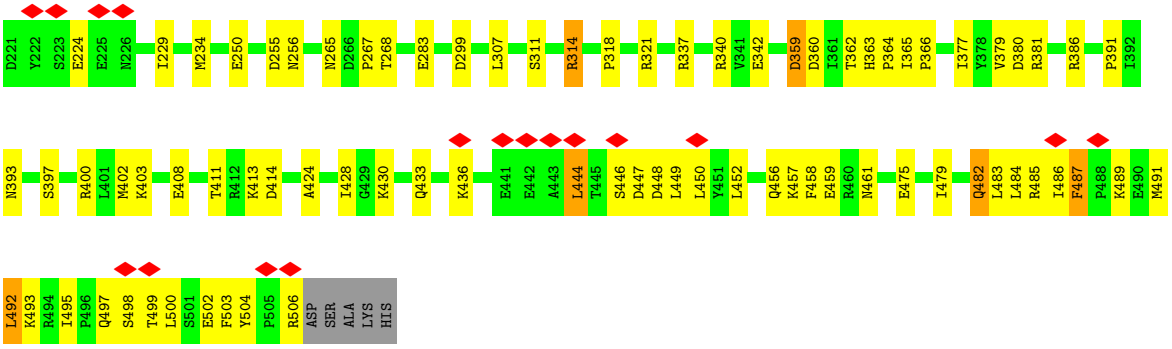
Chain B:



- Molecule 13: V-type proton ATPase subunit B, brain isoform

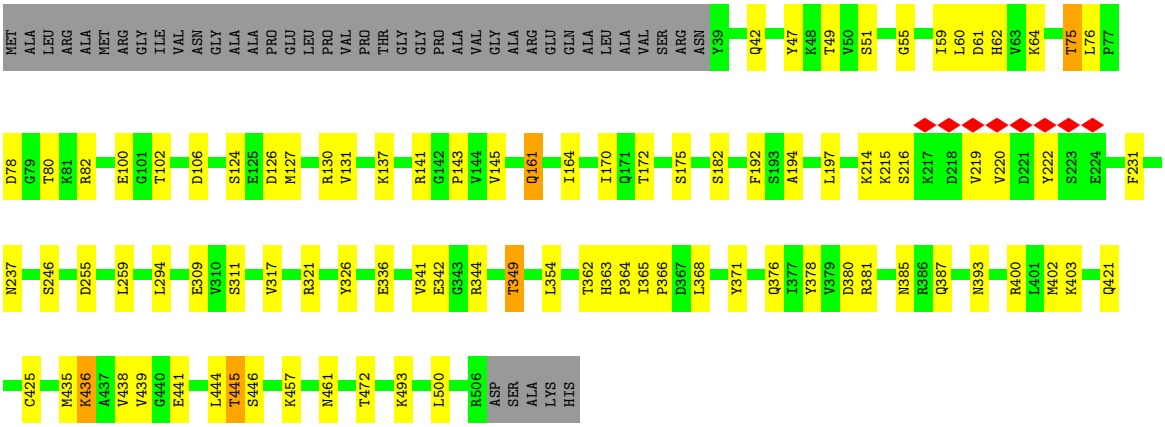
Chain F:





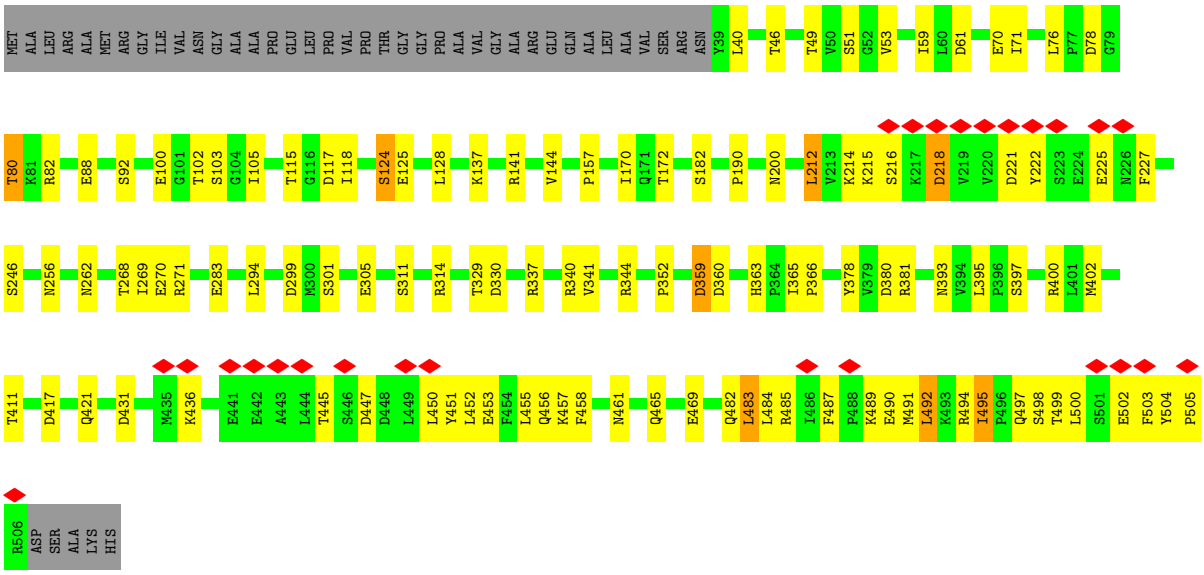
- Molecule 13: V-type proton ATPase subunit B, brain isoform

Chain D:



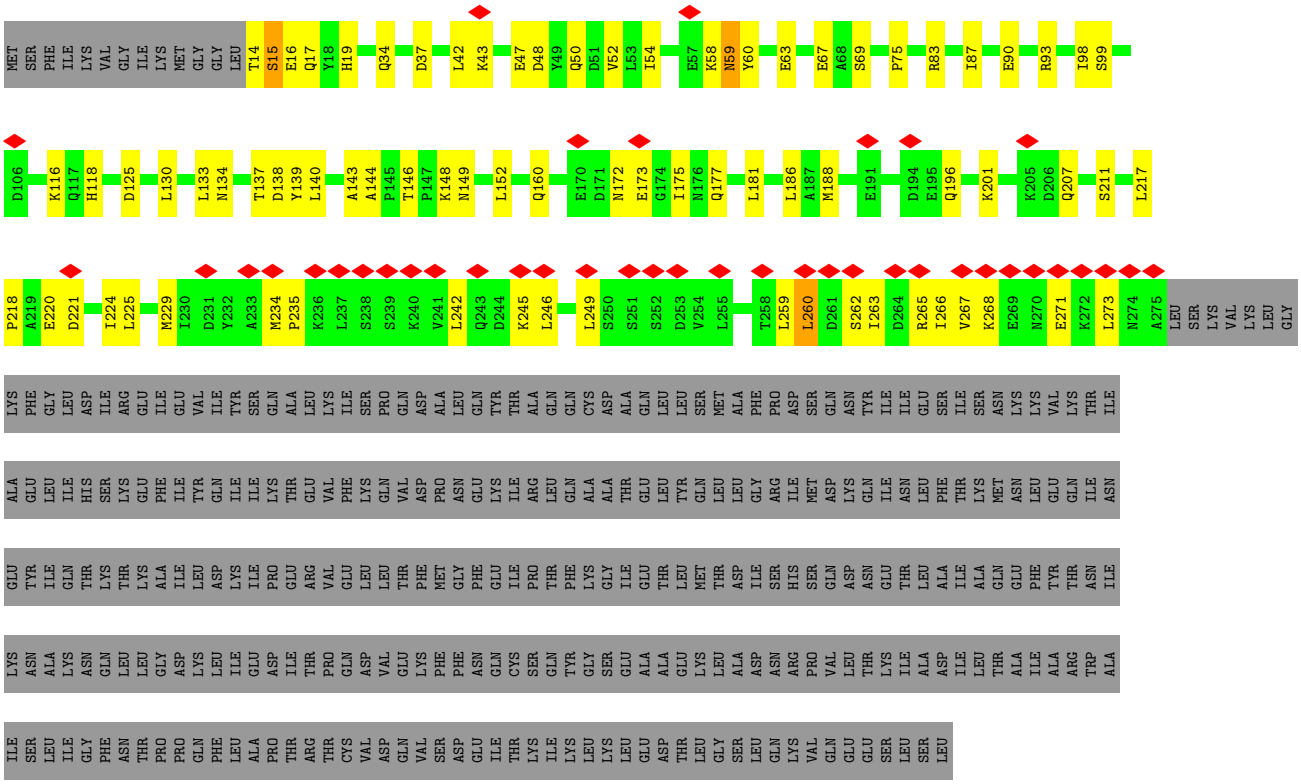
- Molecule 13: V-type proton ATPase subunit B, brain isoform

Chain E:



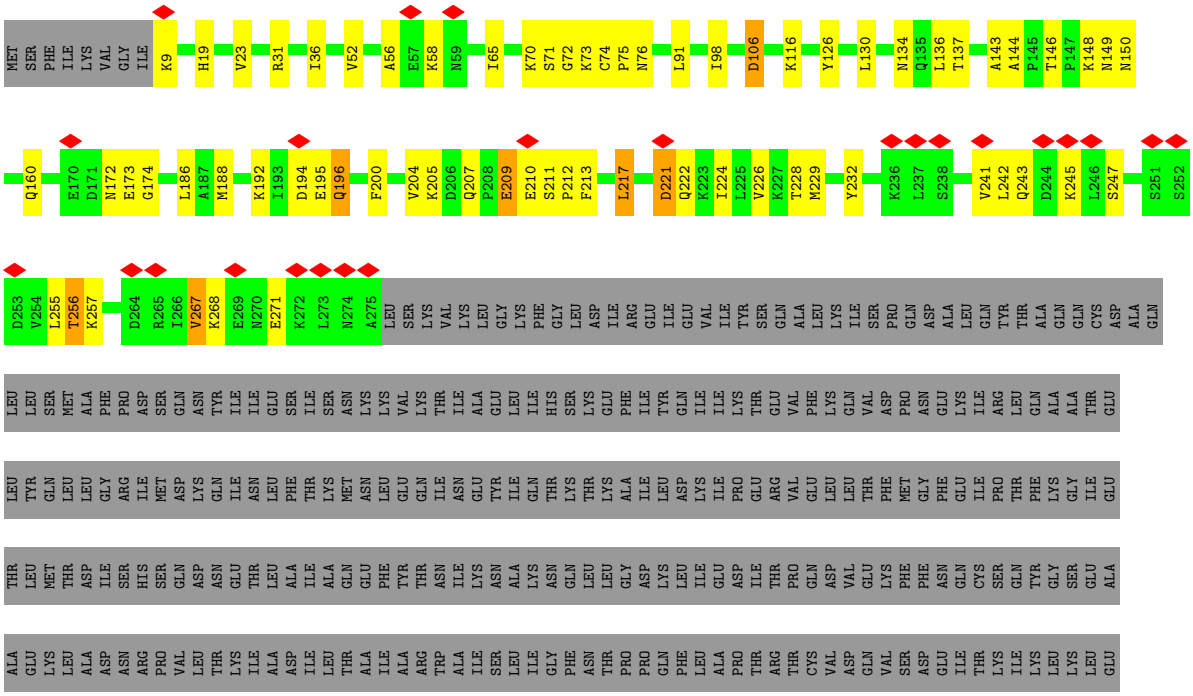
- Molecule 14: SidK

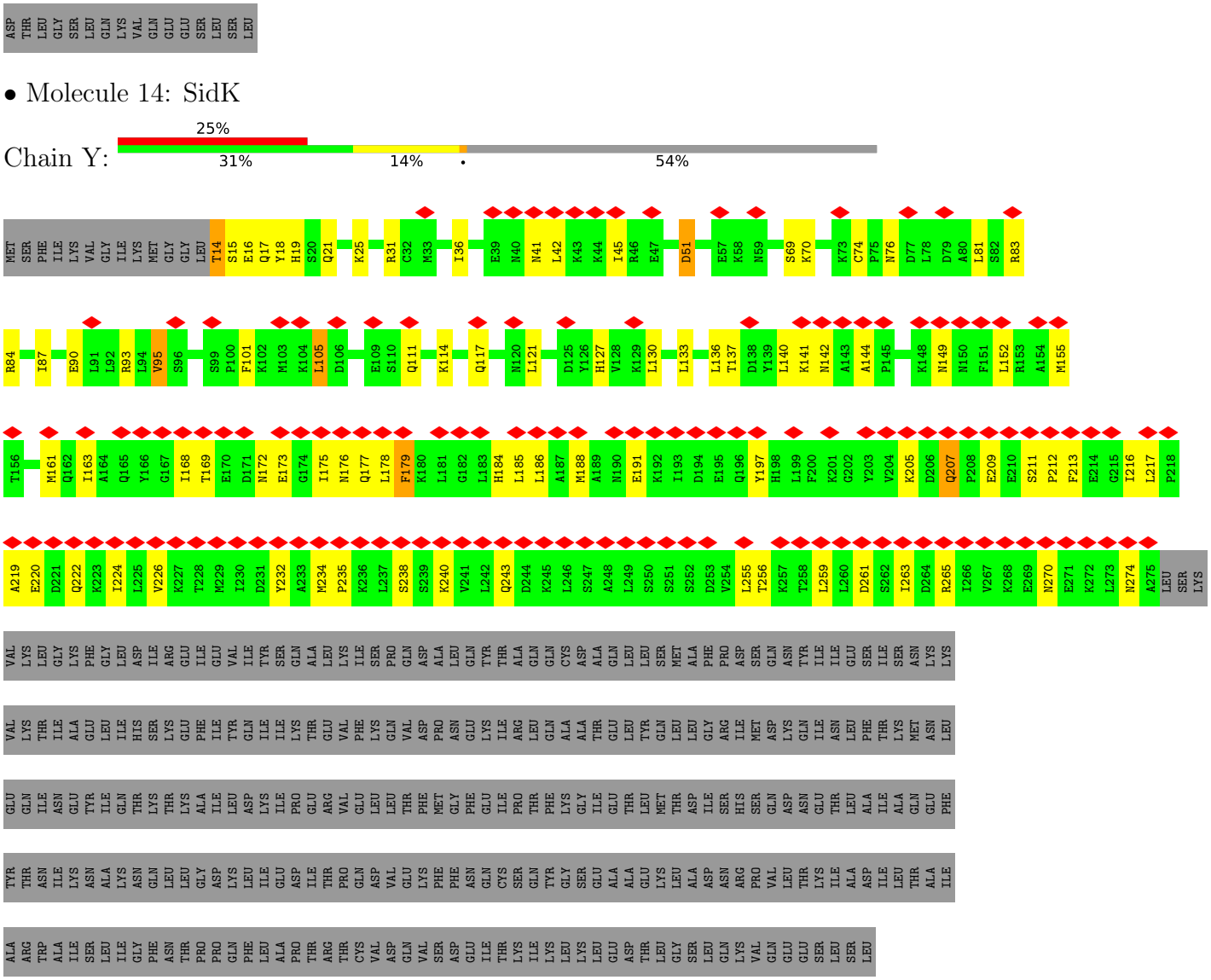
Chain Z:

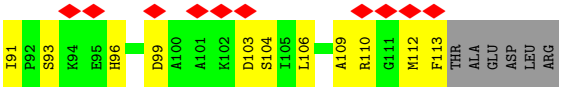


- Molecule 14: SidK

Chain X:

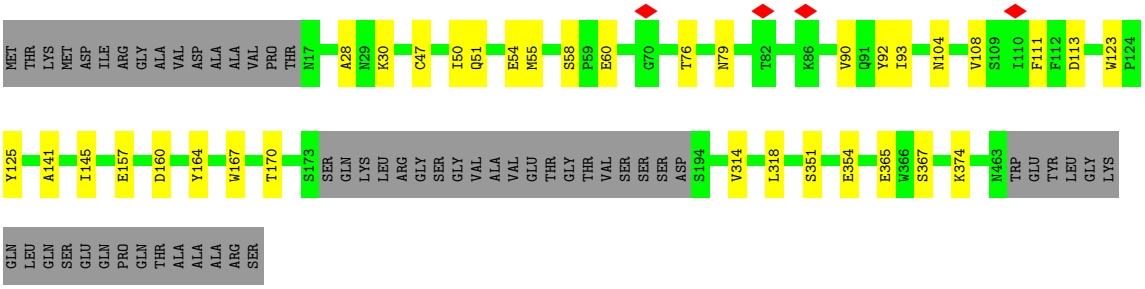



ASP THR LEU GLY SER LEU GLN LYS VAL GLN GLU GLU SER LEU SER LEU
• Molecule 14: SidK
Chain Y:
25%
31%
14%
54%
MET SER PHE ILE LYS VAL GLY ILE LYS MET GLY GLY LEU T14 S15 E16 Q17 Y18 H19 S20 Q21 K25 R31 C32 M33 I36 E39 N40 N41 L42 K43 K44 I45 R46 E47 D51 E57 K58 N59 S69 K70 K73 C74 P75 N76 D77 L78 D79 A80 L81 S82 R83
R84 I87 E90 L91 L92 R93 L94 V95 S96 S99 P100 F101 K102 M103 K104 L105 D106 E109 S110 Q111 K114 Q117 N120 L121 D125 Y126 H127 V128 K129 L130 L133 L136 T137 D138 Y139 L140 K141 N142 A143 A144 P145 K148 N149 N150 F151 L152 R153 A154 M155
T156 M161 Q162 I163 A164 Q165 Y166 G167 I168 T169 E170 D171 N172 E173 G174 I175 N176 Q177 L178 F179 K180 L181 G182 L183 H184 L185 L186 A187 M188 A189 N190 E191 K192 I193 D194 E195 Q196 Y197 H198 L199 F200 K201 G202 Y203 V204 K205 D206 Q207 P208 E209 E210 S211 P212 F213 E214 G215 I216 L217 P218
A219 E220 D221 Q222 K223 I224 L225 V226 K227 T228 M229 I230 D231 Y232 A233 M234 P235 K236 L237 S238 S239 K240 V241 L242 Q243 D244 K245 L246 S247 A248 L249 S250 S251 S252 D253 V254 L255 T256 K257 T258 L259 L260 D261 S262 I263 D264 R265 I266 V267 K268 E269 N270 E271 K272 L273 N274 A275 LEU SER LYS
VAL LYS LEU GLY LYS PHE GLY LEU ASP ILE ARG GLU ILE GLU VAL ILE TYR SER GLN ALA LEU LYS ILE SER PRO GLN ASP ALA LEU GLN TYR THR ALA GLN GLN CYS ASP ALA GLN LEU LEU SER MET ALA PHE PRO ASP SER GLN ASN TYR ILE ILE GLU SER ILE SER ASN LYS LYS
VAL LYS THR ILE ALA GLU LEU ILE HIS SER LYS GLU PHE ILE TYR GLN ILE ILE LYS THR GLU VAL PHE LYS GLN VAL ASP PRO ASN GLU LYS ILE ARG LEU GLN ALA ALA THR GLU LEU TYR GLN LEU LEU GLY ARG ILE MET ASP LYS GLN ILE ASN LEU PHE THR LYS MET ASN LEU
GLU GLN ILE ASN GLU TYR ILE GLN THR LYS THR LYS ALA ILE LEU ASP LYS ILE PRO GLU ARG VAL GLU LEU LEU THR PHE MET GLY PHE GLU ILE PRO THR PHE LYS GLY ILE GLU THR LEU MET THR ASP ILE SER HIS SER GLN ASP ASN GLU THR LEU ALA ILE ALA GLN GLU PHE
TYR THR ASN ILE LYS ASN ALA LYS ASN GLN LEU LEU GLY ASP LYS LEU ILE GLU ASP ILE THR PRO GLN ASP VAL GLU LYS PHE PHE ASN GLN CYS SER GLN TYR GLY SER GLU ALA ALA GLU LYS LEU ALA ASP ASN ARG PRO VAL LEU THR LYS ILE ALA ASP ILE LEU THR ALA ILE
ALA ARG TRP ALA ILE SER LEU ILE GLY PHE ASN THR PRO PRO GLN PHE LEU ALA PRO THR ARG THR CYS VAL ASP GLN VAL SER ASP GLU ILE THR LYS ILE LYS LEU LYS LEU GLU ASP THR LEU GLY SER LEU GLN LYS VAL GLN GLU GLU SER LEU SER LEU
• Molecule 15: V-type proton ATPase subunit D
Chain G:
68%
17%
14%
MET SER GLY K4 D5 E8 R30 R43 Q46 K50 E53 T54 K55 M56 L57 M58 R63 E64 A65 A70 Q85 N88 K89 I94 R95 V101 T105 L106 E110 G115 L121 T122 L134 Y138 E143 L144 L145 V146 E147 L148
S154 D159 K163 R167 R182 T183 L184 E193 R196 R201 L202 K203 E207 L212 K213 S216 GLU LYS ASP LEU GLU GLU GLN ARG ARG ALA ALA GLY GLU VAL LEU GLU PRO ALA ASN LEU LEU ALA GLU GLU LYS ASP GLU ASP LEU LEU PHE GLU
• Molecule 16: V-type proton ATPase subunit F
Chain N:
13%
55%
34%
8%
MET ALA GLY R4 G5 K6 I11 G12 D13 E14 D15 T16 V17 T18 G26 E27 L28 N29 K30 N35 E40 T43 T44 I45 N46 R53 N57 R58 D59 I63 I64 L65 I66 N67 Q68 Y69 I70 M73 V74 R75 L78 D79 A80 H81 I85 P86 L89 E90



• Molecule 17: V-type proton ATPase subunit H

Chain P:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1000000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	28.244	Depositor
Minimum map value	-15.673	Depositor
Average map value	0.016	Depositor
Map value standard deviation	1.165	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: ADP, NAG

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| >5	RMSZ	#|Z| >5
1	R	0.27	0/6306	0.43	0/8534
2	O	0.24	0/1863	0.42	0/2600
3	H	0.34	0/1839	0.44	0/2462
3	I	0.34	0/1839	0.46	0/2462
3	J	0.33	0/1839	0.43	0/2462
4	K	0.31	0/945	0.42	0/1258
4	L	0.34	0/945	0.44	0/1258
4	M	0.32	0/945	0.42	0/1258
5	S	0.28	0/657	0.43	0/902
6	T	0.28	0/674	0.47	0/915
7	U	0.37	0/1716	0.50	1/2333 (0.0%)
8	V	0.44	0/425	0.52	0/582
9	0	0.45	0/1532	0.52	0/2082
10	1	0.45	0/1080	0.50	0/1461
10	2	0.43	0/1080	0.50	0/1461
10	3	0.41	0/1080	0.51	0/1461
10	4	0.40	0/1080	0.49	0/1461
10	5	0.40	0/1080	0.48	0/1461
10	6	0.37	0/1080	0.47	0/1461
10	7	0.38	0/1080	0.50	0/1461
10	8	0.39	0/1080	0.49	0/1461
10	9	0.41	0/1080	0.49	0/1461
11	Q	0.44	0/2910	0.49	0/3940
12	A	0.46	0/4752	0.50	0/6435
12	B	0.49	0/4752	0.49	0/6435
12	C	0.46	0/4752	0.48	0/6435
13	D	0.49	0/3739	0.49	0/5067
13	E	0.48	0/3739	0.51	0/5067
13	F	0.48	0/3739	0.52	0/5067
14	X	0.32	0/2170	0.43	0/2926
14	Y	0.28	0/2145	0.43	0/2893
14	Z	0.29	0/2143	0.42	0/2888

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
15	G	0.34	0/1735	0.44	0/2320
16	N	0.26	0/889	0.42	0/1200
17	P	0.26	0/2119	0.44	0/2955
All	All	0.40	0/70829	0.47	1/95885 (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
3	I	0	1
12	A	0	2
13	E	0	1
13	F	0	1
17	P	0	1
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	U	418	CYS	CA-CB-SG	5.92	124.66	114.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	A	23	GLY	Peptide
12	A	33	ASP	Peptide
13	E	451	TYR	Peptide
13	F	487	PHE	Peptide
3	I	224	PHE	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	R	6147	0	6172	244	0
2	O	1864	0	830	11	0
3	H	1822	0	1886	53	0
3	I	1822	0	1886	39	0
3	J	1822	0	1886	49	0
4	K	938	0	947	42	0
4	L	938	0	947	27	0
4	M	938	0	947	32	0
5	S	631	0	646	20	0
6	T	658	0	652	16	0
7	U	1662	0	1583	45	0
8	V	411	0	401	12	0
9	0	1498	0	1544	48	0
10	1	1065	0	1131	20	0
10	2	1065	0	1131	29	0
10	3	1065	0	1131	31	0
10	4	1065	0	1131	30	0
10	5	1065	0	1131	27	0
10	6	1065	0	1131	40	0
10	7	1065	0	1131	33	0
10	8	1065	0	1131	34	0
10	9	1065	0	1131	32	0
11	Q	2844	0	2782	77	0
12	A	4656	0	4642	97	0
12	B	4656	0	4642	80	0
12	C	4656	0	4642	74	0
13	D	3666	0	3665	55	0
13	E	3666	0	3665	70	0
13	F	3666	0	3665	69	0
14	X	2136	0	2158	44	0
14	Y	2111	0	2134	55	0
14	Z	2110	0	2132	47	0
15	G	1717	0	1829	34	0
16	N	875	0	878	31	0
17	P	2121	0	941	19	0
18	R	14	0	13	1	0
18	S	14	0	13	0	0
18	U	84	0	78	1	0
19	B	27	0	12	2	0
All	All	69755	0	68397	1503	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 11.

The worst 5 of 1503 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)
14:Z:19:HIS:HD1	14:Z:69:SER:HG	1.21	0.89
13:F:446:SER:O	13:F:450:LEU:HB2	1.73	0.88
9:0:77:ILE:HG21	10:1:117:GLY:HA2	1.60	0.84
3:H:22:GLU:HG3	4:K:17:ARG:HH11	1.41	0.84
12:C:314:ASN:HD21	12:C:323:ARG:HG2	1.41	0.83

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	R	747/837 (89%)	701 (94%)	46 (6%)	0	100	100
2	O	373/382 (98%)	348 (93%)	25 (7%)	0	100	100
3	H	223/226 (99%)	217 (97%)	6 (3%)	0	100	100
3	I	223/226 (99%)	208 (93%)	15 (7%)	0	100	100
3	J	223/226 (99%)	212 (95%)	10 (4%)	1 (0%)	34	67
4	K	112/118 (95%)	110 (98%)	2 (2%)	0	100	100
4	L	112/118 (95%)	107 (96%)	5 (4%)	0	100	100
4	M	112/118 (95%)	110 (98%)	2 (2%)	0	100	100
5	S	75/81 (93%)	73 (97%)	2 (3%)	0	100	100
6	T	83/137 (61%)	75 (90%)	8 (10%)	0	100	100
7	U	202/470 (43%)	163 (81%)	39 (19%)	0	100	100
8	V	47/350 (13%)	42 (89%)	5 (11%)	0	100	100
9	0	202/205 (98%)	183 (91%)	19 (9%)	0	100	100
10	1	148/155 (96%)	138 (93%)	10 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	2	148/155 (96%)	138 (93%)	10 (7%)	0	100	100
10	3	148/155 (96%)	137 (93%)	11 (7%)	0	100	100
10	4	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
10	5	148/155 (96%)	137 (93%)	11 (7%)	0	100	100
10	6	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
10	7	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
10	8	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
10	9	148/155 (96%)	139 (94%)	9 (6%)	0	100	100
11	Q	349/351 (99%)	312 (89%)	37 (11%)	0	100	100
12	A	598/617 (97%)	537 (90%)	61 (10%)	0	100	100
12	B	598/617 (97%)	542 (91%)	56 (9%)	0	100	100
12	C	598/617 (97%)	542 (91%)	56 (9%)	0	100	100
13	D	466/511 (91%)	431 (92%)	35 (8%)	0	100	100
13	E	466/511 (91%)	433 (93%)	33 (7%)	0	100	100
13	F	466/511 (91%)	432 (93%)	34 (7%)	0	100	100
14	X	265/573 (46%)	250 (94%)	15 (6%)	0	100	100
14	Y	260/573 (45%)	252 (97%)	8 (3%)	0	100	100
14	Z	258/573 (45%)	248 (96%)	10 (4%)	0	100	100
15	G	211/247 (85%)	205 (97%)	6 (3%)	0	100	100
16	N	108/119 (91%)	101 (94%)	7 (6%)	0	100	100
17	P	423/483 (88%)	328 (78%)	93 (22%)	2 (0%)	29	61
All	All	9132/11192 (82%)	8418 (92%)	711 (8%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	16	MET
17	P	104	ASN
17	P	374	LYS

5.3.2 Protein sidechains (i)

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	R	674/746 (90%)	635 (94%)	39 (6%)	20	50
3	H	198/199 (100%)	194 (98%)	4 (2%)	55	77
3	I	198/199 (100%)	183 (92%)	15 (8%)	13	41
3	J	198/199 (100%)	183 (92%)	15 (8%)	13	41
4	K	99/101 (98%)	92 (93%)	7 (7%)	14	44
4	L	99/101 (98%)	96 (97%)	3 (3%)	41	68
4	M	99/101 (98%)	91 (92%)	8 (8%)	11	38
5	S	69/72 (96%)	69 (100%)	0	100	100
6	T	71/116 (61%)	68 (96%)	3 (4%)	30	59
7	U	182/397 (46%)	164 (90%)	18 (10%)	8	27
8	V	44/308 (14%)	41 (93%)	3 (7%)	16	45
9	0	154/155 (99%)	140 (91%)	14 (9%)	9	32
10	1	107/112 (96%)	100 (94%)	7 (6%)	17	46
10	2	107/112 (96%)	96 (90%)	11 (10%)	7	26
10	3	107/112 (96%)	100 (94%)	7 (6%)	17	46
10	4	107/112 (96%)	96 (90%)	11 (10%)	7	26
10	5	107/112 (96%)	99 (92%)	8 (8%)	13	41
10	6	107/112 (96%)	103 (96%)	4 (4%)	34	62
10	7	107/112 (96%)	101 (94%)	6 (6%)	21	51
10	8	107/112 (96%)	100 (94%)	7 (6%)	17	46
10	9	107/112 (96%)	96 (90%)	11 (10%)	7	26
11	Q	306/306 (100%)	291 (95%)	15 (5%)	25	55
12	A	508/525 (97%)	473 (93%)	35 (7%)	15	45
12	B	508/525 (97%)	479 (94%)	29 (6%)	20	50
12	C	508/525 (97%)	475 (94%)	33 (6%)	17	46
13	D	401/430 (93%)	377 (94%)	24 (6%)	19	49
13	E	401/430 (93%)	372 (93%)	29 (7%)	14	43
13	F	401/430 (93%)	365 (91%)	36 (9%)	9	32
14	X	239/519 (46%)	229 (96%)	10 (4%)	30	59

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	Y	238/519 (46%)	229 (96%)	9 (4%)	33	61
14	Z	237/519 (46%)	230 (97%)	7 (3%)	41	68
15	G	184/212 (87%)	179 (97%)	5 (3%)	44	70
16	N	94/100 (94%)	89 (95%)	5 (5%)	22	52
All	All	7073/8742 (81%)	6635 (94%)	438 (6%)	22	48

5 of 438 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	C	308	ARG
12	B	32	CYS
13	E	495	ILE
12	C	453	SER
12	A	294	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
11	Q	338	GLN
12	B	573	HIS
12	C	231	GLN
12	B	184	ASN
13	D	161	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

9 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	$\#\|Z\| > 2$
18	NAG	S	101	5	14,14,15	0.26	0	17,19,21	0.54	0
18	NAG	U	506	7	14,14,15	0.26	0	17,19,21	0.49	0
18	NAG	U	503	7	14,14,15	0.19	0	17,19,21	0.45	0
18	NAG	U	501	7	14,14,15	0.32	0	17,19,21	0.55	0
18	NAG	R	901	1	14,14,15	0.49	0	17,19,21	0.56	0
19	ADP	B	701	-	24,29,29	0.98	1 (4%)	29,45,45	1.41	5 (17%)
18	NAG	U	504	7	14,14,15	0.32	0	17,19,21	0.58	0
18	NAG	U	505	7	14,14,15	0.21	0	17,19,21	0.38	0
18	NAG	U	502	7	14,14,15	0.28	0	17,19,21	0.56	0

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
18	NAG	S	101	5	-	0/6/23/26	0/1/1/1
18	NAG	U	506	7	-	3/6/23/26	0/1/1/1
18	NAG	U	503	7	-	1/6/23/26	0/1/1/1
18	NAG	U	501	7	-	2/6/23/26	0/1/1/1
18	NAG	R	901	1	-	2/6/23/26	0/1/1/1
19	ADP	B	701	-	-	1/12/32/32	0/3/3/3
18	NAG	U	504	7	-	3/6/23/26	0/1/1/1
18	NAG	U	505	7	-	4/6/23/26	0/1/1/1
18	NAG	U	502	7	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	701	ADP	C5-C4	2.18	1.46	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	701	ADP	C3'-C2'-C1'	3.25	105.87	100.98
19	B	701	ADP	N3-C2-N1	-2.95	124.06	128.68
19	B	701	ADP	PA-O3A-PB	-2.66	123.71	132.83
19	B	701	ADP	C4-C5-N7	-2.48	106.81	109.40
19	B	701	ADP	C2'-C3'-C4'	2.01	106.54	102.64

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

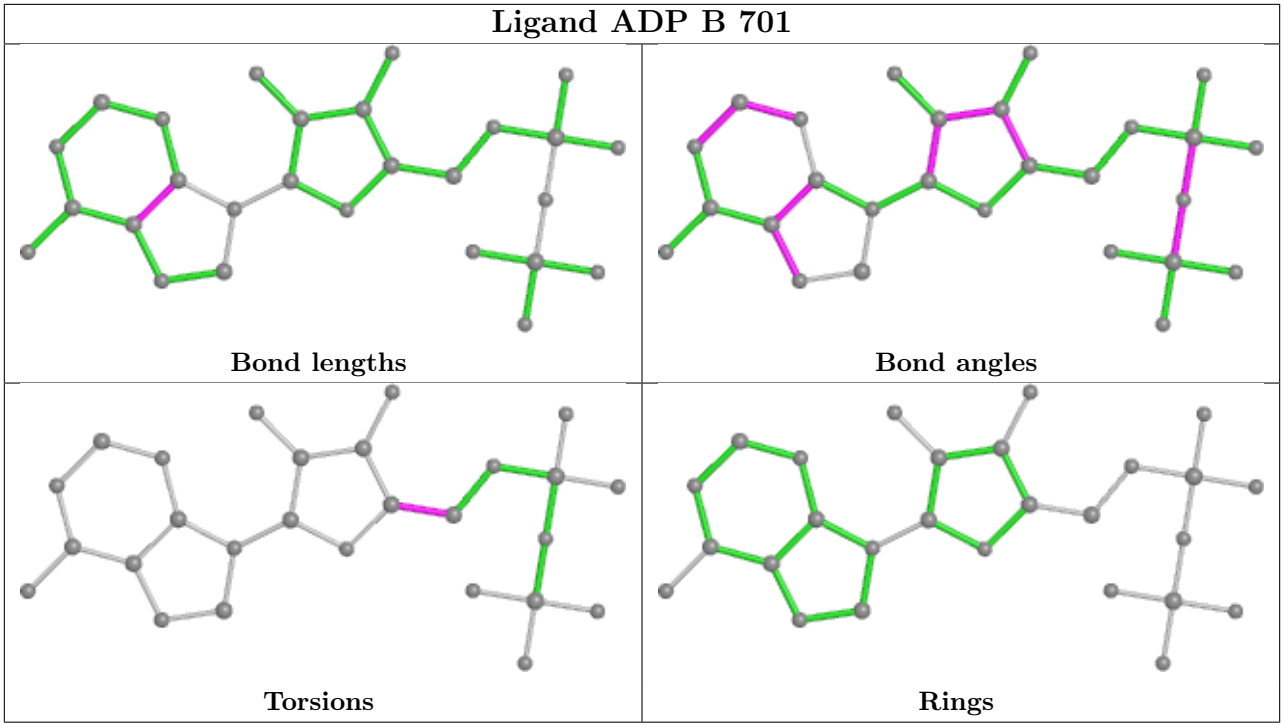
Mol	Chain	Res	Type	Atoms
18	U	501	NAG	C4-C5-C6-O6
18	U	505	NAG	O5-C5-C6-O6
18	U	502	NAG	O5-C5-C6-O6
18	U	506	NAG	O5-C5-C6-O6
18	U	501	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	R	901	NAG	1	0
19	B	701	ADP	2	0
18	U	505	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

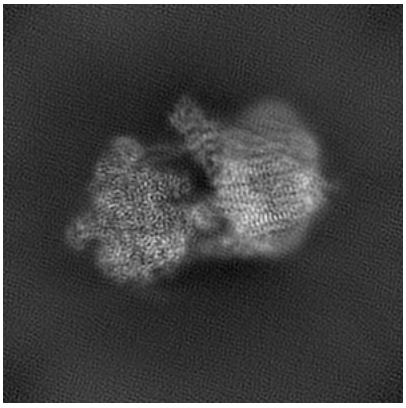
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-21848. These allow visual inspection of the internal detail of the map and identification of artifacts.

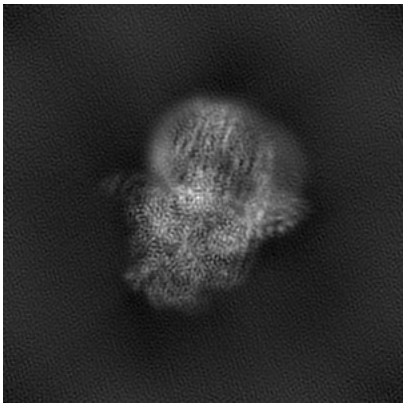
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

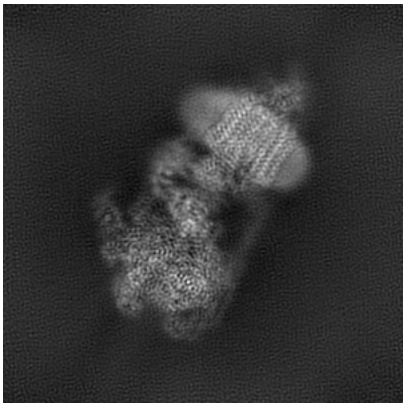
6.1.1 Primary map



X



Y

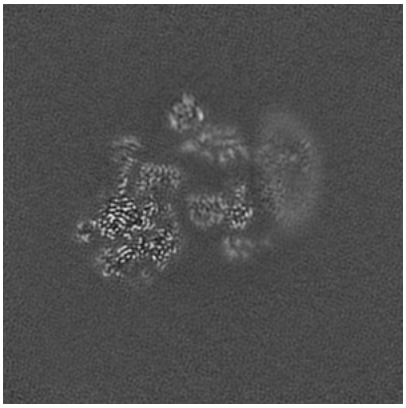


Z

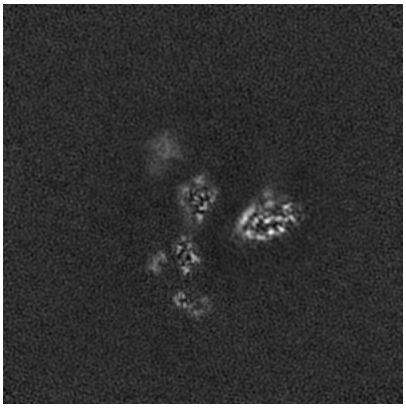
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

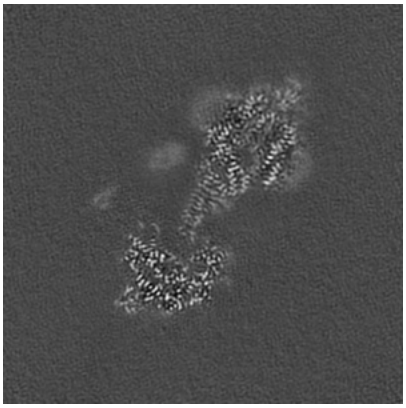
6.2.1 Primary map



X Index: 180



Y Index: 180

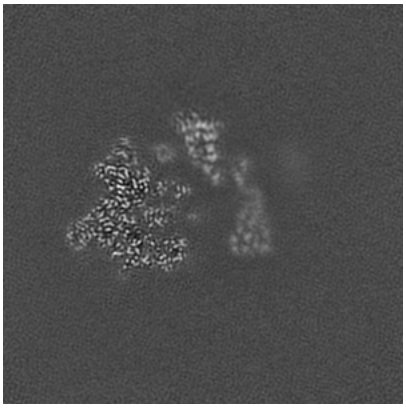


Z Index: 180

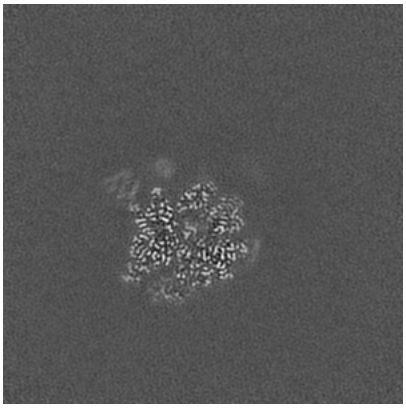
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

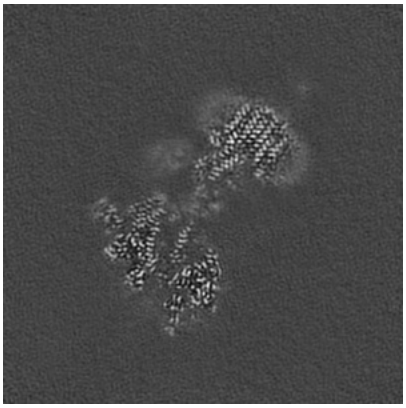
6.3.1 Primary map



X Index: 157



Y Index: 128



Z Index: 167

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

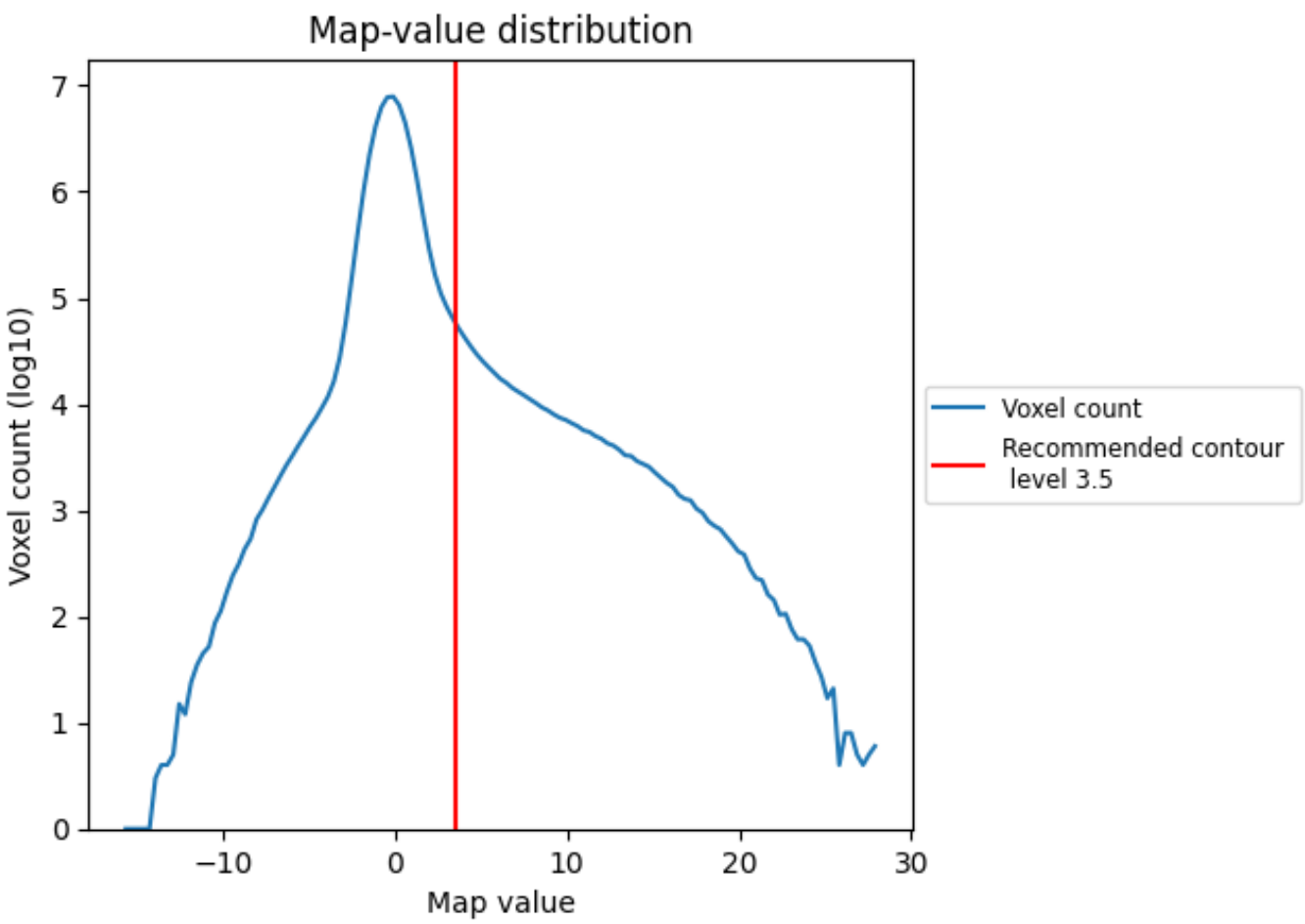
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

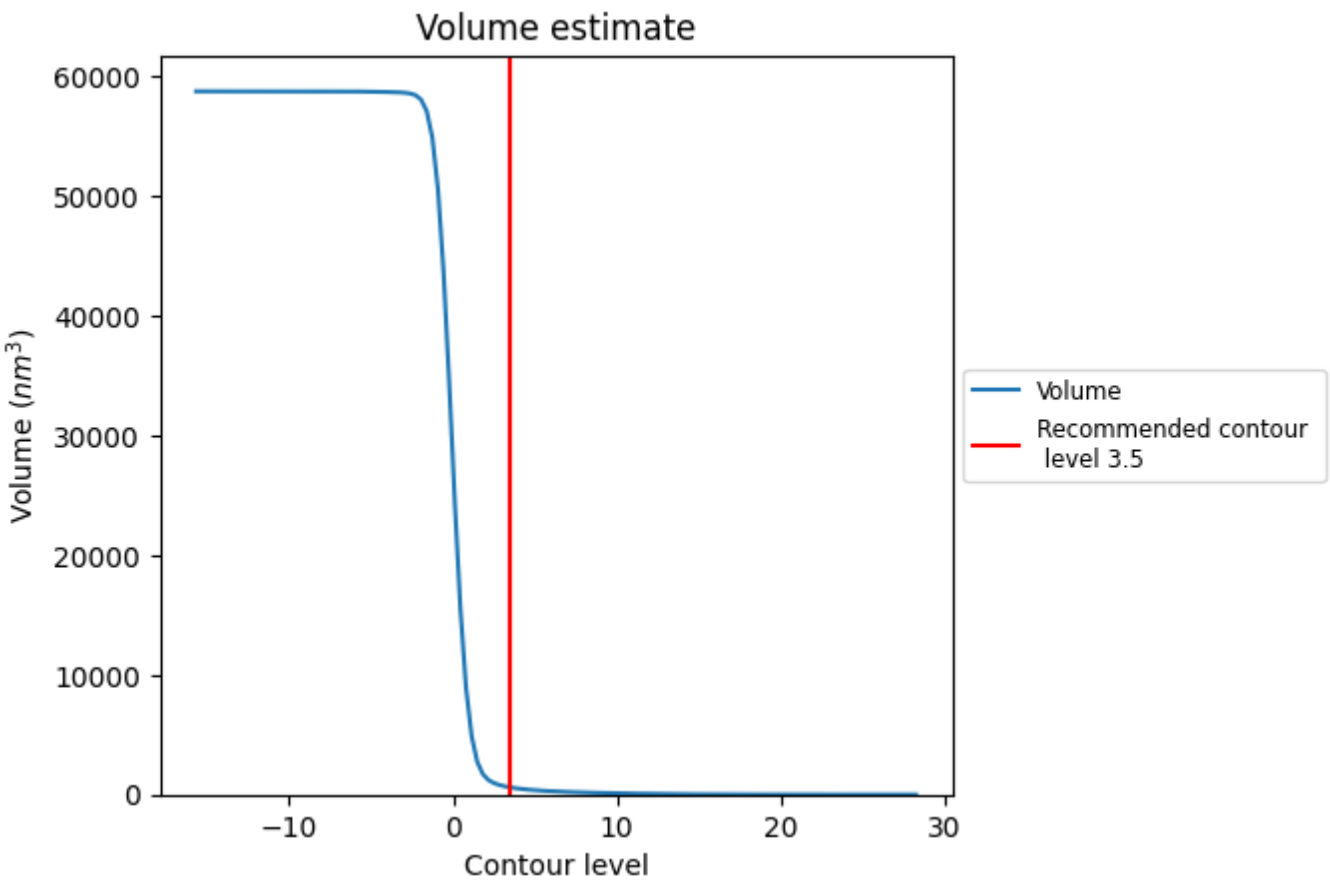
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

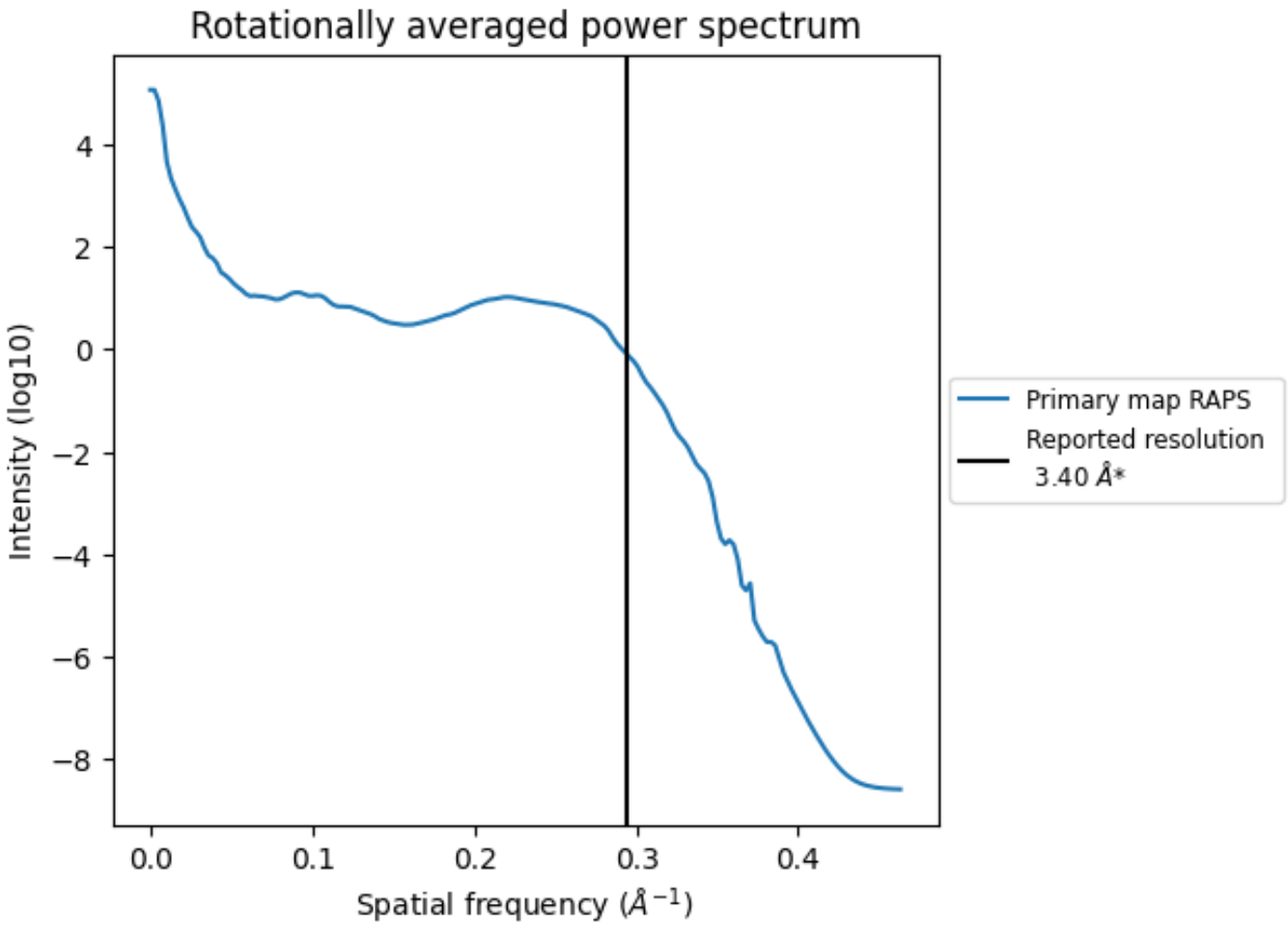
7.2 Volume estimate (i)



The volume at the recommended contour level is 599 nm^3; this corresponds to an approximate mass of 541 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

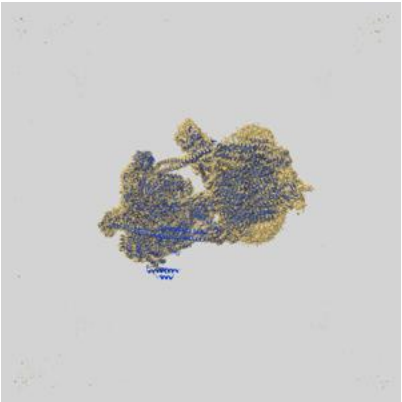
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

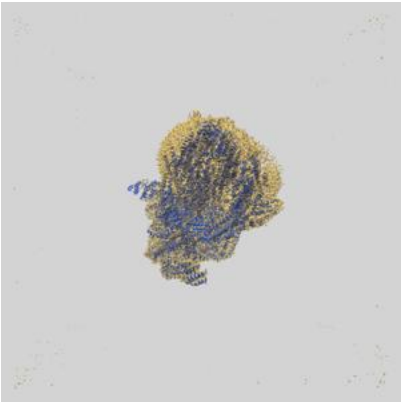
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-21848 and PDB model 6WM3. Per-residue inclusion information can be found in section 3 on page 10.

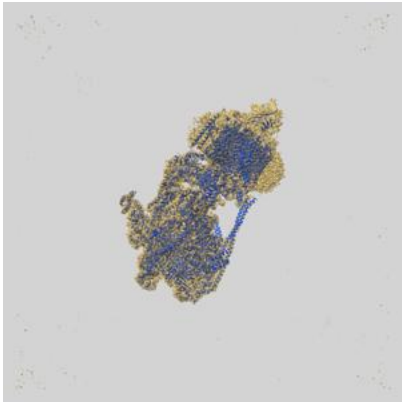
9.1 Map-model overlay (i)



X



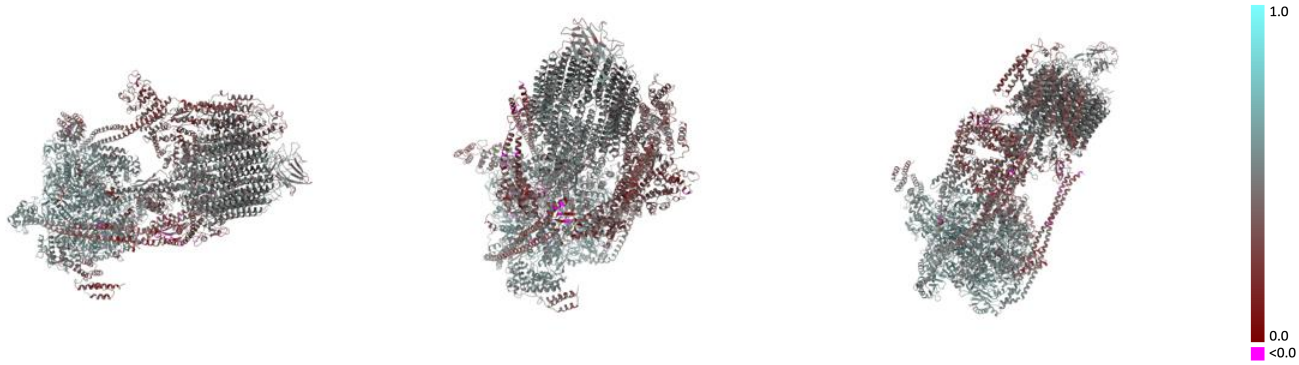
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

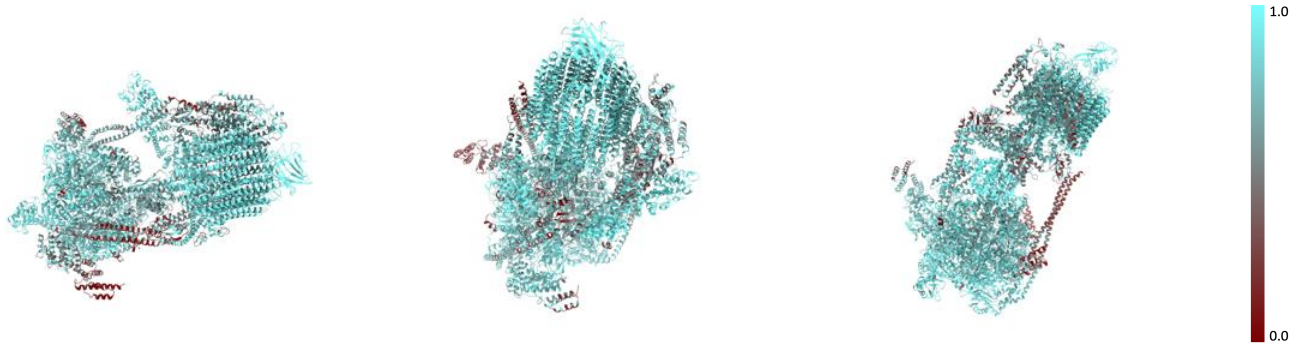
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

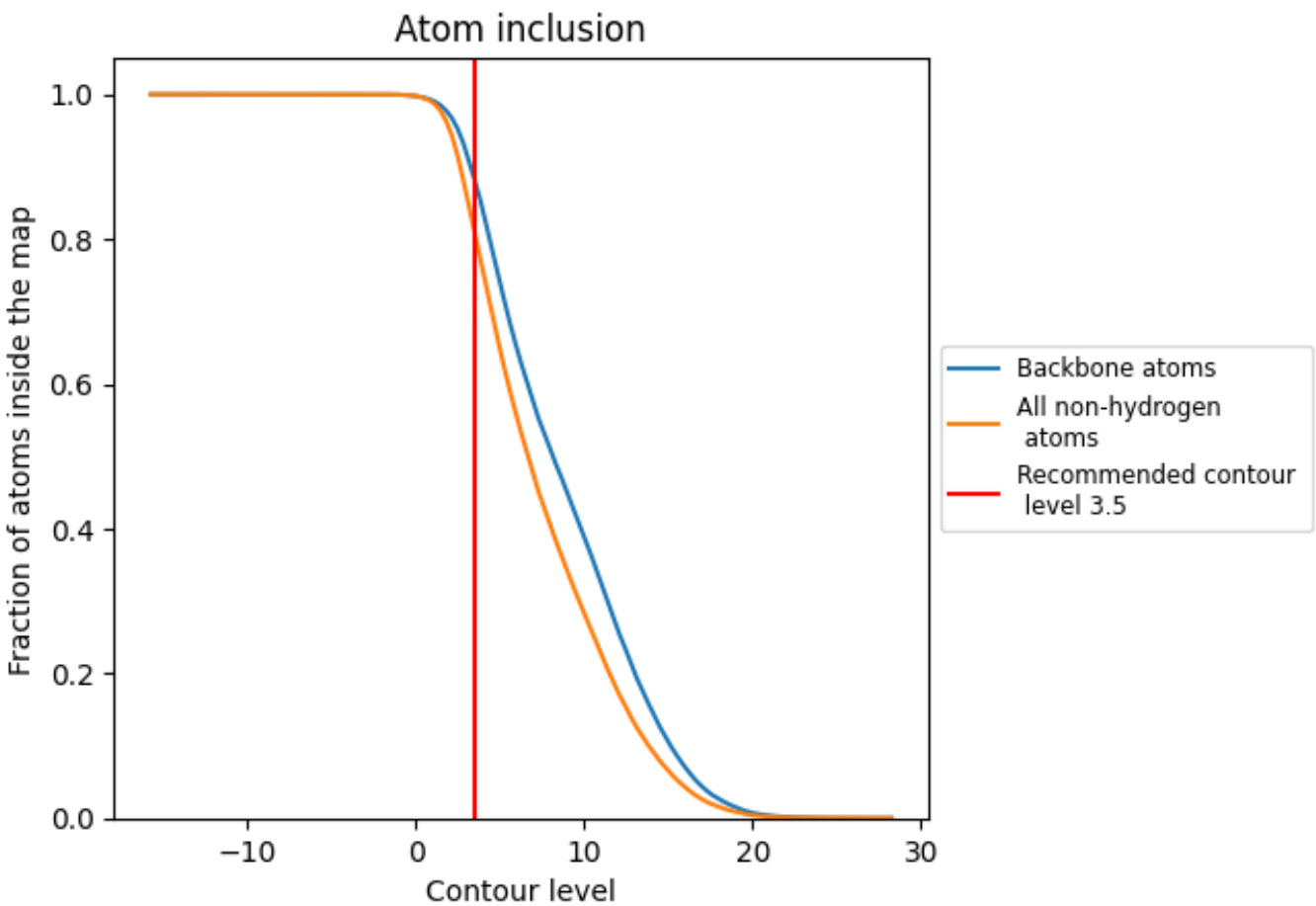
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.5).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8114	0.4770
0	0.9284	0.5020
1	0.9213	0.4950
2	0.9241	0.4830
3	0.9203	0.4790
4	0.9137	0.4720
5	0.9146	0.4730
6	0.8805	0.4650
7	0.8624	0.4730
8	0.8738	0.4820
9	0.9042	0.4930
A	0.8785	0.5390
B	0.9183	0.5680
C	0.8757	0.5490
D	0.9098	0.5700
E	0.8722	0.5420
F	0.8872	0.5480
G	0.8117	0.5050
H	0.8170	0.4710
I	0.7801	0.4820
J	0.7168	0.4680
K	0.7245	0.4150
L	0.6345	0.3970
M	0.5280	0.3870
N	0.6803	0.4170
O	0.6872	0.2830
P	0.9698	0.3510
Q	0.8859	0.4970
R	0.6057	0.3440
S	0.7102	0.3930
T	0.5991	0.3230
U	0.9347	0.4690
V	0.9303	0.4860
X	0.7485	0.4880
Y	0.3924	0.4180
Z	0.6877	0.4610