



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:50 PM UTC

PDB ID : 6REU / pdb_00006reu
EMDB ID : EMD-4857
Title : Cryo-EM structure of Polytomella F-ATP synthase, Rotary substate 3C, focussed refinement of F1 head and rotor
Authors : Murphy, B.J.; Klusch, N.; Yildiz, O.; Kuhlbrandt, W.
Deposited on : 2019-04-12
Resolution : 4.20 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

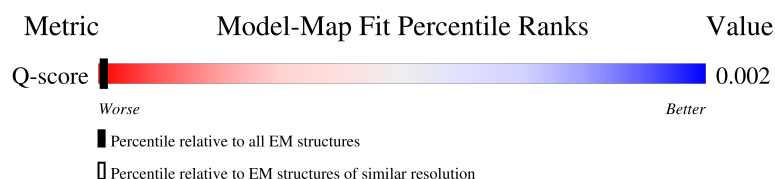
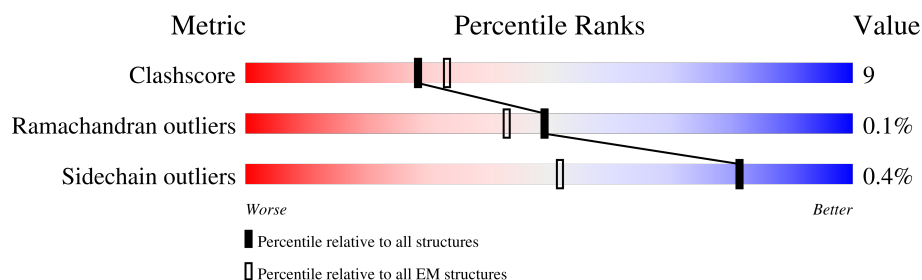
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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.



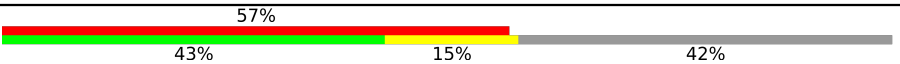
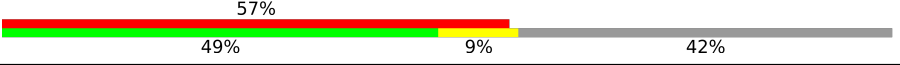
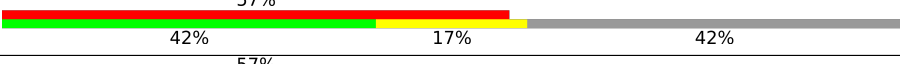
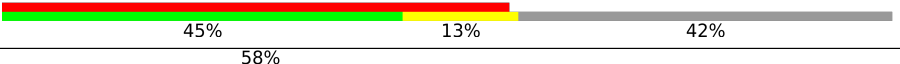
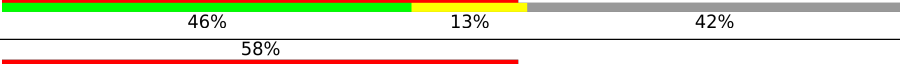
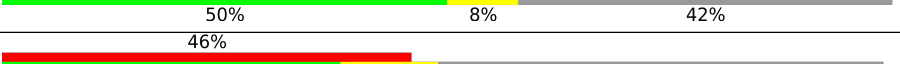
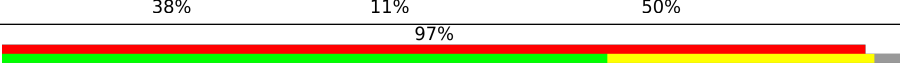
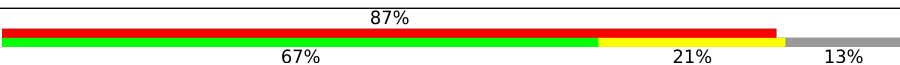
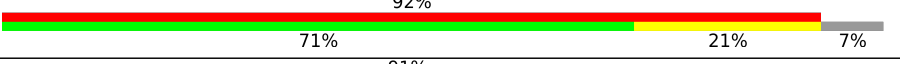
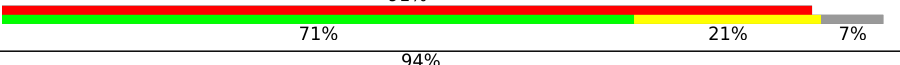
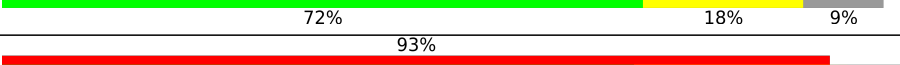
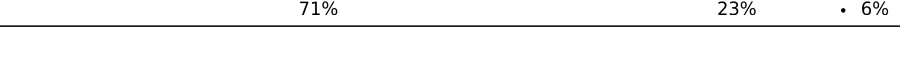
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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 $\leq 5\%$. 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	A	127	57% 41% 17% 42%
1	B	127	57% 38% 20% 42%
1	C	127	58% 41% 17% 42%
1	D	127	57% 45% 13% 42%

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Mol	Chain	Length	Quality of chain
1	E	127	
1	F	127	
1	G	127	
1	H	127	
1	I	127	
1	J	127	
2	P	229	
3	Q	74	
4	R	199	
5	S	317	
6	T	562	
6	U	562	
6	V	562	
7	X	574	
7	Y	574	
7	Z	574	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 33899 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 Mitochondrial ATP synthase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	B	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	C	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	D	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	E	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	F	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	G	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	H	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	I	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	J	74	Total	C	N	O	S	0	0
			514	340	83	88	3		

- Molecule 2 is a protein called Mitochondrial ATP synthase subunit OSCP.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	114	Total	C	N	O	S	0	0
			895	576	147	171	1		

- Molecule 3 is a protein called epsilon: Polytomella F-ATP synthase epsilon subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	72	Total	C	N	O	S	0	0
			561	358	102	99	2		

- Molecule 4 is a protein called Mitochondrial ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	177	Total	C	N	O	S	0	0
			1303	833	213	256	1		

- Molecule 5 is a protein called ATP synthase gamma chain, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	277	Total	C	N	O	S	0	0
			2130	1327	377	416	10		

- Molecule 6 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	478	Total	C	N	O	S	0	0
			3609	2294	640	664	11		
6	U	523	Total	C	N	O	S	0	0
			3980	2537	703	729	11		
6	V	520	Total	C	N	O	S	0	0
			3962	2527	700	724	11		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	266	ARG	LYS	conflict	UNP A0ZW40
U	266	ARG	LYS	conflict	UNP A0ZW40
V	266	ARG	LYS	conflict	UNP A0ZW40

- Molecule 7 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	X	539	Total	C	N	O	S	0	0
			4095	2572	693	817	13		
7	Y	521	Total	C	N	O	S	0	0
			3957	2485	670	789	13		
7	Z	542	Total	C	N	O	S	0	0
			4115	2586	696	820	13		

There are 6 discrepancies between the modelled and reference sequences:

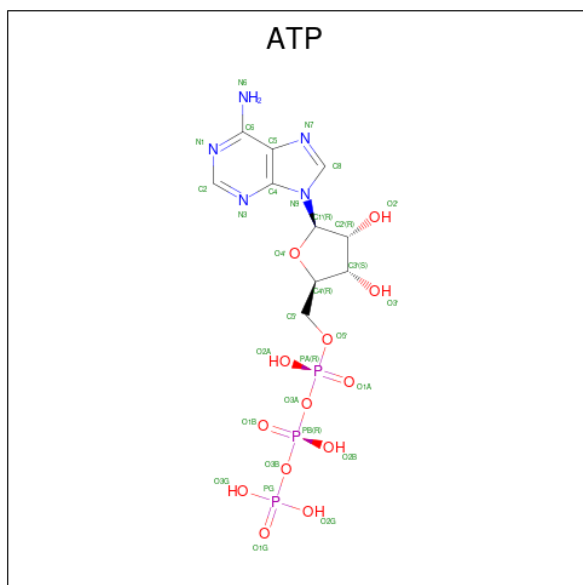
Chain	Residue	Modelled	Actual	Comment	Reference
X	350	ALA	GLY	conflict	UNP A0ZW41
X	387	LEU	ARG	conflict	UNP A0ZW41
Y	350	ALA	GLY	conflict	UNP A0ZW41

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	387	LEU	ARG	conflict	UNP A0ZW41
Z	350	ALA	GLY	conflict	UNP A0ZW41
Z	387	LEU	ARG	conflict	UNP A0ZW41

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



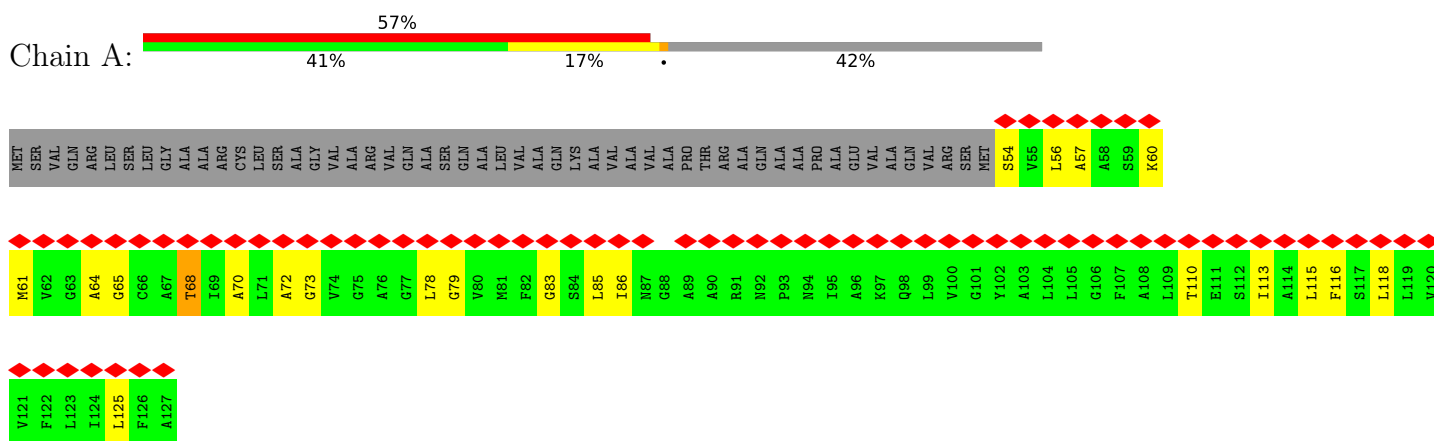
- # ADP

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

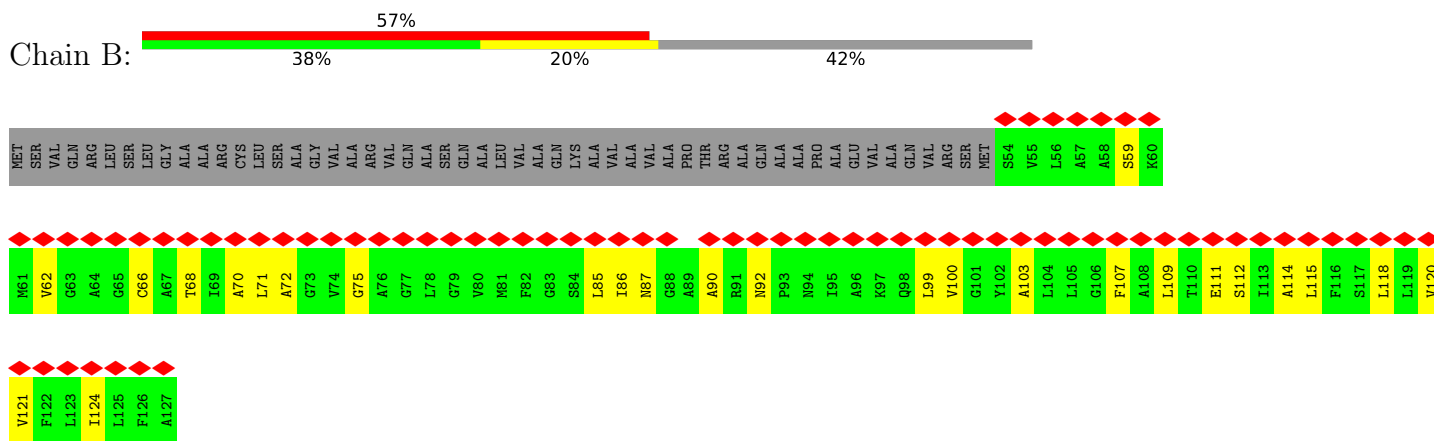
3 Residue-property plots

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.

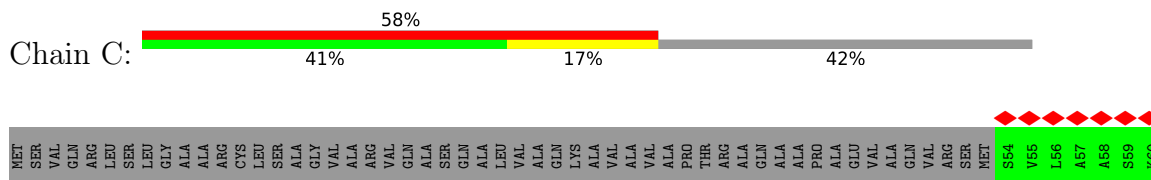
- Molecule 1: Mitochondrial ATP synthase subunit c

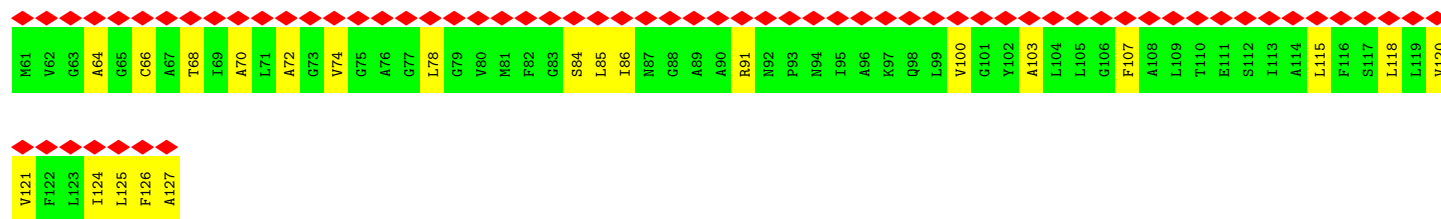


- Molecule 1: Mitochondrial ATP synthase subunit c

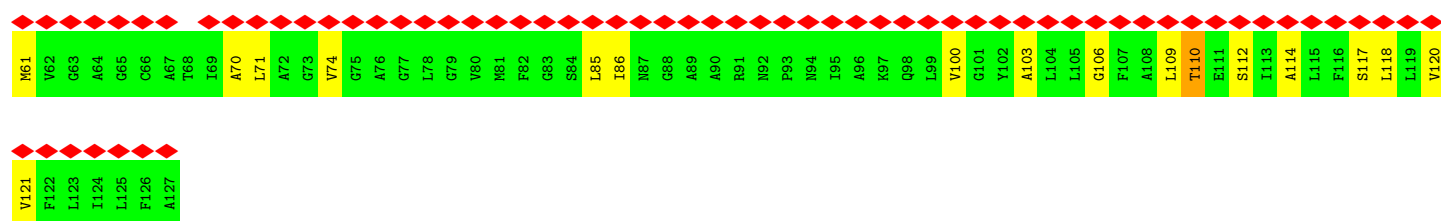
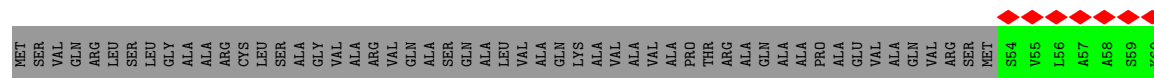
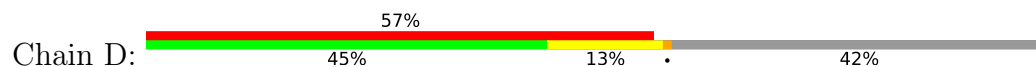


- Molecule 1: Mitochondrial ATP synthase subunit c

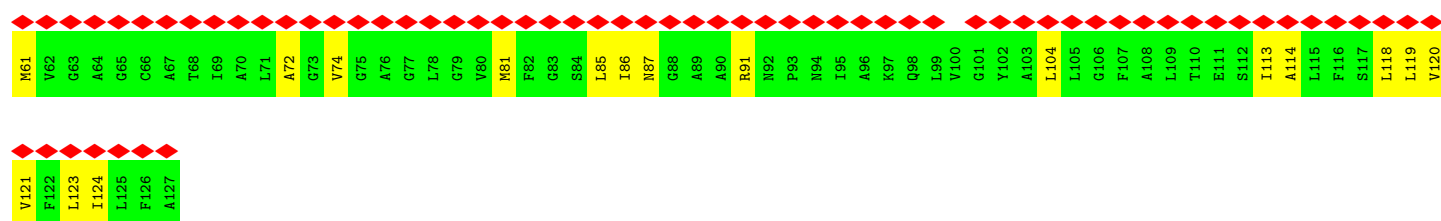
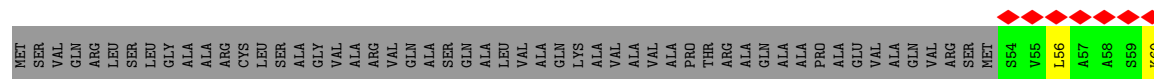
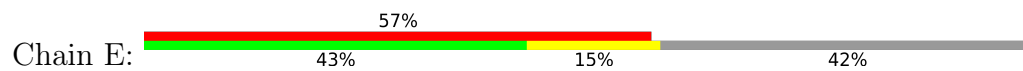




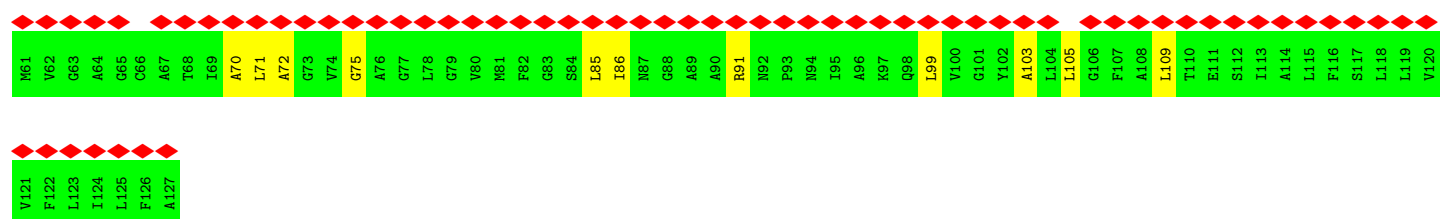
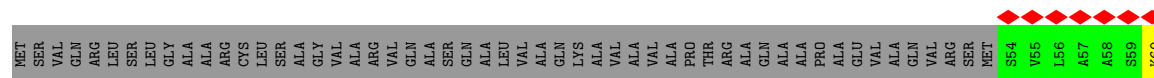
• Molecule 1: Mitochondrial ATP synthase subunit c



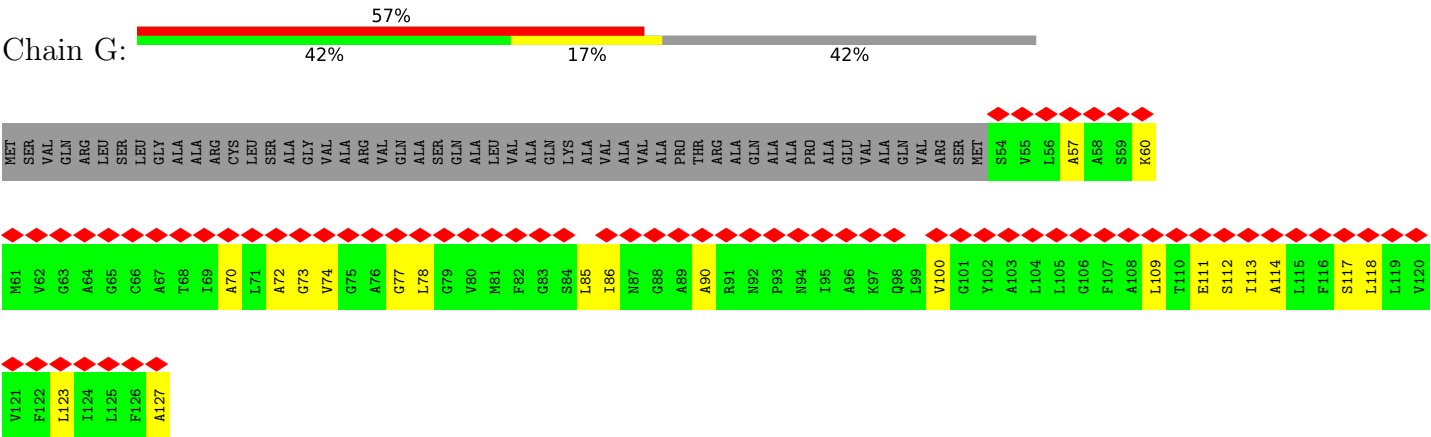
• Molecule 1: Mitochondrial ATP synthase subunit c



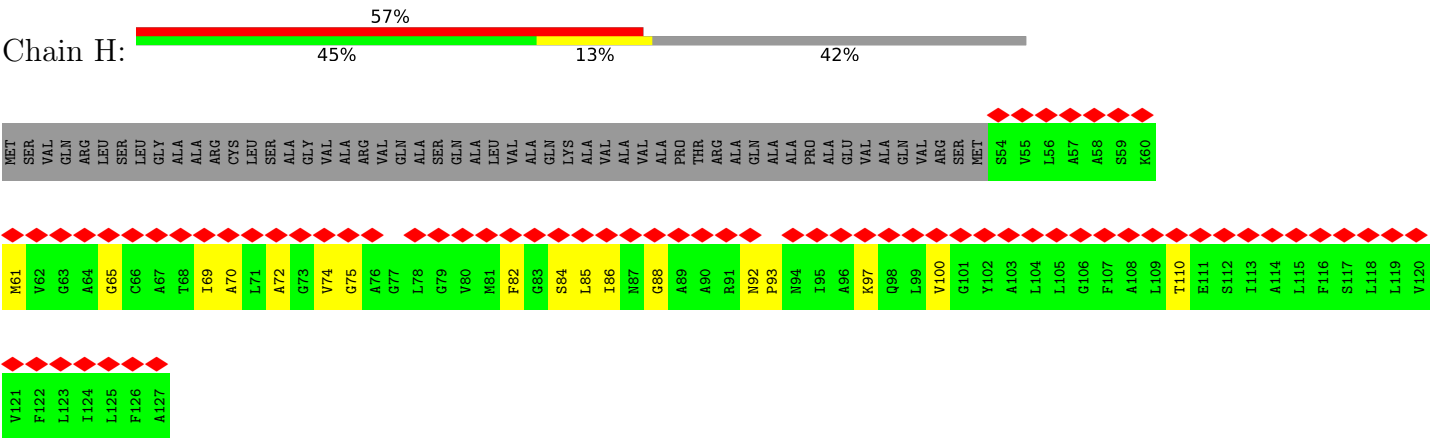
• Molecule 1: Mitochondrial ATP synthase subunit c



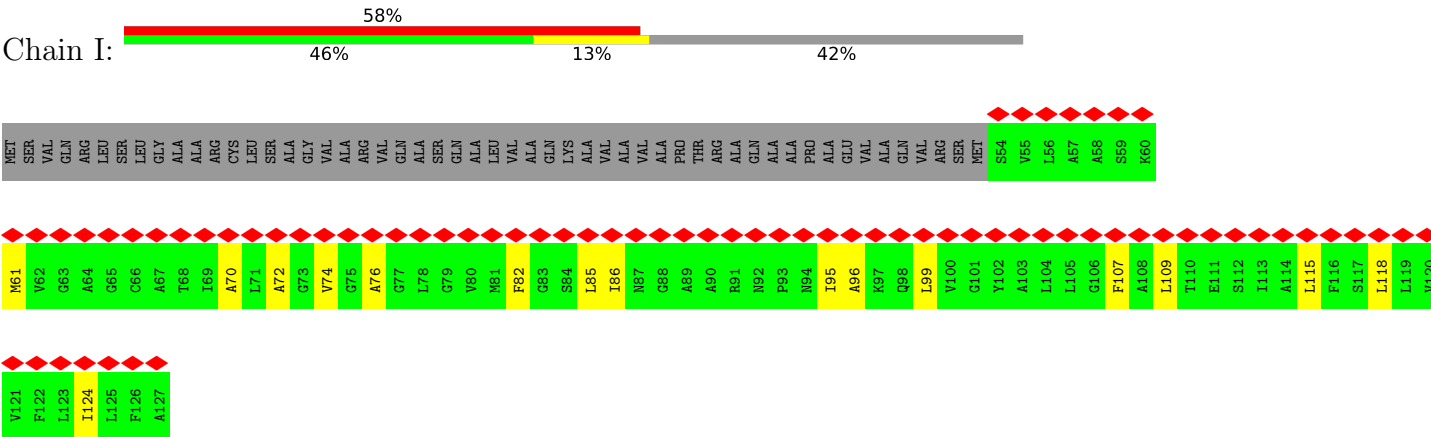
• Molecule 1: Mitochondrial ATP synthase subunit c



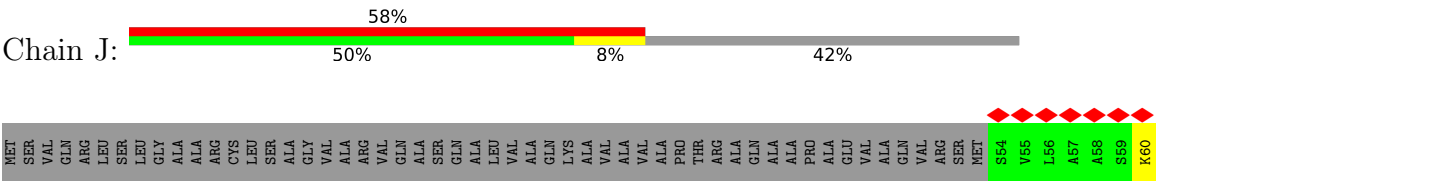
• Molecule 1: Mitochondrial ATP synthase subunit c



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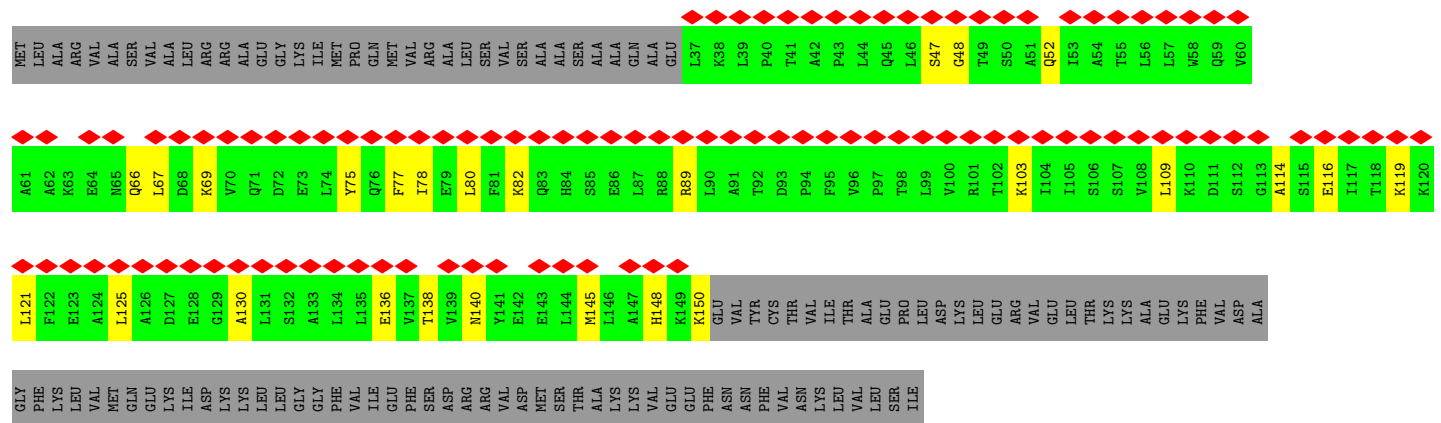
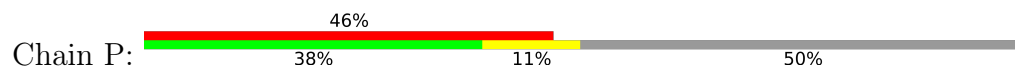


• Molecule 1: Mitochondrial ATP synthase subunit c





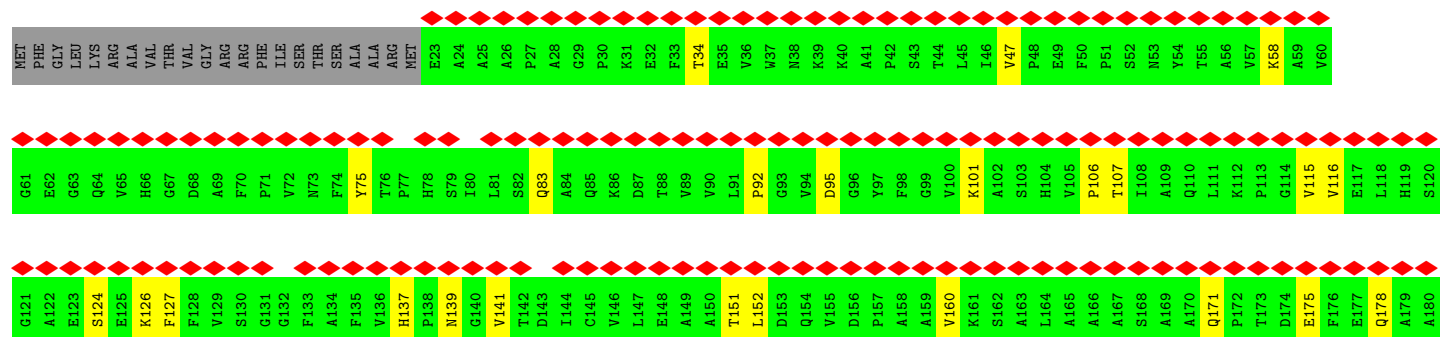
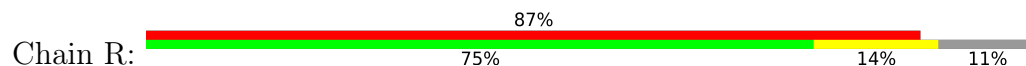
• Molecule 2: Mitochondrial ATP synthase subunit OSCP

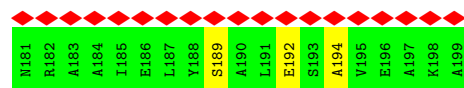


• Molecule 3: epsilon: Polytomella F-ATP synthase epsilon subunit

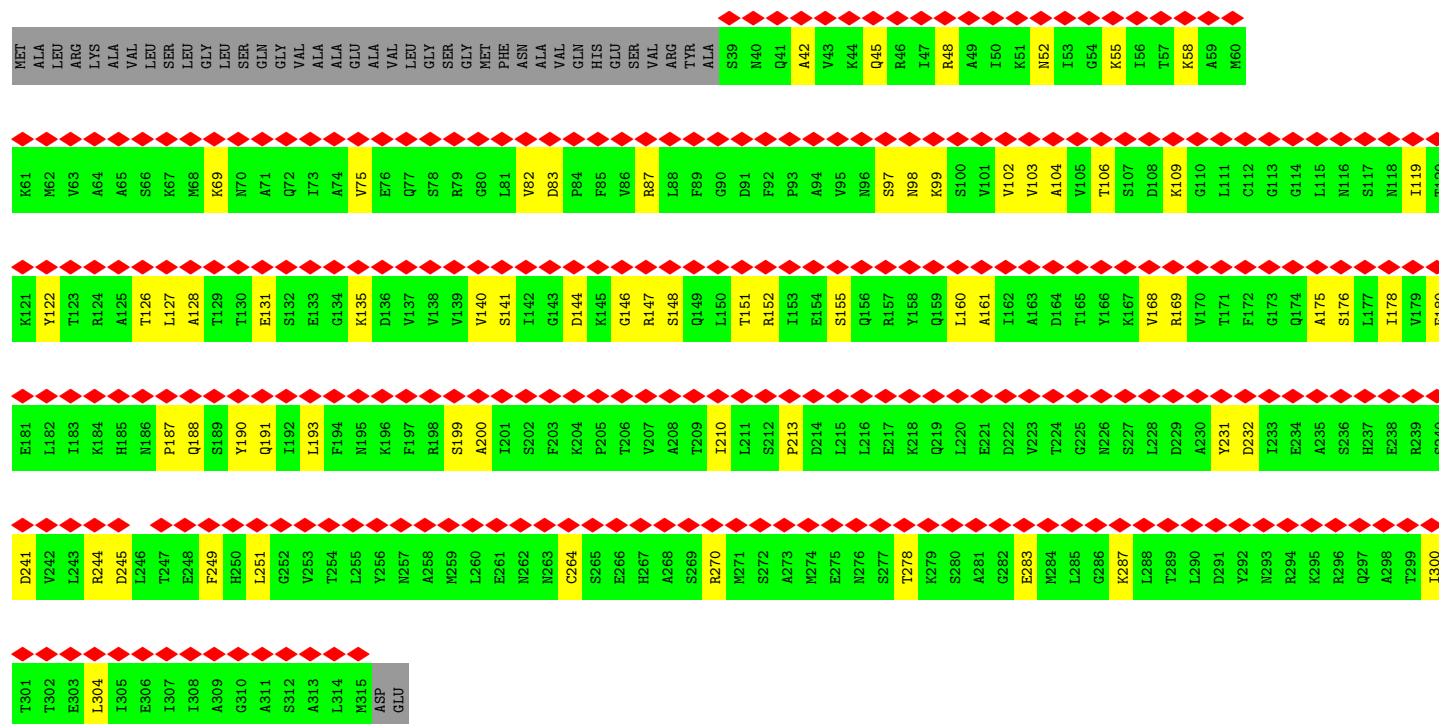
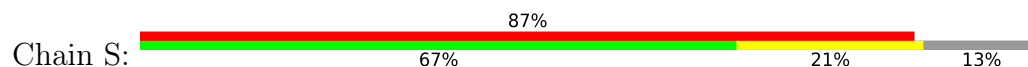


• Molecule 4: Mitochondrial ATP synthase subunit delta

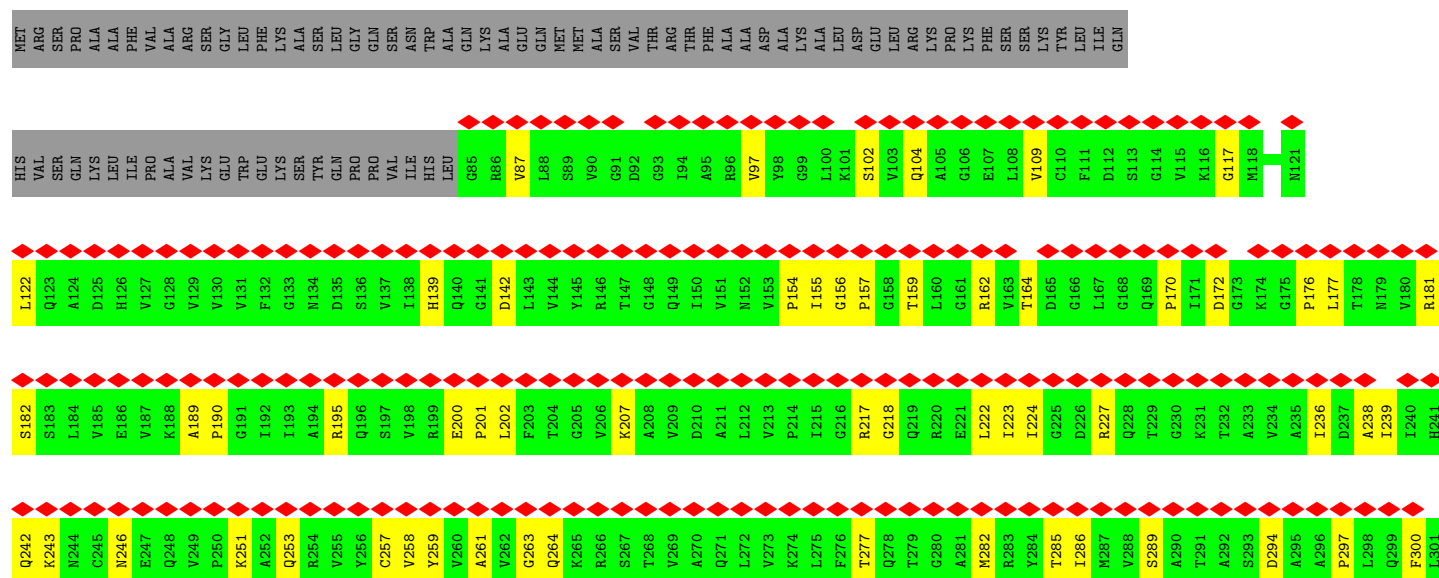
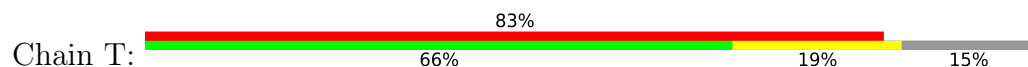


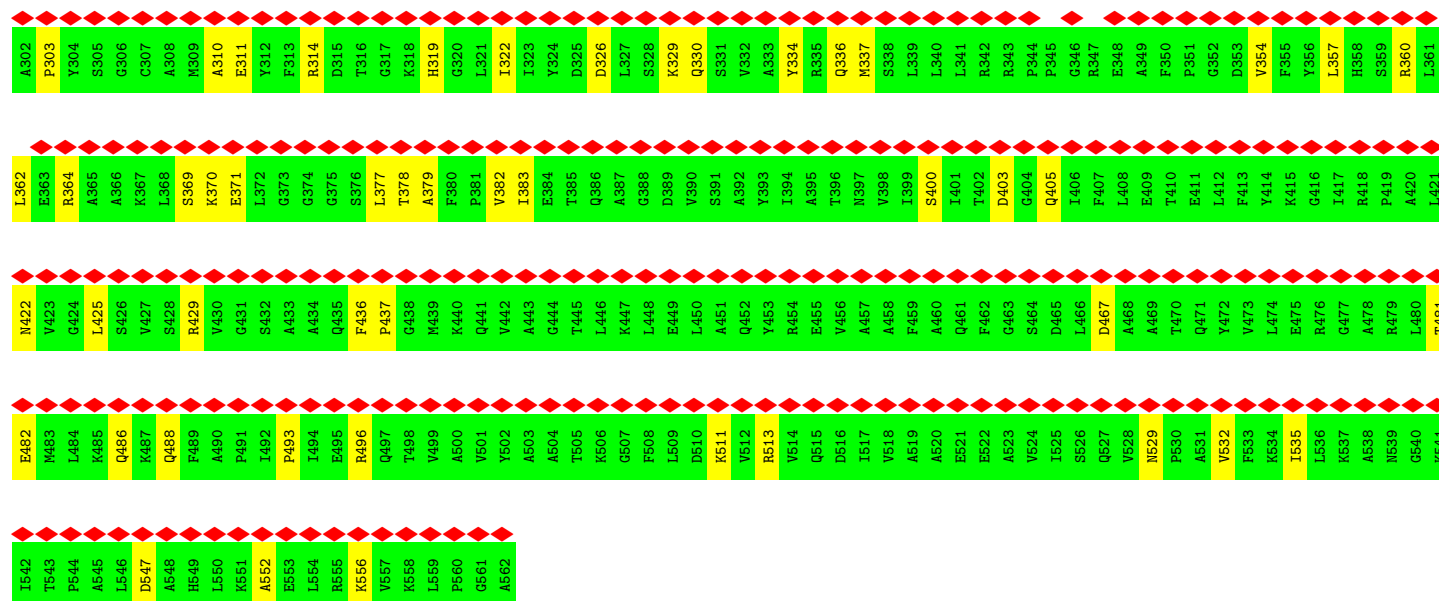


• Molecule 5: ATP synthase gamma chain, mitochondrial

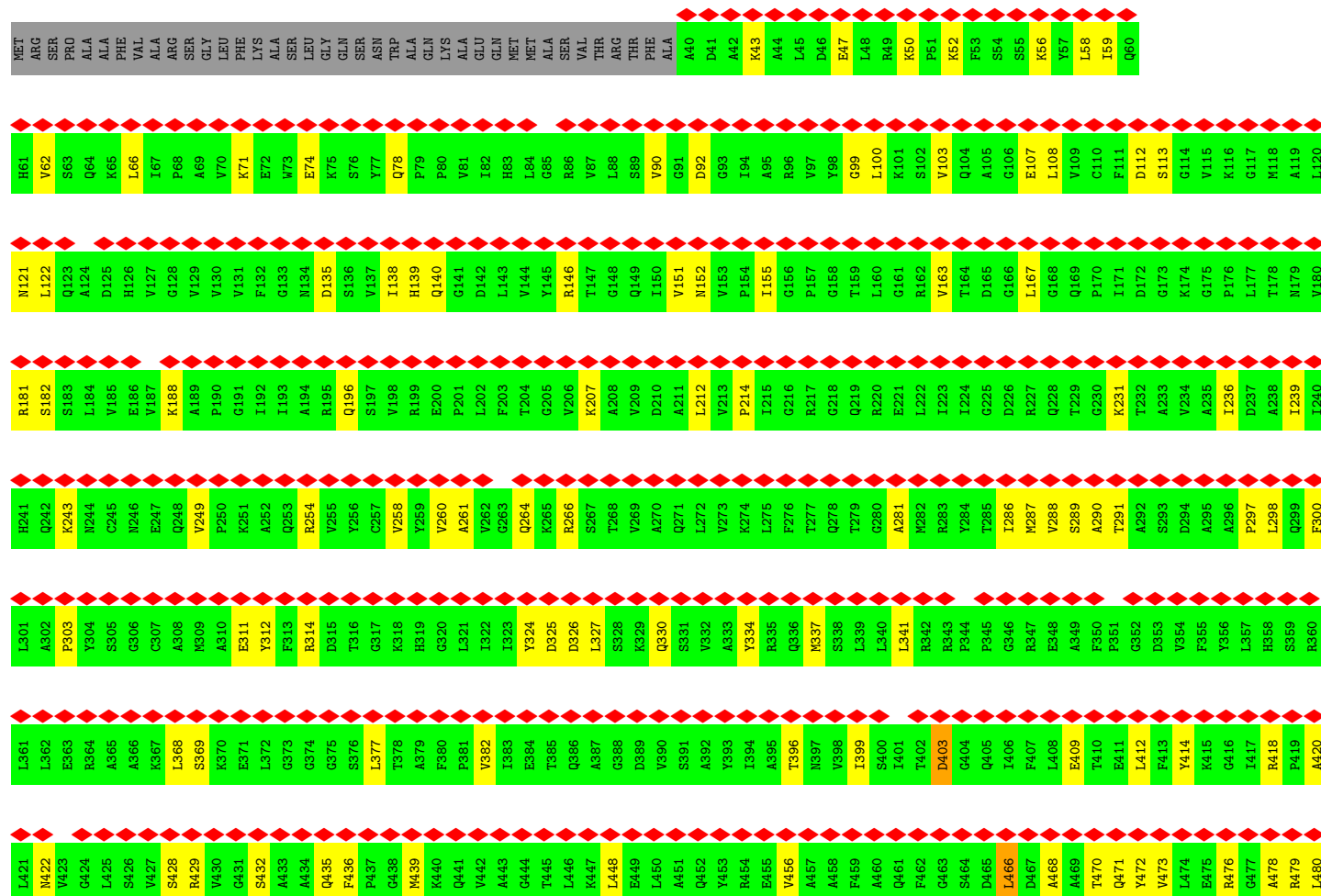
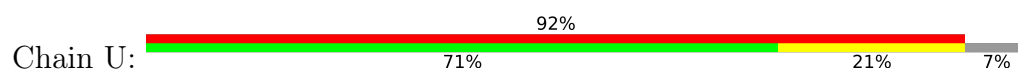


• Molecule 6: ATP synthase subunit alpha





• Molecule 6: ATP synthase subunit alpha



T481 E482 M483 L484 K485 Q486 K487 Q488 F489 A490 P491 I492 P493 I494 E495 R496 Q497 T498 V499 A500 V501 Y502 A503 A504 T505 K506 G507 F508 L509 D510 K511 V512 R513 V514 Q515 D516 I517 V518 A519 A520 E521 E522 A523 V524 I525 S526 Q527 V528 N529 P530 A531 V532 F533 K534 I535 L536 K537 A538 N539 G540

K541 I542 T543 P544 A545 L546 D547 A548 H549 L550 K551 A552 E553 L554 R555 K556 V557 T558 L559 P560 G561 A562

• Molecule 6: ATP synthase subunit alpha

Chain V: 91% 71% 21% 7%

MET ARG SER PRO ALA PHE VAL ALA ARG SER GLY LEU PHE LYS ALA SER LEU GLY GLN SER ASN TRP ALA GLN LYS ALA GLU GLN MET MET MET ALA SER VAL THR THR PHE ALA ASP ALA K43 A44 L45 D46 E47 Y98 L48 R49 K50 F51 K52 F53 S54 S55 K56 K57 V57 L58 I59 Q60

H61 V62 S63 Q64 K65 L66 I67 P68 A69 V70 K71 E72 W73 E74 K75 S76 Y77 Q78 F79 P80 V81 I82 H83 H84 G85 R86 V87 L88 S89 V90 G91 D92 G93 I94 A95 R96 V97 Y98 G99 I100 K101 S102 V103 Q104 A105 G106 E107 L108 V109 G110 F111 D112 S113 G114 V115 K116 G117 M118 A119 L120

N121 L122 Q123 A124 I125 H126 V127 G128 A129 V130 V131 F132 G133 W134 D135 S136 V137 I138 H139 Q140 G141 D142 L143 V144 Y145 R146 T147 G148 Q149 I150 V151 N152 V153 P154 I155 G156 P157 G158 T159 L160 G161 V163 T164 D165 G166 L167 G168 Q169 P170 I171 D172 G173 K174 G175 P176 L177 T178 N179 V180

R181 S183 L184 V185 E186 V187 K188 A189 P190 G191 I192 I193 A194 R195 Q196 S197 V198 R199 E200 P201 L202 F203 T204 G205 V206 K207 A208 V209 D210 A211 L212 V213 P214 I215 G216 R217 G218 Q219 R220 E221 T223 T224 G225 D226 R227 Q228 T229 Q230 K231 T232 A233 V234 A235 T236 D237 L238 S239 T240

H241 Q242 K243 W244 C245 W246 E247 Q248 V249 P250 K251 A252 Q253 R254 V255 V256 C257 V258 Y259 V260 A261 V262 G263 G264 R265 R266 S267 T268 V269 A270 Q271 L272 V273 K274 L275 F276 T277 Q278 T279 A281 M282 R283 Y284 T285 G286 M287 V288 S289 A290 T291 A292 S293 D294 A295 A296 P297 L298 Q299 F300

L301 A302 P303 Y304 S305 G306 C307 A308 K309 M309 E311 Y312 F313 R314 D315 D316 G317 H318 H319 G320 L321 L322 I323 Y324 D325 D326 L327 S328 K329 S331 V332 A333 Y334 R335 Q336 K337 S338 L339 L340 L341 R342 R343 P344 P345 G346 R347 E348 A349 F350 P351 G352 D353 V354 F355 Y356 L357 H358 S359 R360

L361 L362 E363 R364 A365 A366 K367 L368 S369 F369 A370 E371 L372 G373 G374 G375 S376 L377 T378 A379 F380 P381 V382 I383 E384 T385 Q386 A387 G388 D389 V390 S391 A392 Y393 L394 A395 T396 A397 T398 T399 S400 A401 T402 D403 A404 Q405 D406 F407 L408 A409 E411 L412 F413 Y414 K415 O416 L417 R418 P419 A420

L421 H422 V423 Q424 L425 S426 W427 A428 R429 A430 G431 S432 A433 A434 Q435 F436 P437 Q438 M439 K440 Q441 V442 A443 A444 Q445 T446 L447 K448 E449 L450 A451 Q452 Y453 R454 S455 V456 A457 A458 F459 A460 Q461 Q462 Q463 Q464 D465 L466 S467 D467 L468 A469 T470 Q471 Y472 W473 L474 E475 R476 Q477 A478 R479 L480

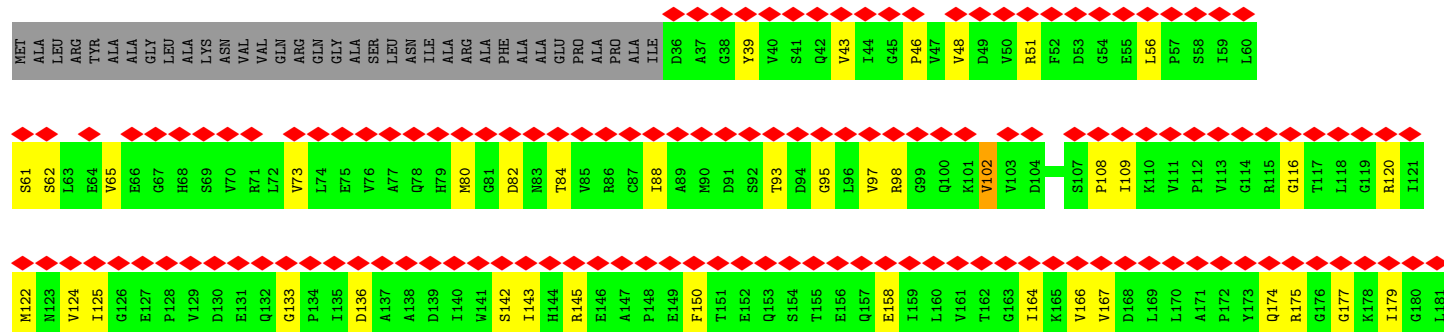
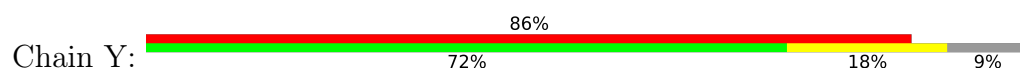
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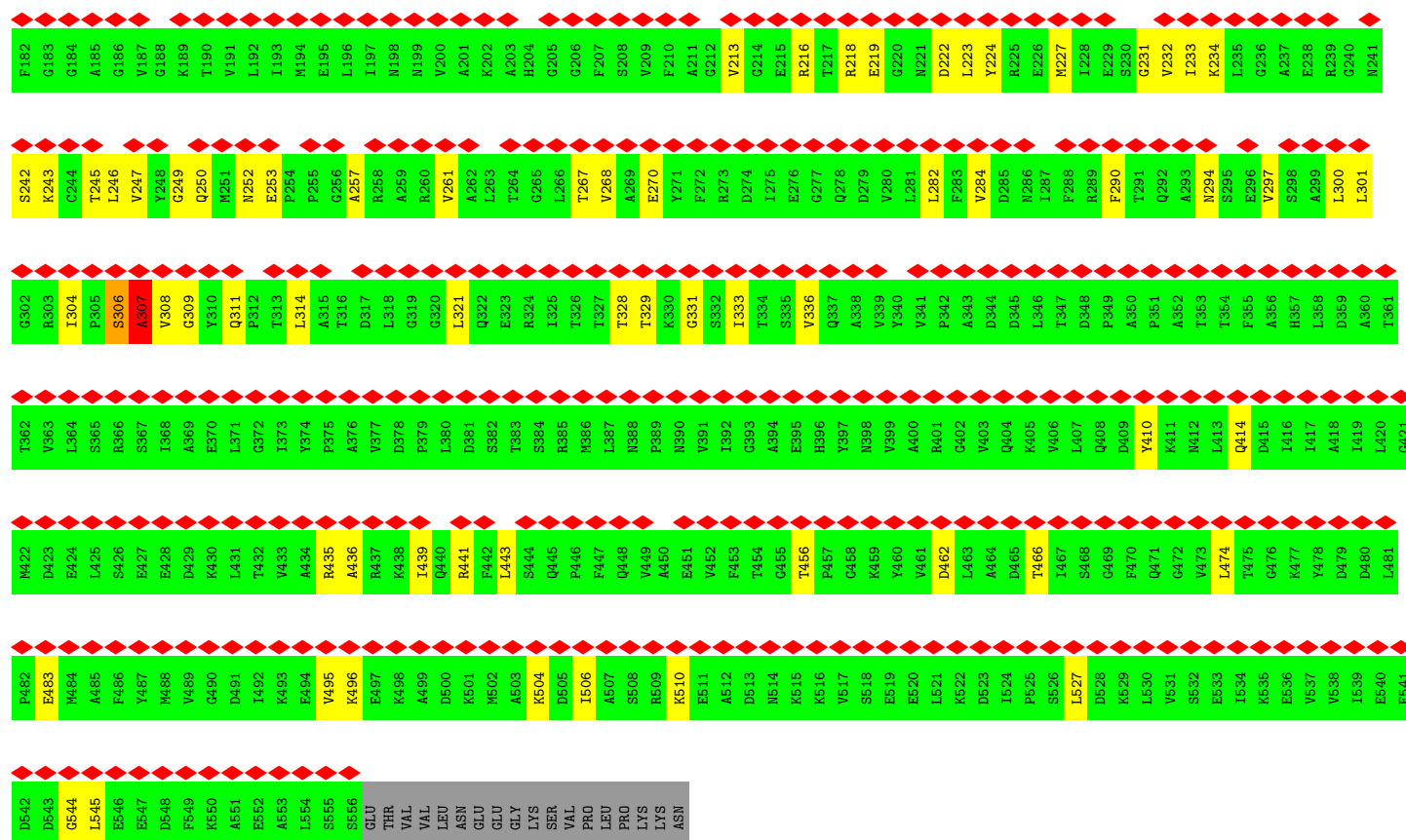
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• Molecule 7: ATP synthase subunit beta

Chain X: 94% 68% 26% 6%

- Molecule 7: ATP synthase subunit beta







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8173	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 ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.134	Depositor
Minimum map value	-0.083	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	518.4, 518.4, 518.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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	A	0.23	0/520	0.53	0/704
1	B	0.19	0/520	0.47	0/704
1	C	0.25	0/519	0.57	0/701
1	D	0.27	0/520	0.48	0/704
1	E	0.24	0/520	0.49	0/704
1	F	0.20	0/520	0.42	0/704
1	G	0.19	0/520	0.48	0/704
1	H	0.22	0/520	0.47	0/704
1	I	0.21	0/520	0.49	0/704
1	J	0.23	0/520	0.52	0/704
2	P	0.32	0/908	0.54	0/1229
3	Q	0.28	0/574	0.53	0/774
4	R	0.24	0/1336	0.48	0/1827
5	S	0.27	0/2153	0.55	0/2901
6	T	0.30	0/3667	0.59	1/4965 (0.0%)
6	U	0.28	0/4049	0.58	4/5481 (0.1%)
6	V	0.31	0/4031	0.57	0/5456
7	X	0.28	0/4155	0.57	1/5630 (0.0%)
7	Y	0.30	0/4015	0.54	0/5440
7	Z	0.32	0/4176	0.55	1/5659 (0.0%)
All	All	0.28	0/34263	0.55	7/46399 (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
2	P	0	1
7	X	0	1
7	Y	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	Z	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	U	66	LEU	CA-C-N	6.37	124.25	120.24
6	U	66	LEU	C-N-CA	6.37	124.25	120.24
6	T	467	ASP	CA-C-O	-6.10	111.78	120.51
7	Z	308	VAL	N-CA-C	5.87	121.55	109.34
7	X	419	ILE	N-CA-C	-5.29	108.34	113.53

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	148	HIS	Mainchain
7	X	307	ALA	Peptide
7	Y	307	ALA	Peptide
7	Z	307	ALA	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	514	0	554	18	0
1	B	514	0	554	22	0
1	C	514	0	553	18	0
1	D	514	0	554	13	0
1	E	514	0	554	16	0
1	F	514	0	554	13	0
1	G	514	0	554	17	0
1	H	514	0	554	15	0
1	I	514	0	554	16	0
1	J	514	0	554	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	895	0	934	19	0
3	Q	561	0	565	16	0
4	R	1303	0	1266	18	0
5	S	2130	0	2180	43	0
6	T	3609	0	3732	71	0
6	U	3980	0	4119	86	0
6	V	3962	0	4105	88	0
7	X	4095	0	4113	95	0
7	Y	3957	0	3967	67	0
7	Z	4115	0	4138	87	0
8	T	31	0	12	1	0
8	U	31	0	12	1	0
8	V	31	0	12	1	0
9	T	1	0	0	0	0
9	U	1	0	0	0	0
9	V	1	0	0	0	0
9	X	1	0	0	0	0
9	Z	1	0	0	0	0
10	X	27	0	12	3	0
10	Z	27	0	12	0	0
All	All	33899	0	34718	649	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 9.

The worst 5 of 649 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)
7:X:498:LYS:O	7:X:502:MET:HG3	1.11	1.25
7:X:498:LYS:O	7:X:502:MET:CG	2.03	1.05
6:V:222:LEU:HD13	6:V:381:PRO:HG2	1.47	0.95
6:V:222:LEU:CD1	6:V:381:PRO:HG2	2.08	0.82
7:X:484:MET:SD	7:X:502:MET:HE3	2.20	0.81

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	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
1	B	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
1	C	71/127 (56%)	69 (97%)	2 (3%)	0	100	100
1	D	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
1	E	72/127 (57%)	68 (94%)	4 (6%)	0	100	100
1	F	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
1	G	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
1	H	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
1	I	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
1	J	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
2	P	112/229 (49%)	103 (92%)	9 (8%)	0	100	100
3	Q	70/74 (95%)	62 (89%)	8 (11%)	0	100	100
4	R	175/199 (88%)	159 (91%)	16 (9%)	0	100	100
5	S	275/317 (87%)	261 (95%)	14 (5%)	0	100	100
6	T	476/562 (85%)	448 (94%)	28 (6%)	0	100	100
6	U	521/562 (93%)	493 (95%)	28 (5%)	0	100	100
6	V	518/562 (92%)	490 (95%)	27 (5%)	1 (0%)	43	77
7	X	537/574 (94%)	498 (93%)	38 (7%)	1 (0%)	43	77
7	Y	519/574 (90%)	490 (94%)	26 (5%)	3 (1%)	21	58
7	Z	540/574 (94%)	496 (92%)	43 (8%)	1 (0%)	43	77
All	All	4462/5497 (81%)	4200 (94%)	256 (6%)	6 (0%)	49	82

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	X	308	VAL

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Mol	Chain	Res	Type
7	Y	308	VAL
7	Z	308	VAL
7	Y	307	ALA
6	V	92	ASP

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	50/86 (58%)	49 (98%)	1 (2%)	48	65
1	B	50/86 (58%)	50 (100%)	0	100	100
1	C	50/86 (58%)	50 (100%)	0	100	100
1	D	50/86 (58%)	49 (98%)	1 (2%)	48	65
1	E	50/86 (58%)	50 (100%)	0	100	100
1	F	50/86 (58%)	50 (100%)	0	100	100
1	G	50/86 (58%)	50 (100%)	0	100	100
1	H	50/86 (58%)	50 (100%)	0	100	100
1	I	50/86 (58%)	50 (100%)	0	100	100
1	J	50/86 (58%)	50 (100%)	0	100	100
2	P	99/196 (50%)	98 (99%)	1 (1%)	68	75
3	Q	56/58 (97%)	55 (98%)	1 (2%)	51	66
4	R	134/151 (89%)	134 (100%)	0	100	100
5	S	235/265 (89%)	234 (100%)	1 (0%)	84	82
6	T	378/448 (84%)	377 (100%)	1 (0%)	86	84
6	U	419/448 (94%)	418 (100%)	1 (0%)	87	85
6	V	418/448 (93%)	416 (100%)	2 (0%)	81	81
7	X	447/469 (95%)	444 (99%)	3 (1%)	76	78
7	Y	430/469 (92%)	428 (100%)	2 (0%)	81	81
7	Z	449/469 (96%)	448 (100%)	1 (0%)	87	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3565/4281 (83%)	3550 (100%)	15 (0%)	81	82

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	V	163	VAL
7	Y	456	THR
6	V	213	VAL
7	Z	363	VAL
7	X	209	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
7	Z	199	ASN
7	Z	294	ASN
6	U	140	GLN
6	T	405	GLN
7	Z	322	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	$\# Z > 2$
8	ATP	U	1001	9	32,33,33	1.34	4 (12%)	48,52,52	1.78	8 (16%)
8	ATP	T	1001	9	32,33,33	1.28	5 (15%)	48,52,52	1.76	8 (16%)
10	ADP	Z	601	9	28,29,29	1.36	5 (17%)	43,45,45	1.89	10 (23%)
8	ATP	V	1001	9	32,33,33	1.31	5 (15%)	48,52,52	1.80	10 (20%)
10	ADP	X	601	9	28,29,29	1.36	4 (14%)	43,45,45	1.93	10 (23%)

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
8	ATP	U	1001	9	-	0/22/38/38	0/3/3/3
8	ATP	T	1001	9	-	4/22/38/38	0/3/3/3
10	ADP	Z	601	9	-	2/16/32/32	0/3/3/3
8	ATP	V	1001	9	-	2/22/38/38	0/3/3/3
10	ADP	X	601	9	-	3/16/32/32	0/3/3/3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	U	1001	ATP	C5-C4	4.56	1.47	1.39
8	V	1001	ATP	C5-C4	4.48	1.47	1.39
10	X	601	ADP	C5-C4	4.32	1.46	1.39
8	T	1001	ATP	C5-C4	4.21	1.46	1.39
10	Z	601	ADP	C5-C4	4.16	1.46	1.39

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	U	1001	ATP	C5-C4-N3	-6.31	118.03	126.72
10	X	601	ADP	C5-C4-N3	-6.13	118.28	126.72
10	Z	601	ADP	C5-C4-N3	-5.72	118.84	126.72
8	T	1001	ATP	C5-C4-N3	-5.64	118.95	126.72
8	V	1001	ATP	C5-C4-N3	-5.49	119.16	126.72

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

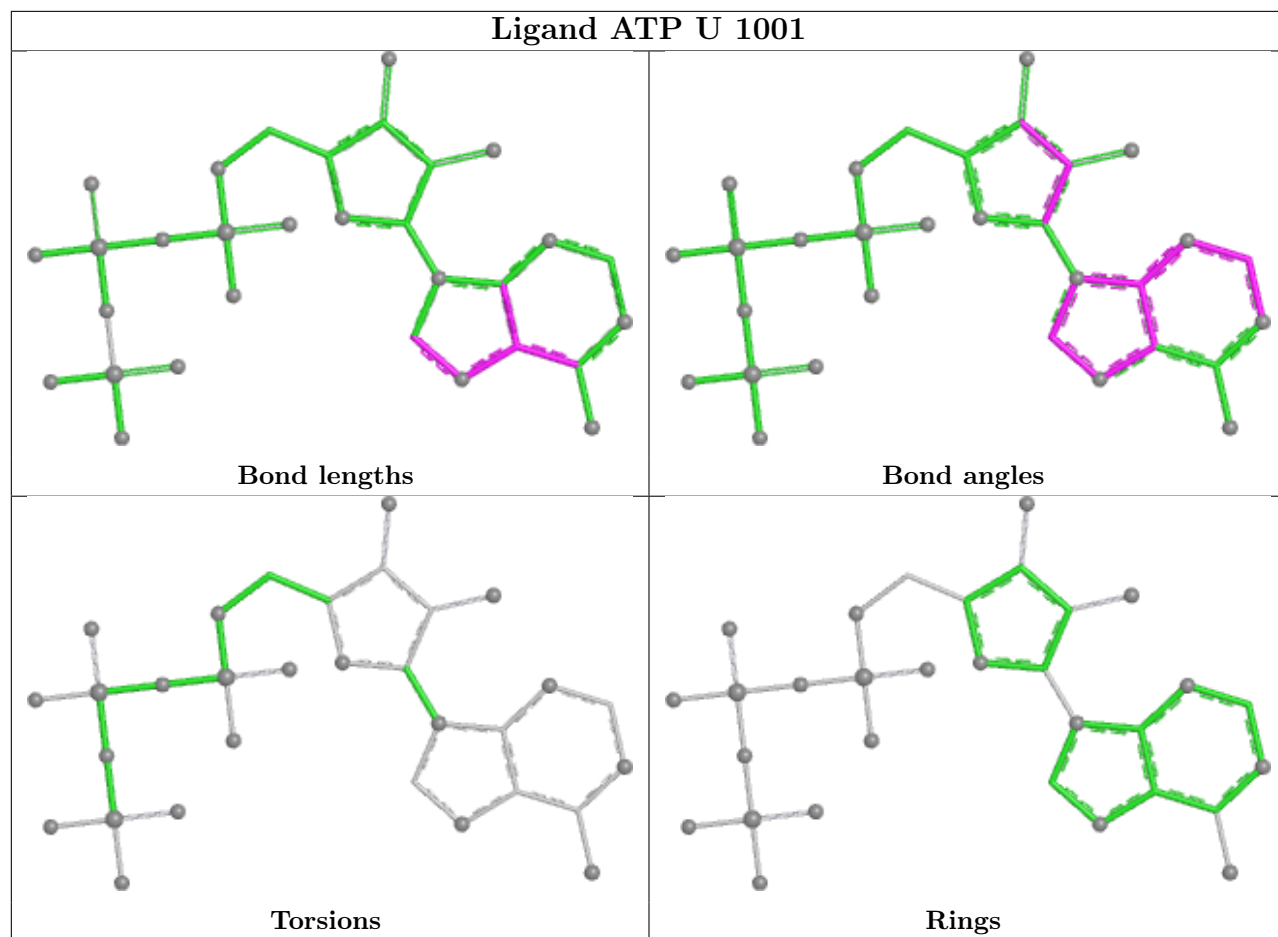
Mol	Chain	Res	Type	Atoms
8	T	1001	ATP	O4'-C4'-C5'-O5'
10	X	601	ADP	C5'-O5'-PA-O1A
8	T	1001	ATP	C3'-C4'-C5'-O5'
8	T	1001	ATP	PA-O3A-PB-O1B
10	X	601	ADP	C5'-O5'-PA-O2A

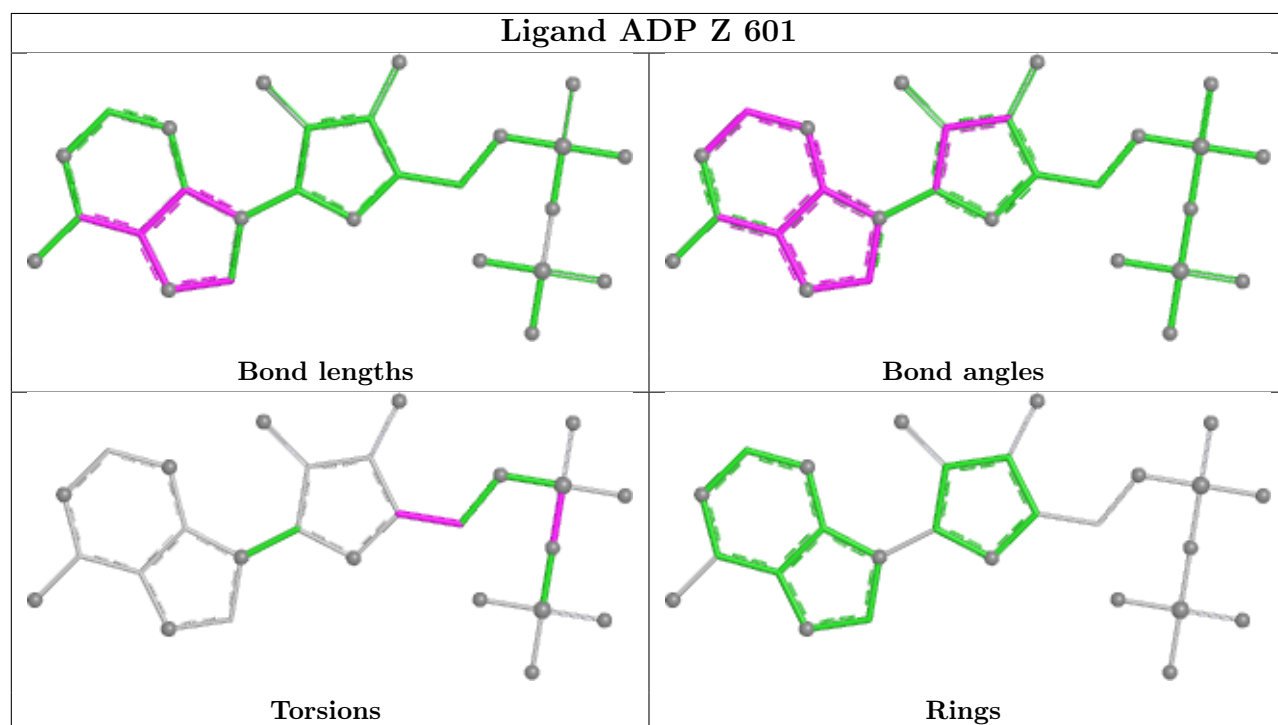
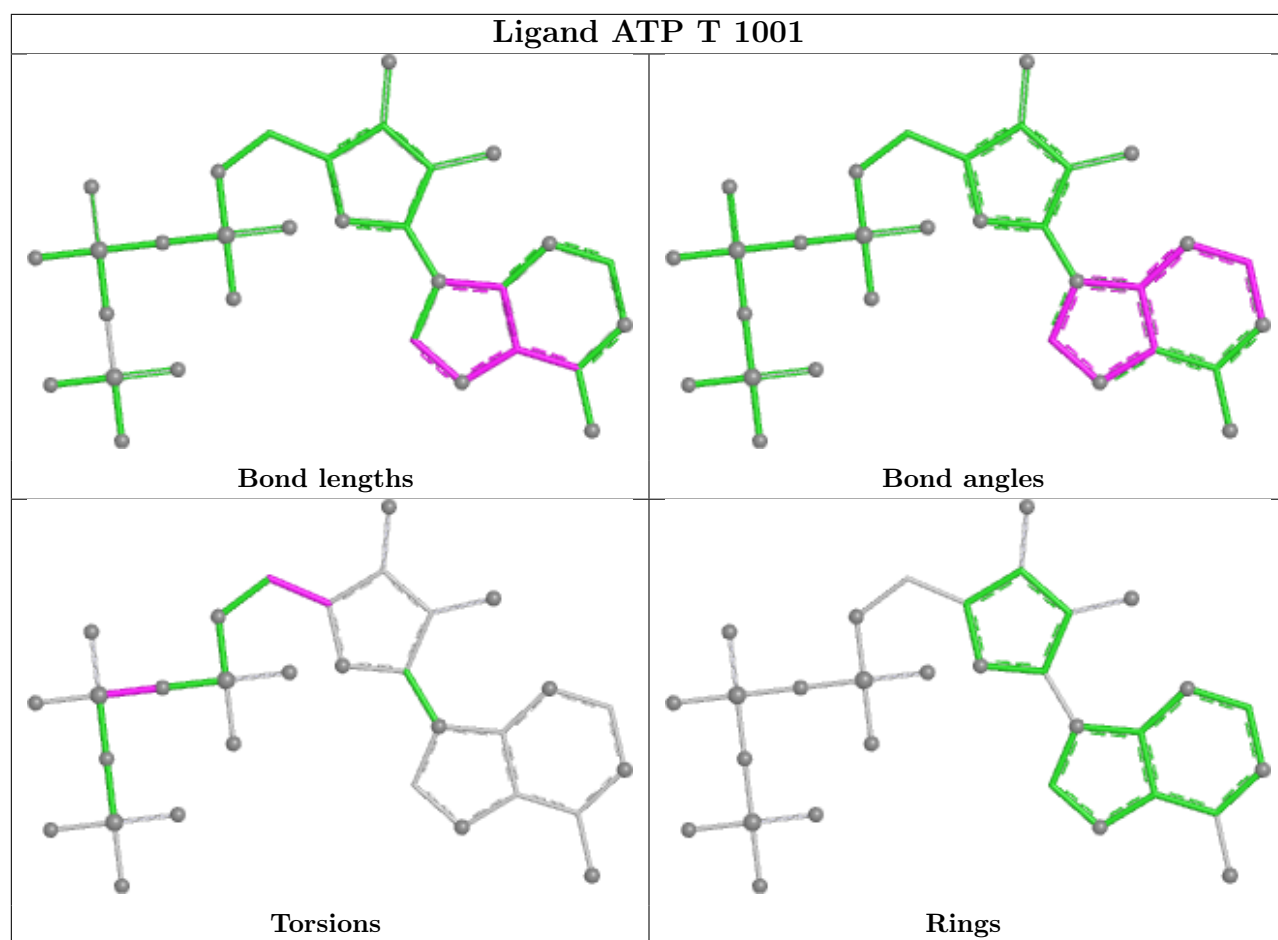
There are no ring outliers.

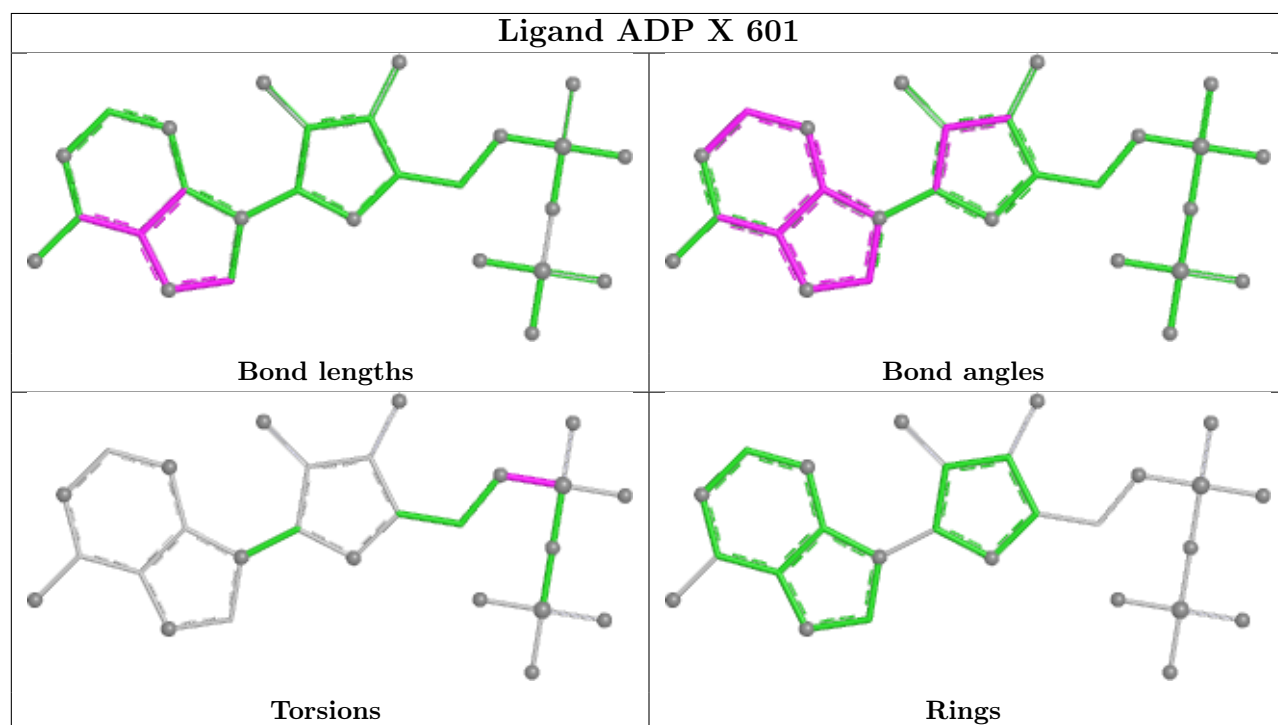
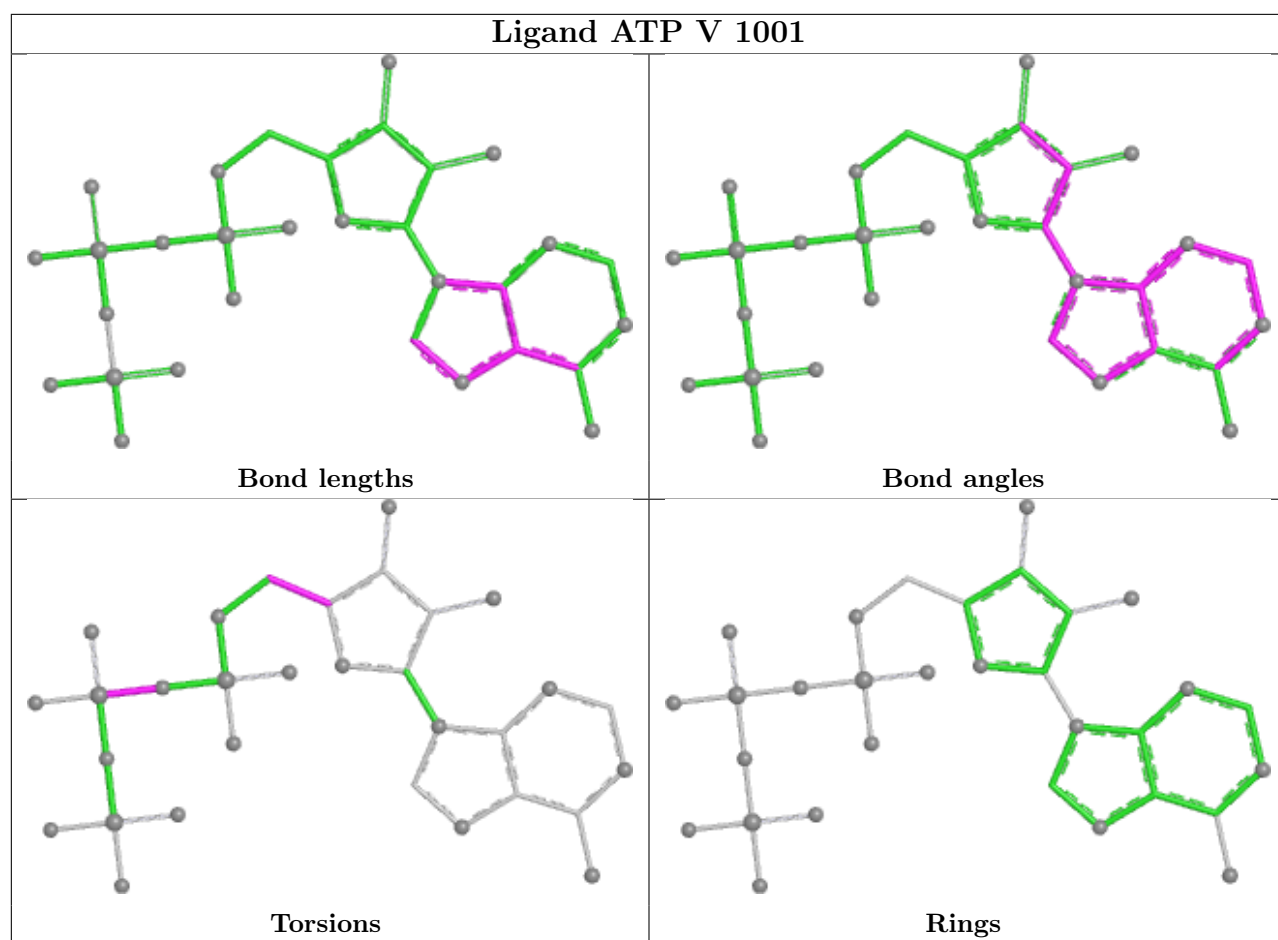
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	U	1001	ATP	1	0
8	T	1001	ATP	1	0
8	V	1001	ATP	1	0
10	X	601	ADP	3	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 than 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	126:PHE	C	127:ALA	N	3.47

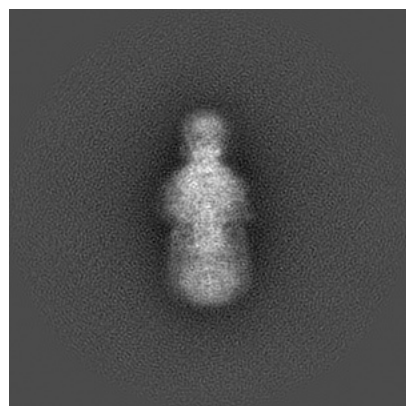
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4857. These allow visual inspection of the internal detail of the map and identification of artifacts.

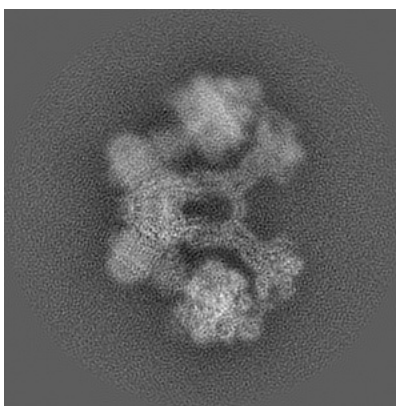
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

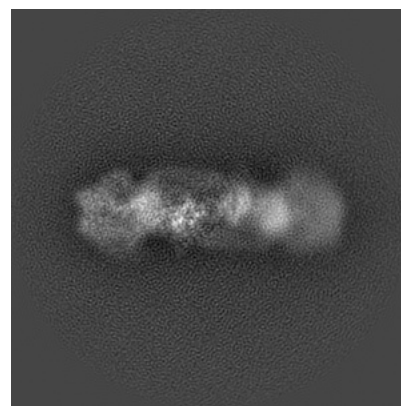
6.1.1 Primary map



X

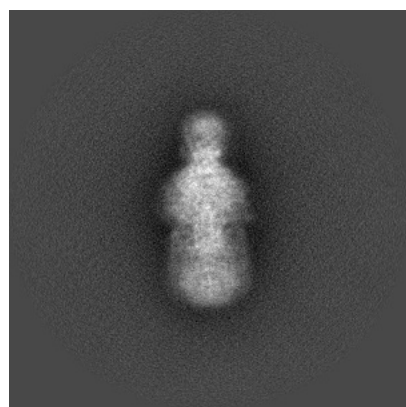


Y

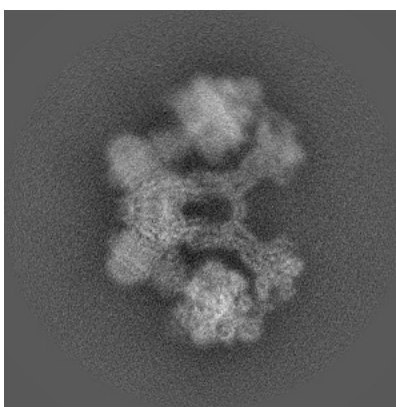


Z

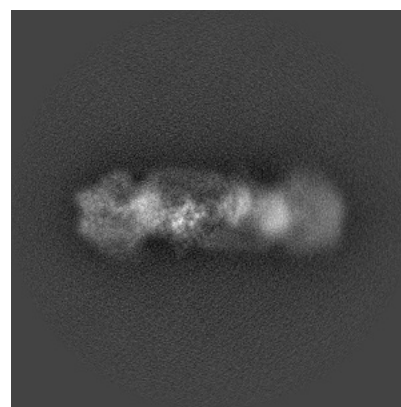
6.1.2 Raw map



X



Y

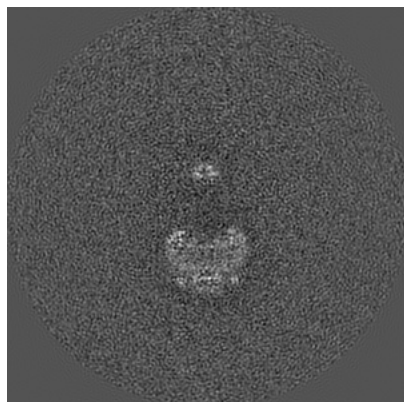


Z

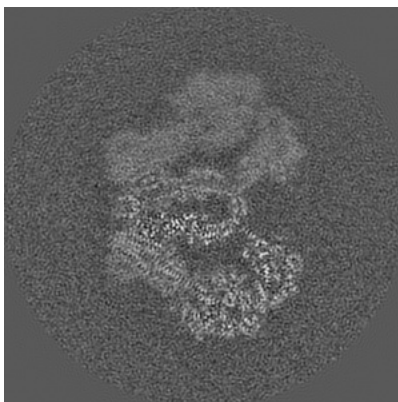
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

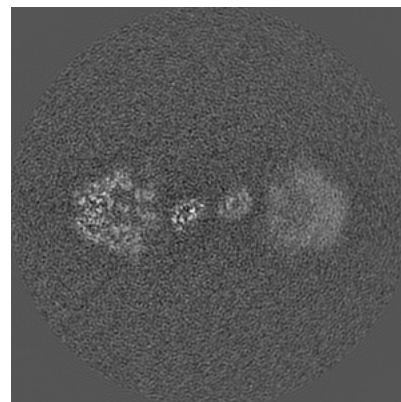
6.2.1 Primary map



X Index: 240

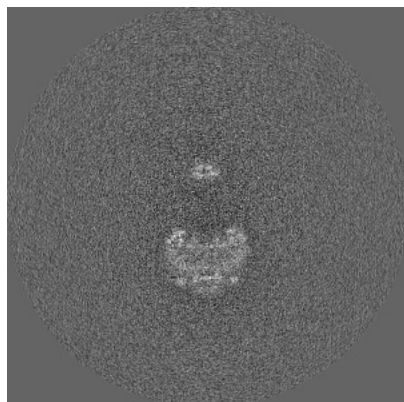


Y Index: 240

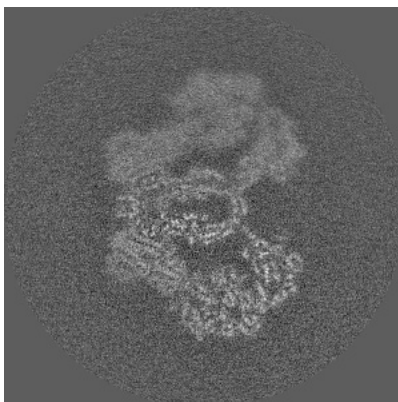


Z Index: 240

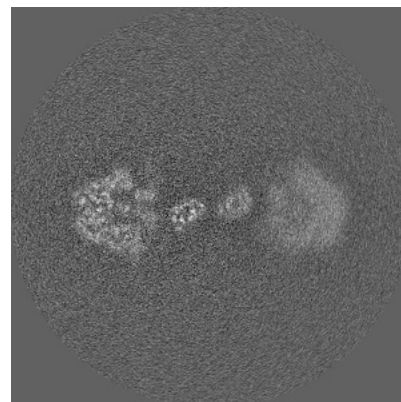
6.2.2 Raw map



X Index: 240



Y Index: 240

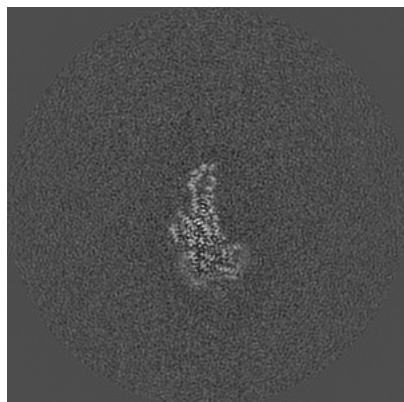


Z Index: 240

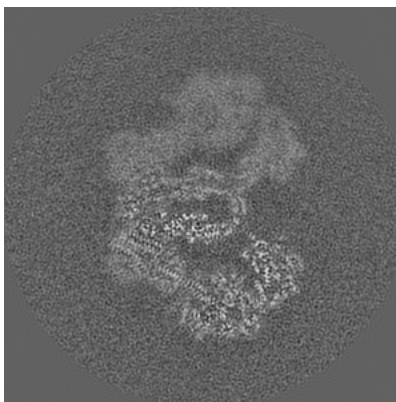
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

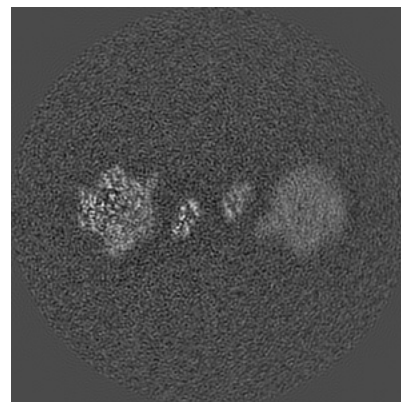
6.3.1 Primary map



X Index: 216

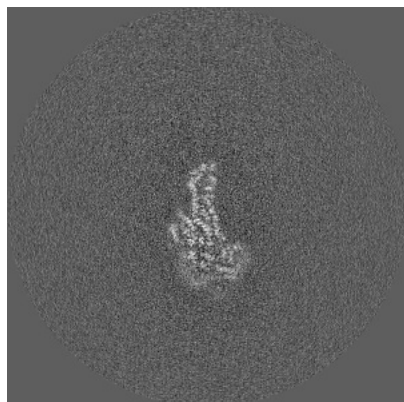


Y Index: 241

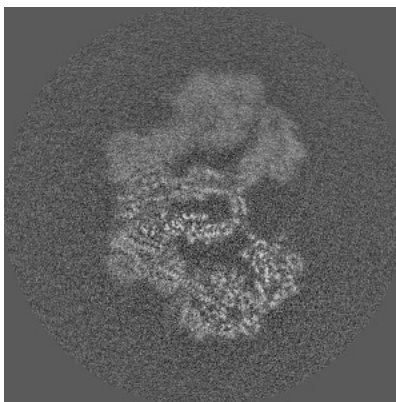


Z Index: 263

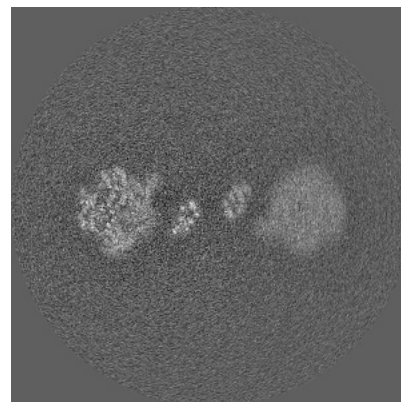
6.3.2 Raw map



X Index: 216



Y Index: 241

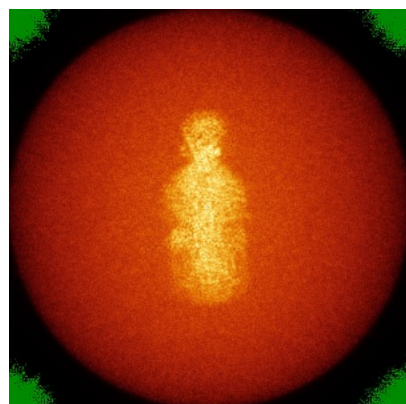


Z Index: 262

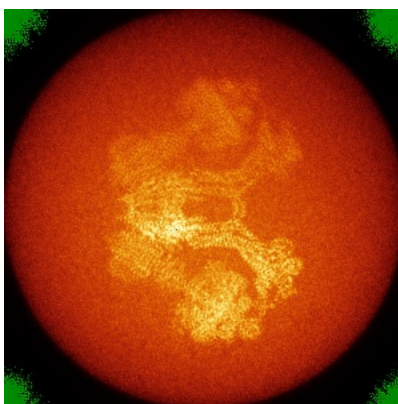
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

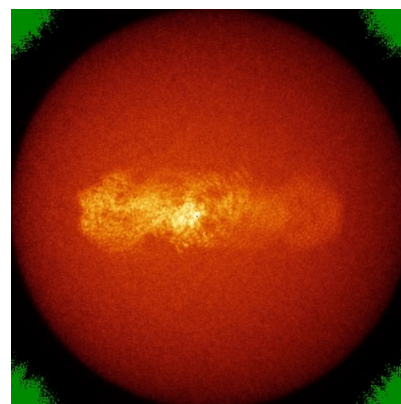
6.4.1 Primary map



X

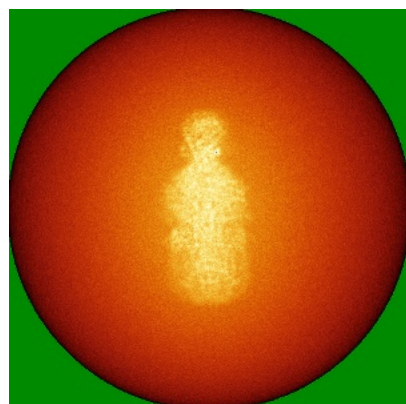


Y

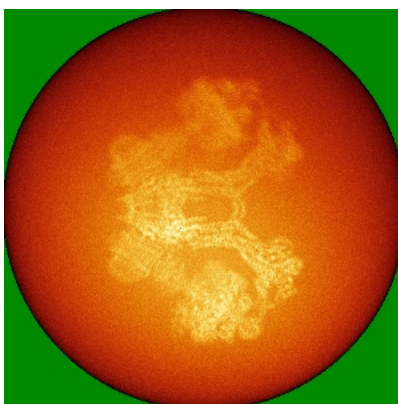


Z

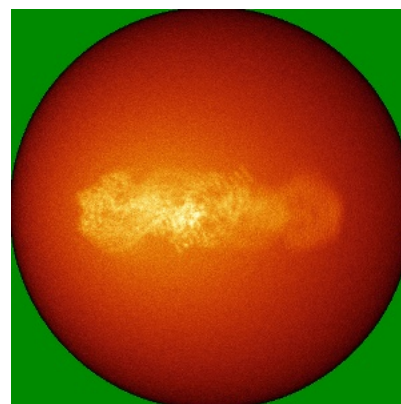
6.4.2 Raw map



X



Y

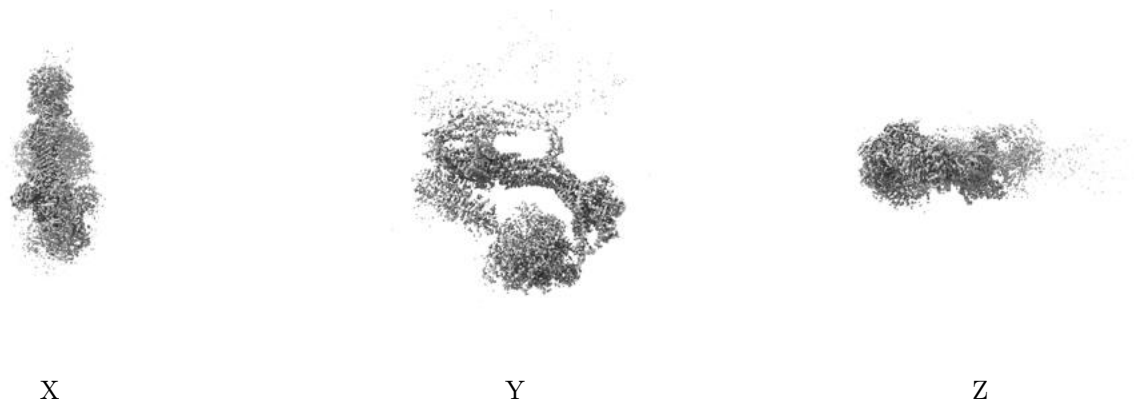


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

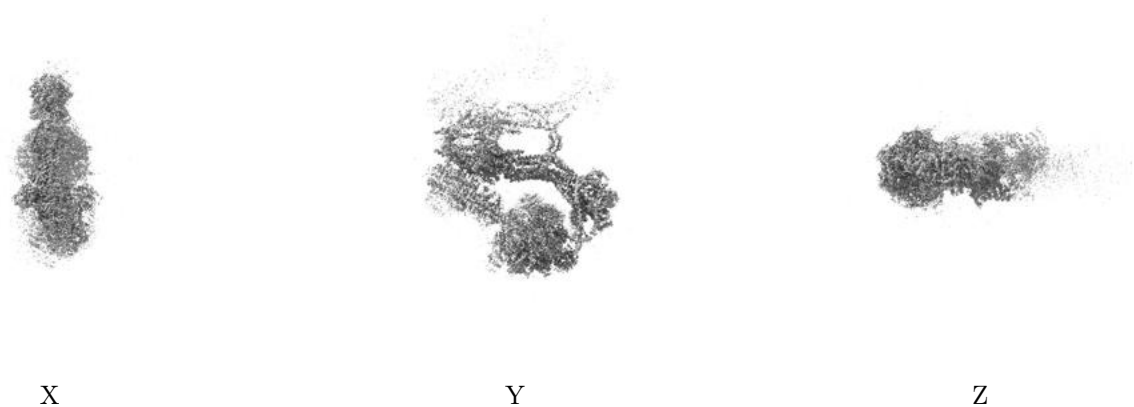
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

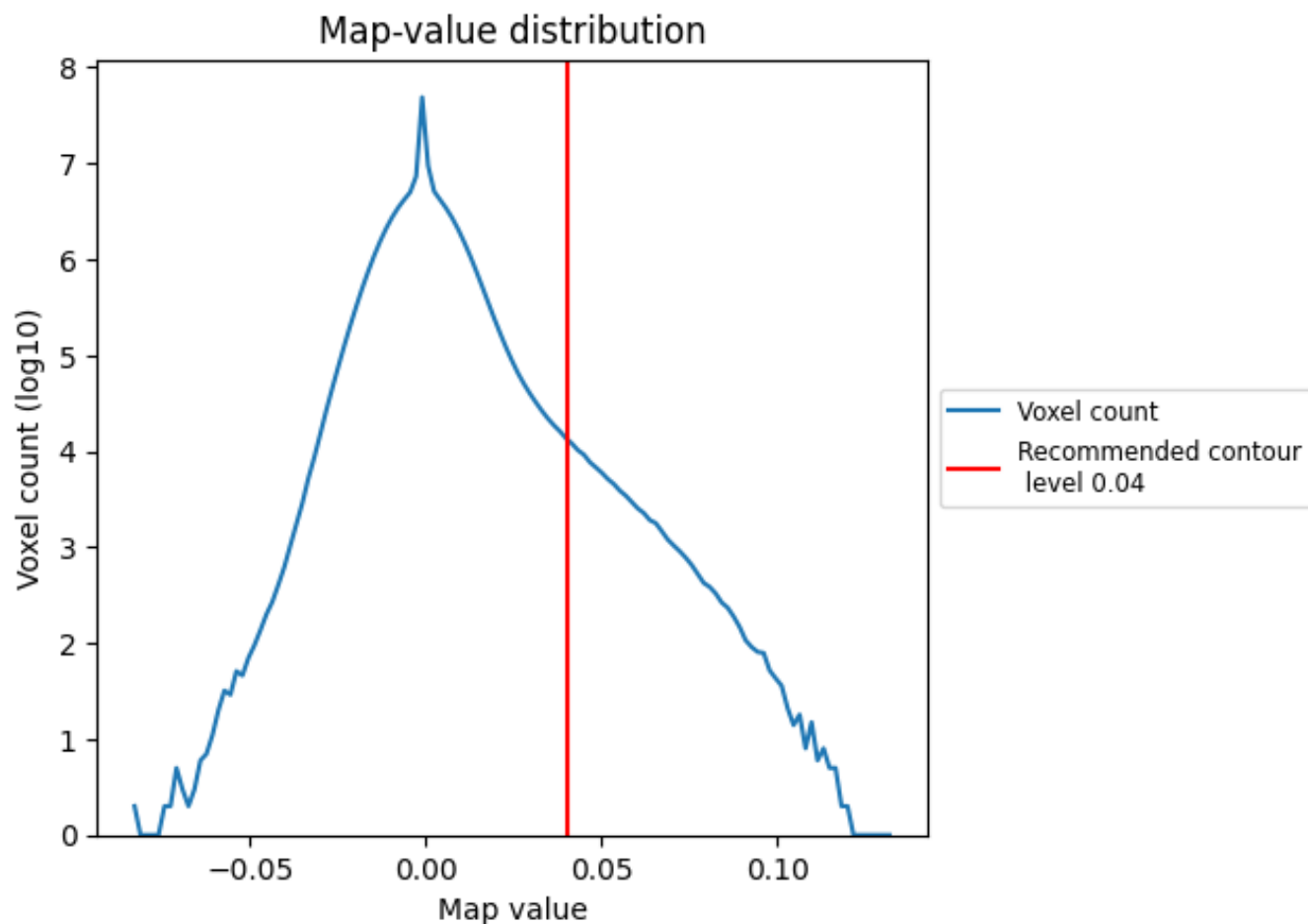
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

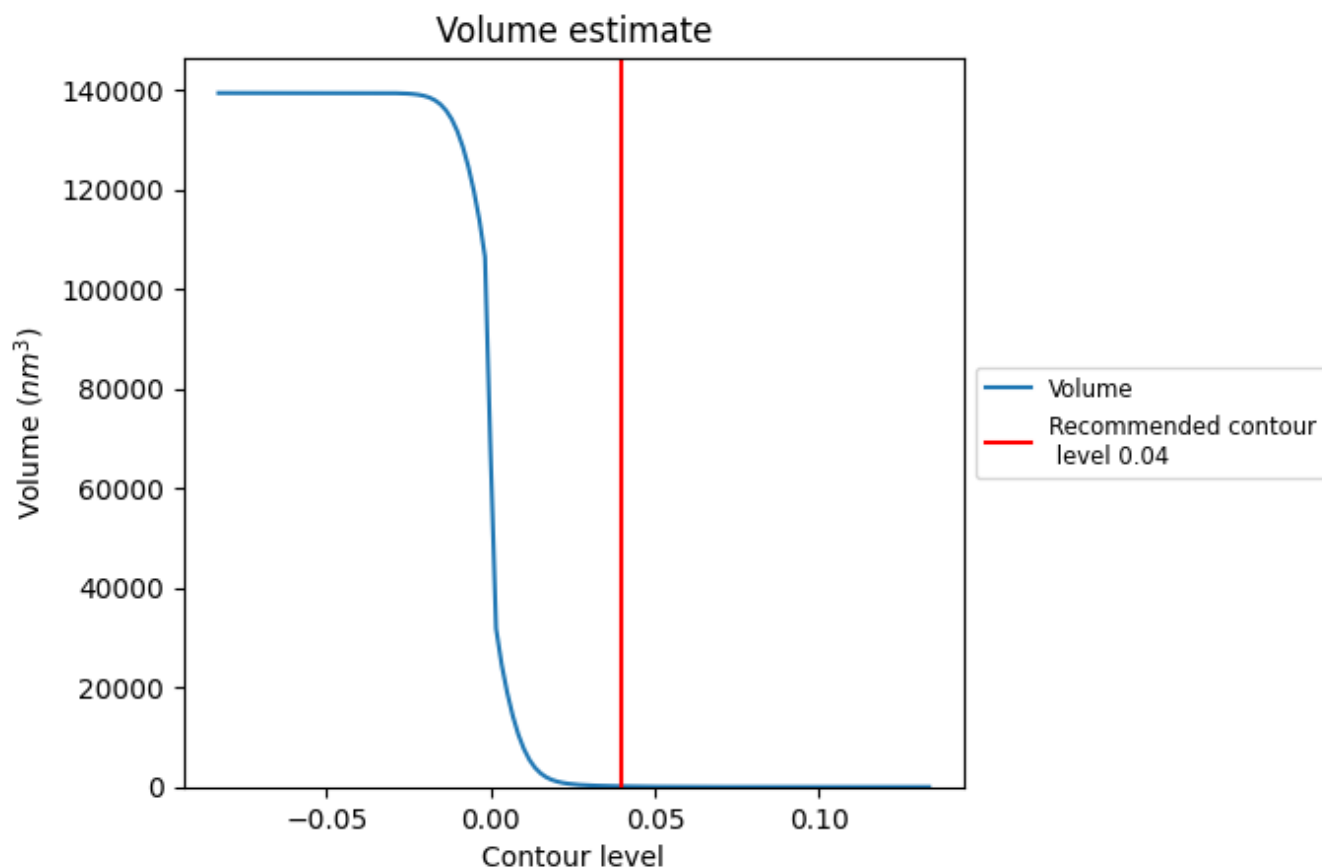
This section contains the results of statistical analysis of the map.

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.

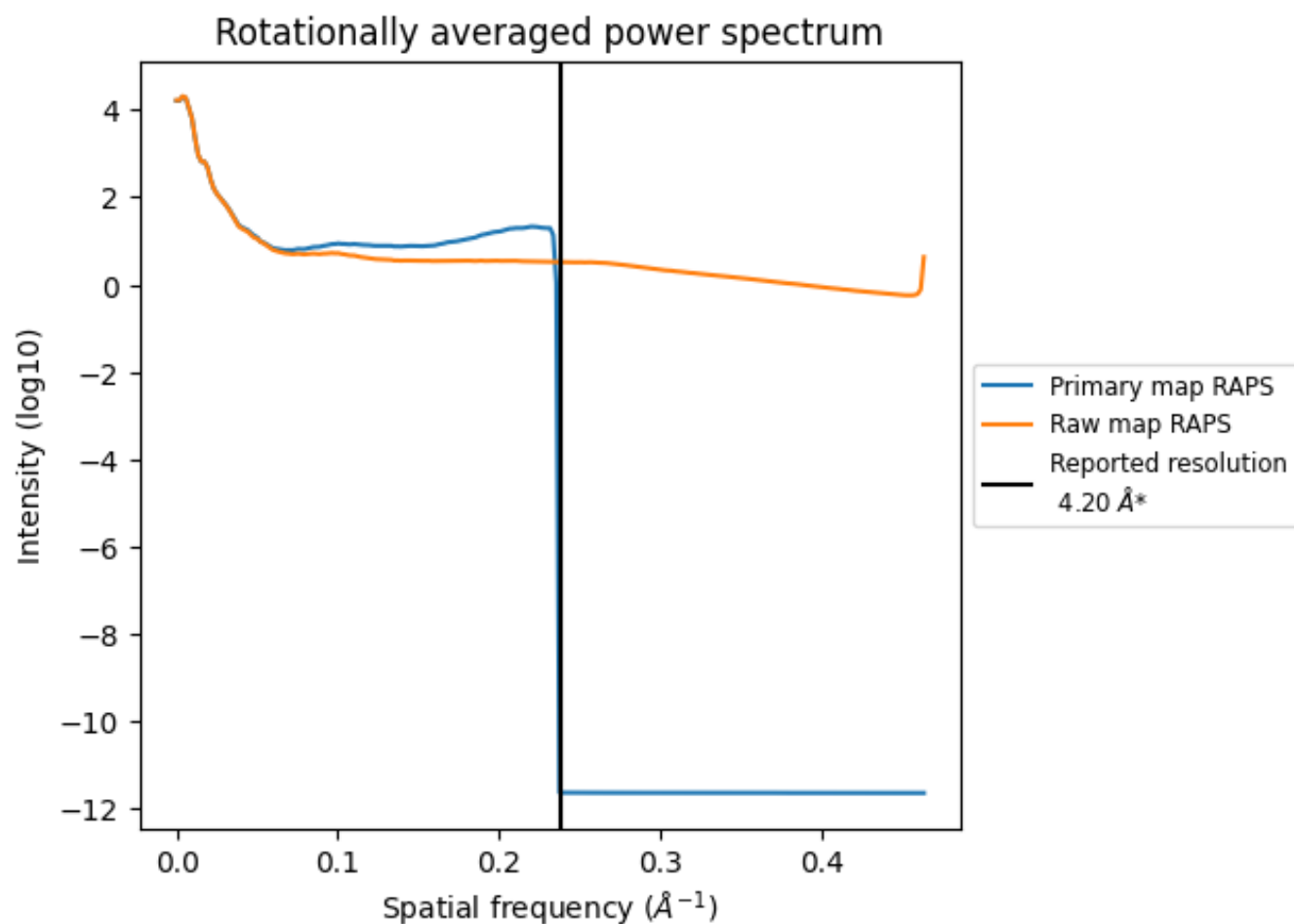
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 129 nm³; this corresponds to an approximate mass of 116 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 ⓘ

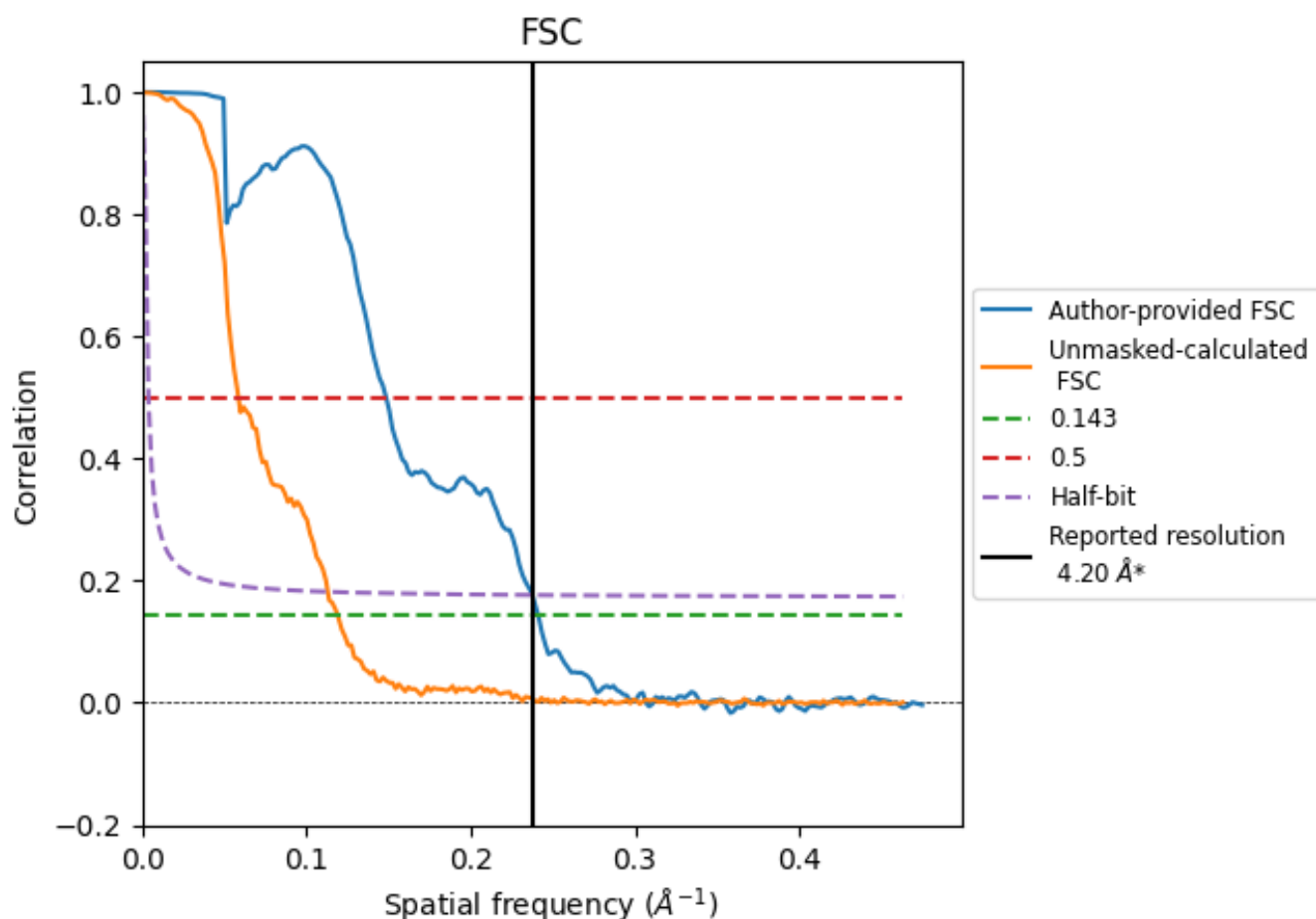


*Reported resolution corresponds to spatial frequency of $0.238 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

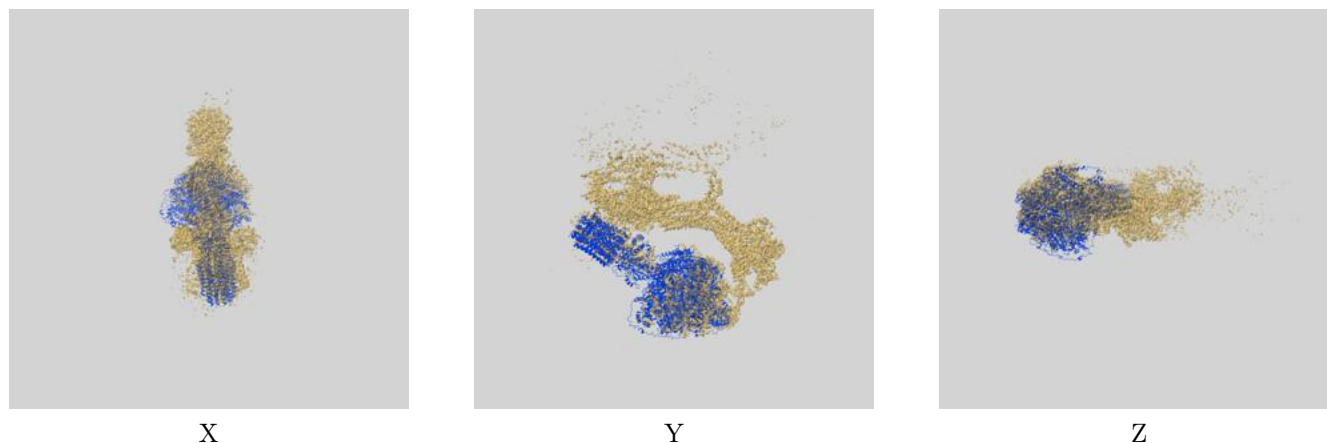
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.15	6.74	4.21
Unmasked-calculated*	8.41	17.09	8.85

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.41 differs from the reported value 4.2 by more than 10 %

9 Map-model fit [i](#)

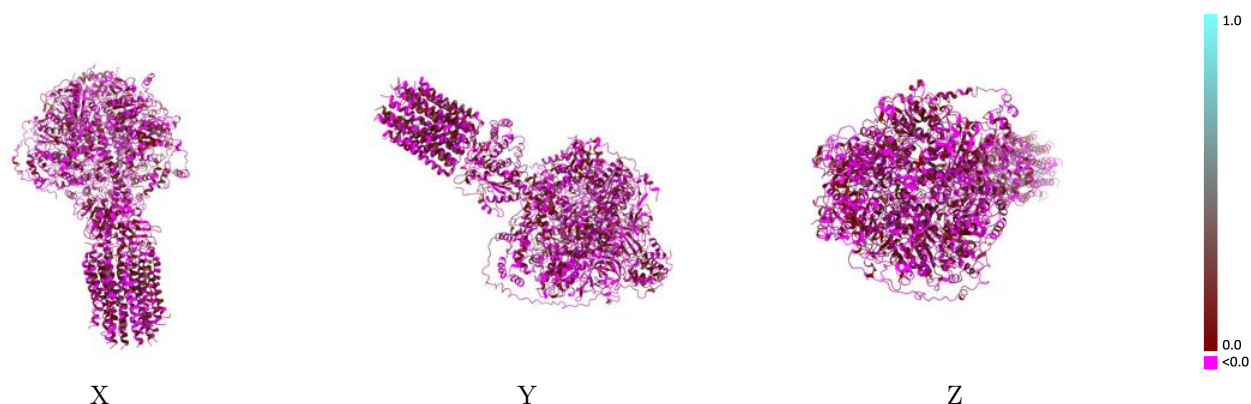
This section contains information regarding the fit between EMDB map EMD-4857 and PDB model 6REU. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.04 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](#)

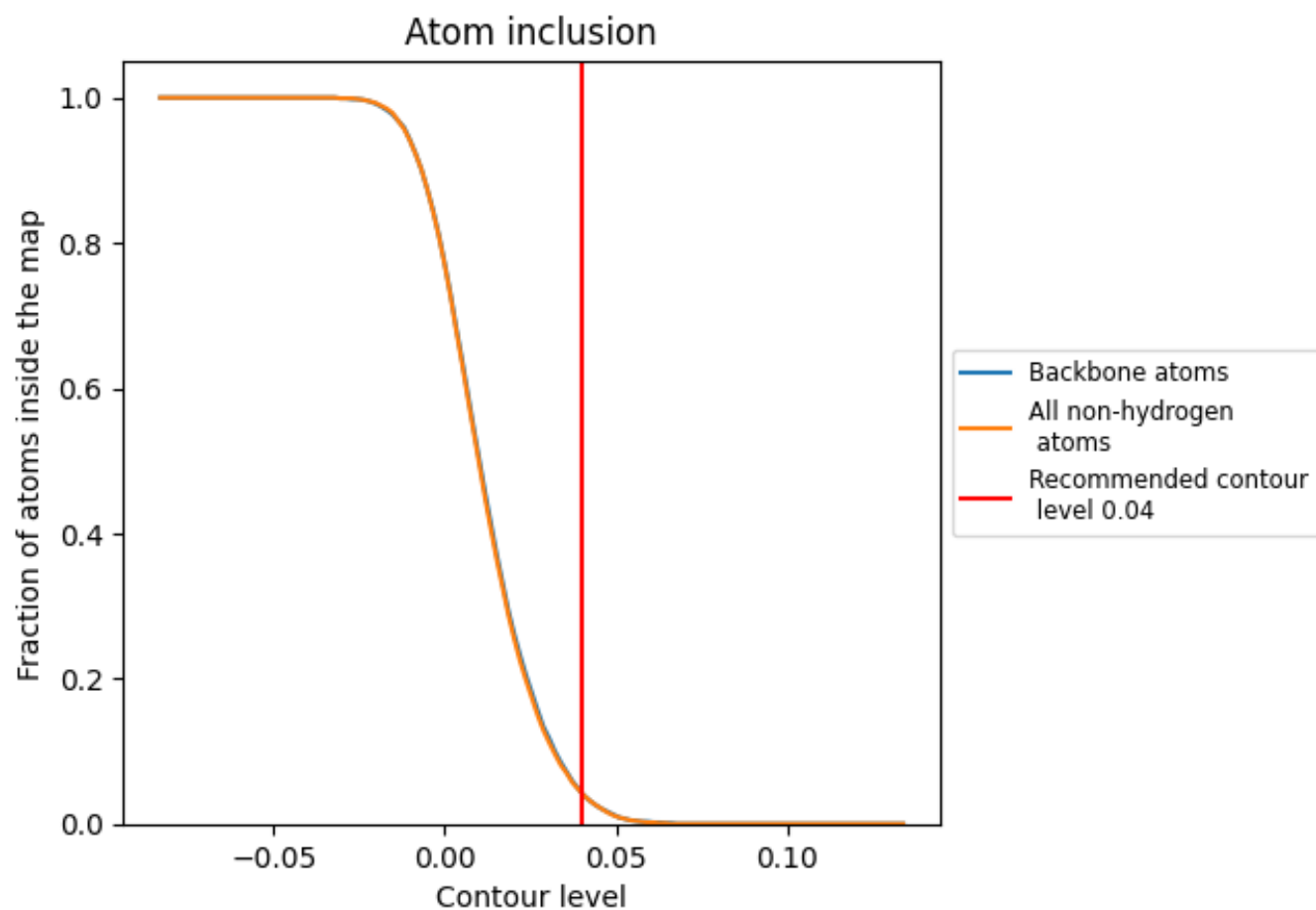


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 4% of all backbone atoms, 4% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.0420	 0.0020
A	 0.0120	 0.0220
B	 0.0140	 0.0290
C	 0.0100	 -0.0090
D	 0.0550	 0.0640
E	 0.0370	 -0.0400
F	 0.0590	 0.0880
G	 0.0630	 0.0190
H	 0.0650	 0.0090
I	 0.0120	 -0.0100
J	 0.0040	 0.0310
P	 0.0910	 0.0200
Q	 0.0170	 0.0020
R	 0.0420	 0.0160
S	 0.0290	 -0.0030
T	 0.0490	 -0.0040
U	 0.0330	 -0.0020
V	 0.0490	 -0.0200
X	 0.0190	 -0.0030
Y	 0.0760	 0.0270
Z	 0.0360	 -0.0150

