wwPDB EM Validation Summary Report (i)

Feb 13, 2024 – 01:55 AM EST

PDB ID	:	3IYG
EMDB ID	:	EMD-5148
Title	:	Ca model of bovine TRiC/CCT derived from a 4.0 Angstrom cryo-EM map
Authors	:	Cong, Y.; Baker, M.L.; Ludtke, S.J.; Frydman, J.; Chiu, W.
Deposited on	:	2009-11-28
Resolution	:	4.00 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 (i)) were used in the production of this report:

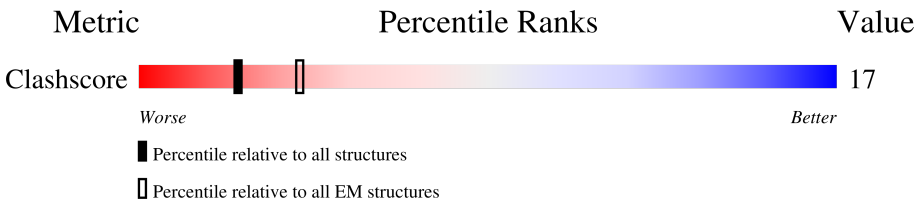
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.00 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

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	Q	512	47% 97% .
2	G	515	50% 98% .
3	Z	517	51% 97% .
4	D	518	47% 96% .
5	B	513	48% 95% 5%
6	E	515	50% 97% .
7	A	529	55% 98% .
8	H	515	50% 98% .

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 4134 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 T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
1	Q	512	512	512	0	512

- Molecule 2 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
2	G	515	515	515	0	515

- Molecule 3 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
3	Z	517	517	517	0	517

- Molecule 4 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
4	D	518	518	518	0	518

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	134	VAL	GLU	conflict	UNP Q2T9X2
D	486	LEU	GLN	conflict	UNP Q2T9X2

- Molecule 5 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
5	B	513	513	513	0	513

- Molecule 6 is a protein called T-complex protein 1 subunit.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
6	E	515	515	515	0	515

- Molecule 7 is a protein called T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
7	A	529	529	529	0	529

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	440	LEU	PRO	conflict	UNP Q32L40

- Molecule 8 is a protein called T-complex protein 1 subunit eta.

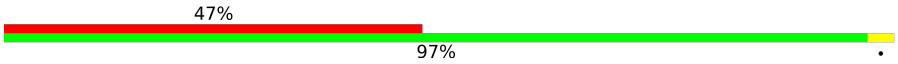
Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
8	H	515	515	515	0	515

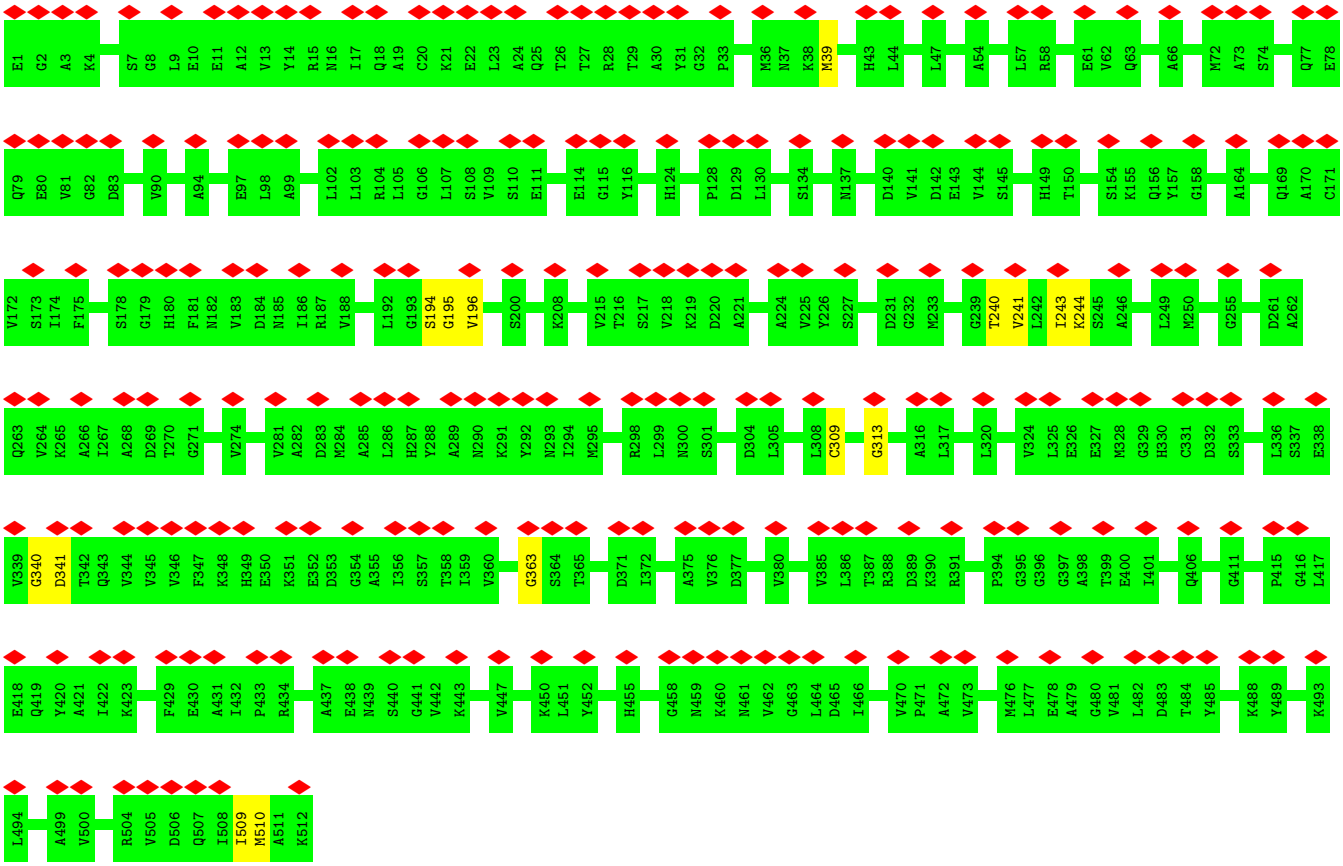
3 Residue-property plots (i)

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: T-complex protein 1 subunit theta

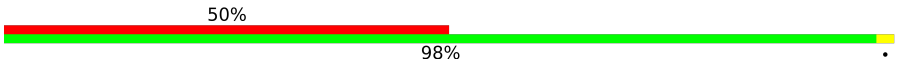
Chain Q:

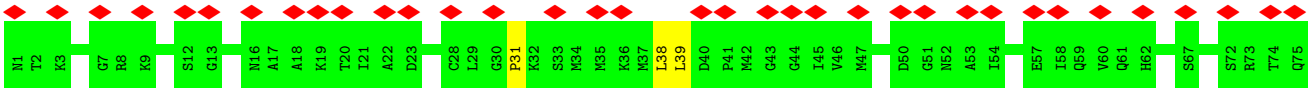


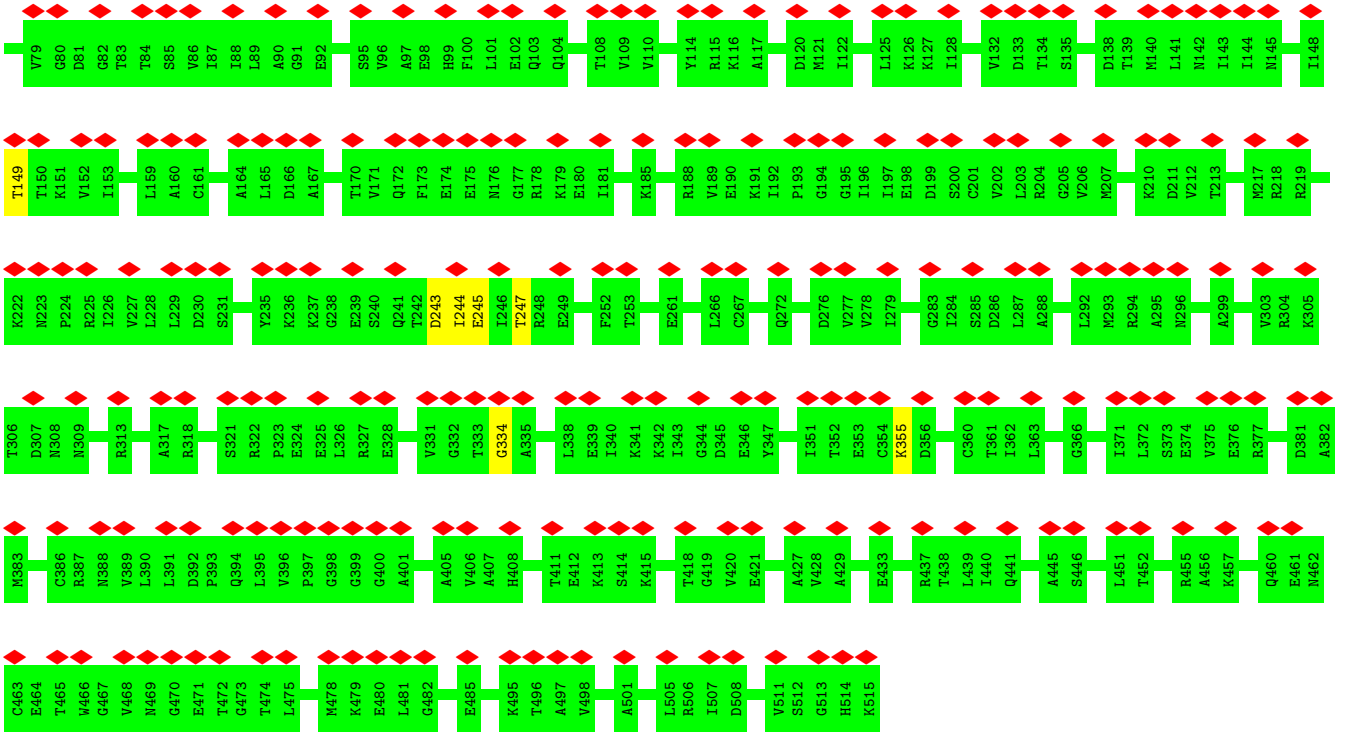


• Molecule 2: T-complex protein 1 subunit gamma

Chain G:

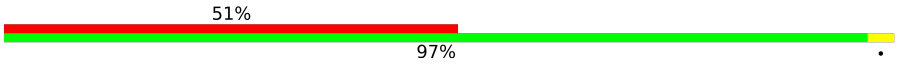


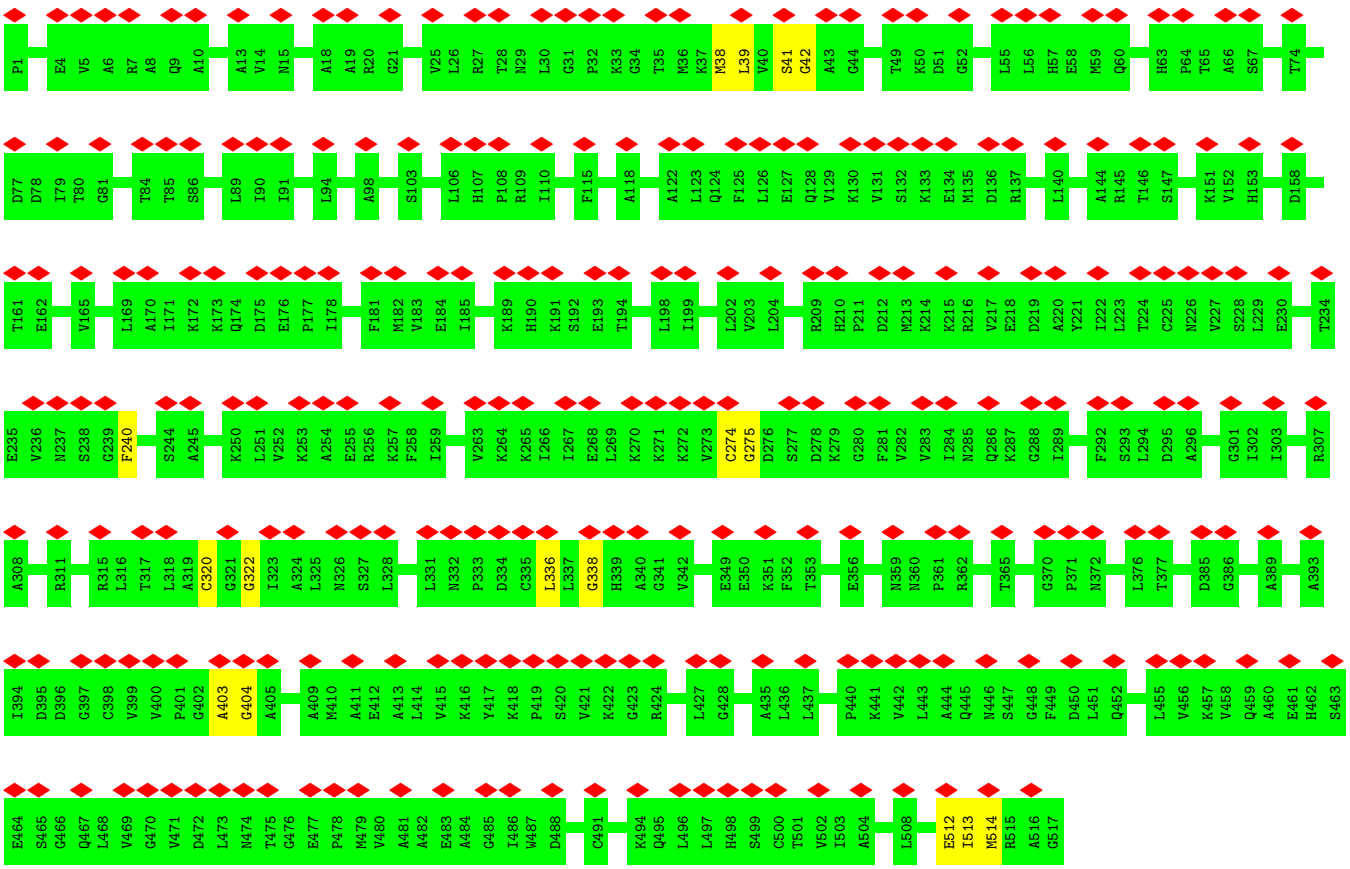




- Molecule 3: T-complex protein 1 subunit zeta

Chain Z:





• Molecule 4: T-complex protein 1 subunit delta

Chain D: 47% 96%

S1 A2 Y3 Q4 D5 R6 P9 A10 R13 N16 I17 S18 A19 D25 A26 I27 R28 T29 K34 G35 M36 D37 K38 M39 I40 Q41 D42 G43 K44 G45 I49 T50 N51 D52 G53 A54 T55 I56 L57 K58 Q59 A67 L73 S74 K75 A76 Q77 D78 I79 E80 A81 G82

D83 G84 V88 V89 I90 I91 A92 C99 T100 K101 L102 L103 G106 I107 H108 P109 T110 I111 I112 S113 E114 K122 G123 I124 L127 T128 D129 M130 L136 S137 D138 R139 E140 T141 L142 L143 N144 S145 T148 S152 K153 Q157 Y158 S159 P164 D168 V173 I174

D175 P176 A177 T178 A179 T180 S181 V182 D183 L184 R185 D186 I187 V190 K191 K192 L193 G194 G195 T196 D199 L202 V203 E204 G205 L206 V207 L208 K211 V212 A213 G216 I217 T218 R219 V220 A223 K224 L227 F230 C231 L232 S233 A234 P235 K236 T237 D238 M239 D240 I243

V244 V245 S246 D247 Y248 V249 Q250 M251 D252 R253 V254 L255 R256 E257 E258 R259 A260 Y261 I262 L263 N264 L265 V266 K267 K270 K271 T272 G273 C274 L278 I279 Q280 K281 S282 D286 A287 L288 S289 A292 L293 L296 N297 K298 M299 K300 I301 M302 V303 I307 E308 R309 E310 D311 I312

E313 F314 I315 C316 K317 T318 I319 G320 T321 K322 P323 V324 V327 T331 A332 D333 M334 L335 A338 E342 E343 V344 S345 L346 N347 K351 T356 G357 C358 A359 S360 P361 T364 I367 V368 V369 R370 G371 S372 N373 V376 I377 E381 R382 D386 V390 K396

A399 A402 G405 A406 E410 L411 R414 L415 T416 E417 L422 S423 G424 M425 E426 S427 I430 R431 A432 F433 A436 M437 E438 V439 S442 A448 G449 L450 I453 R460 N461 R462 H463 A464 Q465 G466 E467 K468 T469 T470 G471 I472 M473 V474 R475 K476 I482

L483 E484 V487 V488 Q489 P490 S494 L498 T499 L500 A501 T502 E503 T504 S507 K510 I511 D512 D513 V514 V515 N516 T517 R518

• Molecule 5: T-complex protein 1 subunit beta

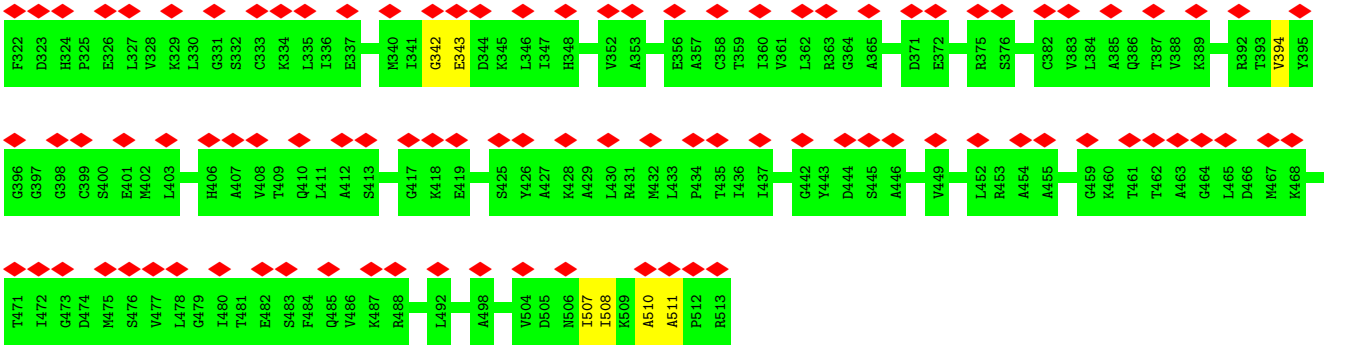
Chain B: 48% 95% 5%

A1 G2 A3 D4 E5 E6 A11 S14 S15 F16 A19 I20 A21 I22 G23 V26 K27 G31 P32 K33 D36 K37 I38 L39 S42 G43 R44 S47 L48 M49 V50 T51 N52 D53 G54 A55 T56 I57 L58 P66 A67 A68 K69 V70 L71 V72 D73 M74 S75 D79

D80 E81 V82 G83 D84 G85 S88 V89 L92 A93 A94 R98 E101 S102 L103 I104 A105 K106 K107 I114 A115 G116 W117 R118 E119 A120 A123 A124 R125 V133 E139 V140 D145 L146 M147 A150 G151 T152 T153 L154 S155 S156 K157 T160 H161 H162 K163 D164 H165

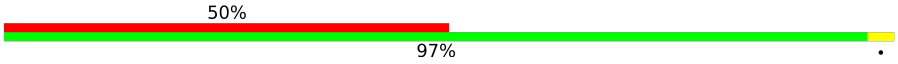
F166 T167 K168 L169 A170 V171 E172 A173 V174 L175 R176 L177 K178 G179 S180 G181 N182 L183 E184 A185 I186 H187 V188 I189 K190 K191 G194 A197 D198 S199 D202 E203 G204 F205 K210 Q215 P216 I219 E220 N221 A222 K223 I224 L225 I226 T229 G230 M231 D232 K235 I236 K237

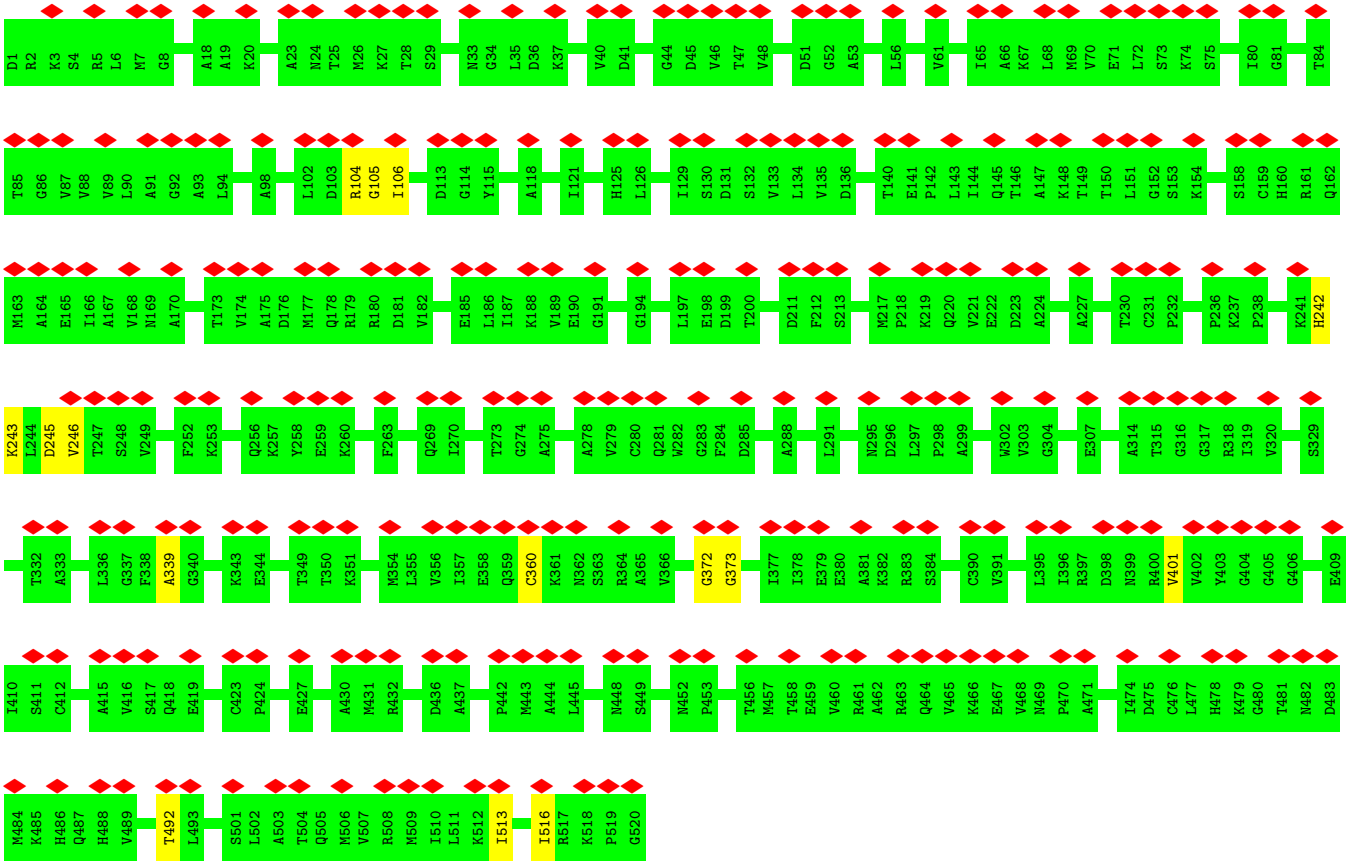
I238 F239 G240 S241 R242 V243 R244 V245 V251 I254 E260 K265 R268 I269 L270 K271 H272 G273 I274 N275 C276 F277 R280 I283 Y284 N285 Y286 P287 E288 Q289 L290 F291 G292 A293 E300 H301 A302 V305 R309 L312 V313 T314 G315 G316 E317 I318 A319 S320 T321



- Molecule 6: T-complex protein 1 subunit

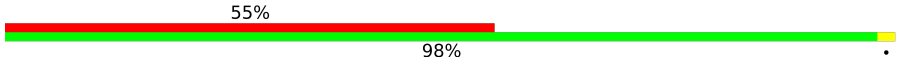
Chain E:

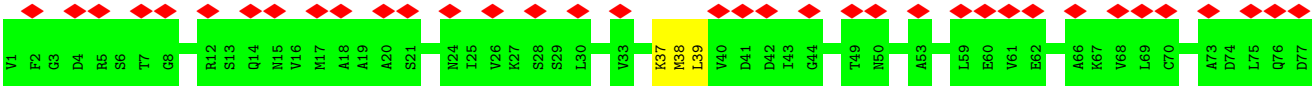




- Molecule 7: T-complex protein 1 subunit alpha

Chain A:





V80 G81 D82 G83 S86 V87 V88 I89 I90 L95 K96 N97 A98 V102 K103 Q104 S110 Y115 C119 K120 E121 A122 V123 I126 S127 E128 N129 L130 I131 I132 N133 T134 D135 E136 L137 G138 R139 D140 C141 L142 A146 K147 T148 S149 M150 S151 S152 K153 V154 I155

N158 G159 D160 F161 F162 A163 V166 V167 D168 A169 A172 I173 K174 Y175 T176 D177 Q181 P182 R183 Y184 P185 V186 N187 S188 I189 N190 R197 S198 Q199 M200 E201 S202 M203 L204 I205 N206 G207 Y208 A209 C212 V213 V214 G215 S216 Q217 G218 K221 R222 I223 V224 N225 A226 L231

L235 Q236 K237 T238 K239 M240 K241 L242 G243 V247 I248 K253 L254 D255 Q256 Q259 D263 E267 R268 I269 Q270 A274 T275 G276 A277 N278 V279 I280 L281 T282 T283 G284 D287 L291 K292 G298 A299 M300 A301 V302 V305 D309 I313 A314 K315 A316 S317

G318 A319 T320 V321 L322 S323 T324 L325 A326 N327 L328 E329 G330 E331 E332 T333 F334 E335 A336 S337 M338 L339 G340 Q341 A342 E343 E344 V345 V346 Q347 E348 R349 I350 C351 D352 D353 E354 L355 I356 K359 N360 T361 K362 T365 S366 A367 S368 L371 R372 G373 D376 F377 M378 E381 M382

E383 H387 D388 C391 V392 V393 K394 R395 V396 S399 K400 S401 G406 V409 E410 A411 A412 L413 S414 L417 E418 N419 T422 S423 M424 G425 S426 R427 L430 A431 I432 A433 E434 R437 S438 L439 N444 T445 L446 A447 V448 N449 A450 A451 Q452 D453 V458 R462

A463 F464 H465 A468 Q469 V470 N471 P472 E473 R474 K475 N476 L477 G481 L482 D483 G487 K488 P489 R490 D491 N492 K493 Q494 A495 G496 V497 F498 E499 P500 T501 I502 V503 K506 S507 L508 K509 F510 A511 T512 E513 A514 T517 I518 L519 R520 I521 D522 I525 K526 L527 H528 P529

- Molecule 8: T-complex protein 1 subunit eta

Chain H: 50% 98%

K1 E2 G3 T4 D5 S6 S7 Q8 G9 I10 S15 N16 I17 S18 A19 C20 I23 A24 E25 A26 V27 R28 T29 T30 L31 G32 P33 R34 G35 M36 D37 I40 V41 D42 G45 K46 A47 S50 N51 D52 G53 L57 L60 D61 V62 V63 H64 T69 L70 V71 D72 I73

S76 V81 G82 D83 G84 T85 T86 S87 V88 T89 L90 L91 A92 A93 K97 Y102 V103 E104 E105 G106 L107 I111 A115 F116 R117 T118 A119 A123 V124 N125 K126 I127 K128 E129 I130 A131 V132 T133 V134 K135 K136 E137 Q142 R143 K144 K148 C149 A150 M151 T152 A153

S156 S160 Q161 A164 F165 F166 A167 K168 M169 V170 V171 M175 M176 L177 D178 D179 L180 L181 Q182 G187 I188 K189 K190 V191 Q192 E197 E198 S199 Q200 L201 V202 A203 A206 F207 K208 K209 A214 G215 Q219 P220 K221 K222 Y223 H224 N225 P226 M227 I228 A229 E234

L235 E236 A239 A244 E245 I246 T250 V251 E252 D253 Y254 Q255 A256 I257 V258 D259 A260 N263 I264 L265 L269 E270 K271 H274 S275 G276 A277 K278 V279 V280 L284 P285 I286 G287 D288 V289 A290 T291 Q292 Y293 F294 A295 D298 M299 F300 C301 A302 G303 R304 V305 P306 E307

E308 D309 L310 M314 M315 G318 T323 N326 S330 D331 V332 L333 G334 R335 G336 Q337 V338 F339 R348 Y349 N350 G354 G355 P356 K357 A358 K359 T360 L365 R366 G367 G368 F372 M373 T376 E377 R378 S379 A383 I384 M385 I386 A390 I391 V396 V397 A398

G401 A402 I403 E404 M405 E406 L407 S408 L411 I418 P419 G420 K421 Q422 Q423 L424 L425 I426 G427 A428 L433 E434 I435 I436 P437 D442 N443 A444 G445 F446 D447 A448 N453 K454 L455 R456 H459 A460 Q461 G462 G463 G467 N471 T472 E473 D474 I475 N478 F479 E480

A481 F482 V483 W484 E485 P486 A487 I491 N492 A493 L494 S498 E499 A500 A501 C502 V505 S506 V507 T510 I511 K512 N513 P514 R515

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	101000	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	each micrograph	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	18	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	7.456	Depositor
Minimum map value	-3.019	Depositor
Average map value	0.055	Depositor
Map value standard deviation	0.377	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	307.2, 307.2, 153.6	wwPDB
Map dimensions	256, 256, 128	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	Q	512	0	0	11	0
2	G	515	0	0	9	0
3	Z	517	0	0	15	0
4	D	518	0	0	17	0
5	B	513	0	0	21	0
6	E	515	0	0	12	0
7	A	529	0	0	9	0
8	H	515	0	0	7	0
All	All	4134	0	0	72	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 17.

The worst 5 of 72 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)
4:D:232:LEU:CA	4:D:288:LEU:CA	2.22	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:520:ARG:CA	8:H:36:MET:CA	2.25	1.14
3:Z:41:SER:CA	5:B:510:ALA:CA	2.26	1.13
1:Q:243:ILE:CA	4:D:243:ILE:CA	2.27	1.12
5:B:1:ALA:CA	5:B:511:ALA:CA	2.30	1.08

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

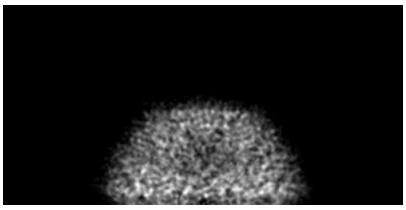
6 Map visualisation (i)

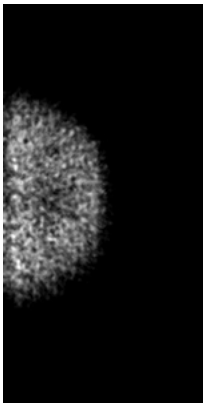
This section contains visualisations of the EMDB entry EMD-5148. These allow visual inspection of the internal detail of the map and identification of artifacts.

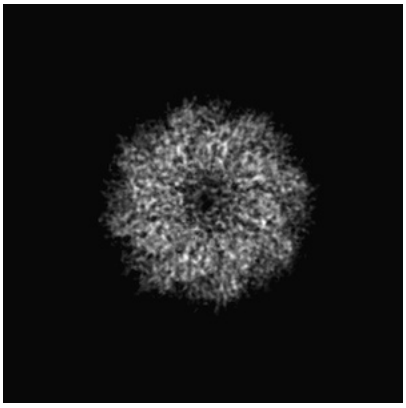
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

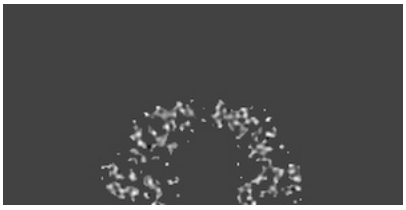

Y


Z

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

6.2 Central slices (i)

6.2.1 Primary map


X Index: 128

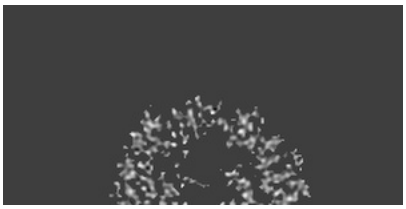
Y Index: 128

Z Index: 64

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: 116

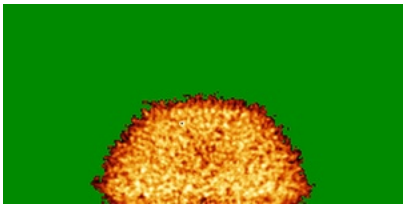
Y Index: 150

Z Index: 9

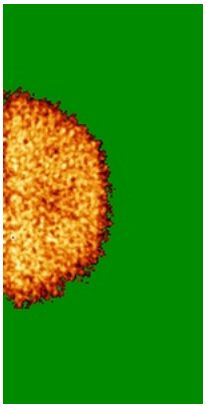
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

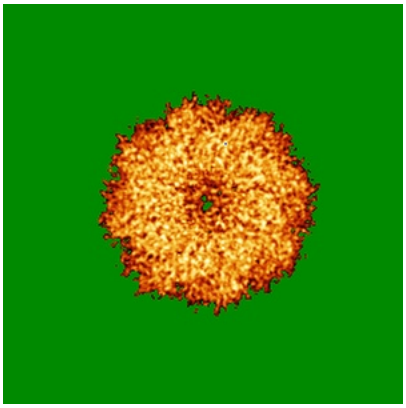
6.4.1 Primary map



X



Y



Z

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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

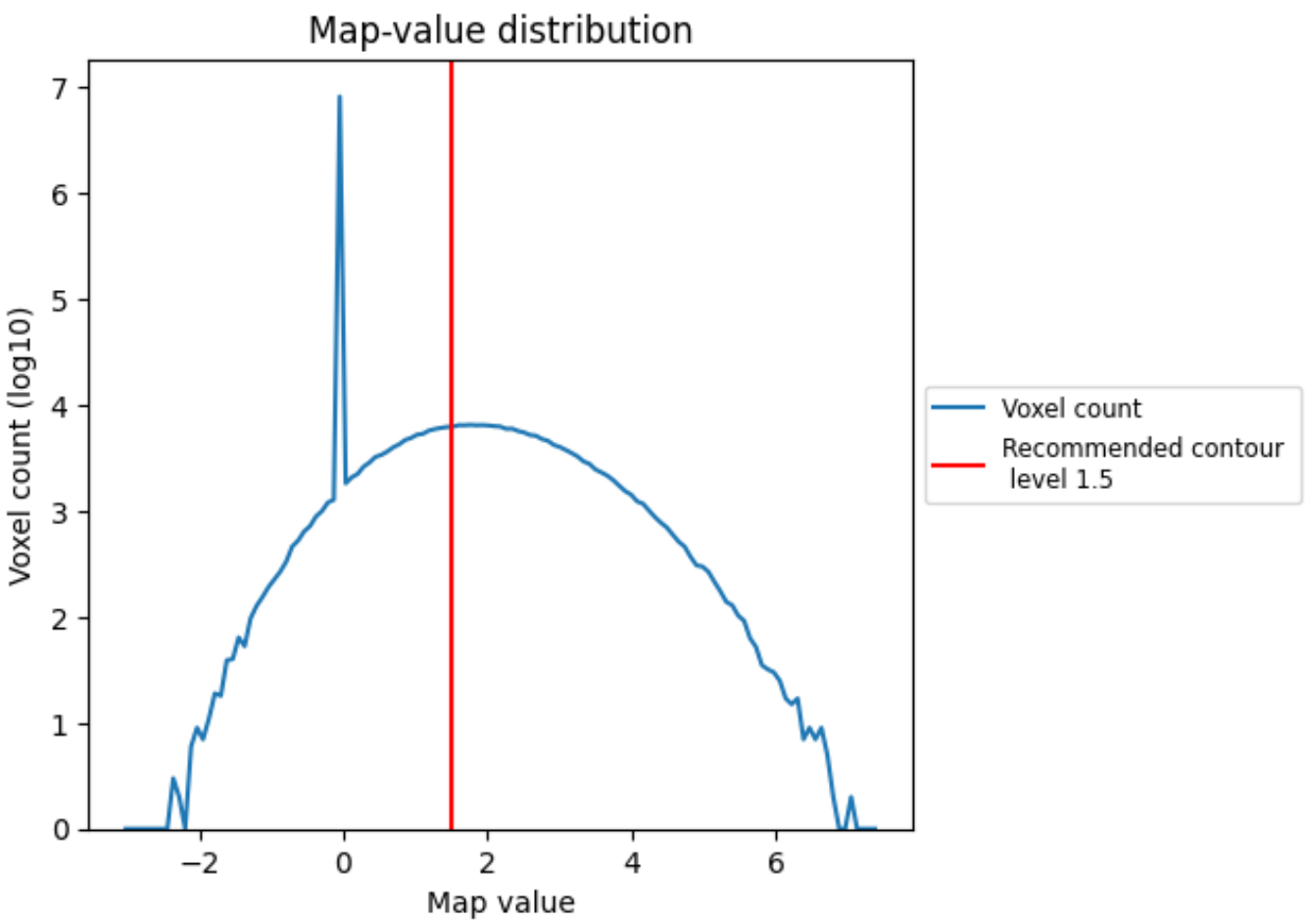
6.6 Mask visualisation (i)

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

7 Map analysis (i)

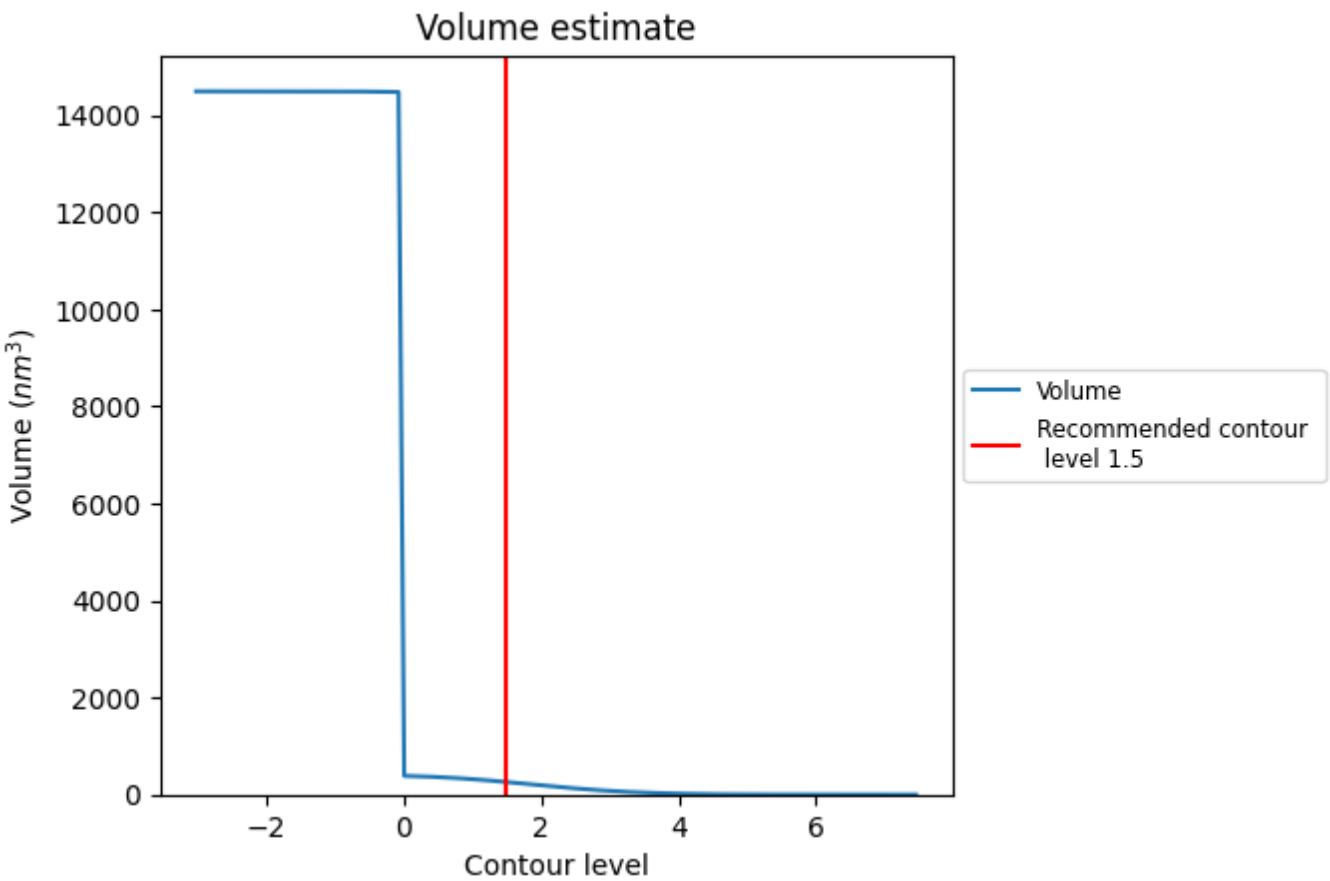
This section contains the results of statistical analysis of the map.

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 258 nm^3; this corresponds to an approximate mass of 233 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)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

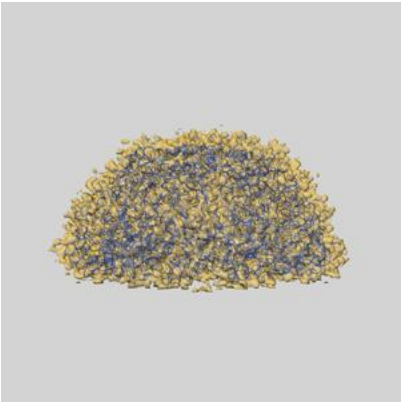
8 Fourier-Shell correlation (i)

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

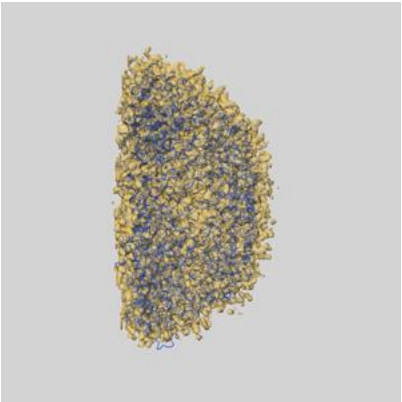
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-5148 and PDB model 3IYG. Per-residue inclusion information can be found in section 3 on page 5.

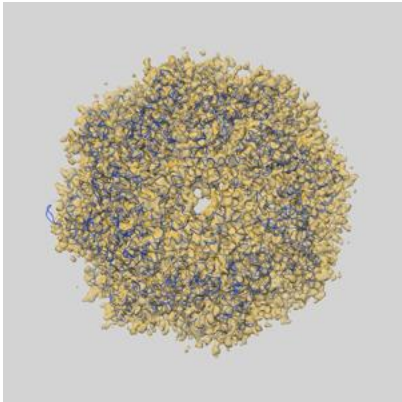
9.1 Map-model overlay (i)



X



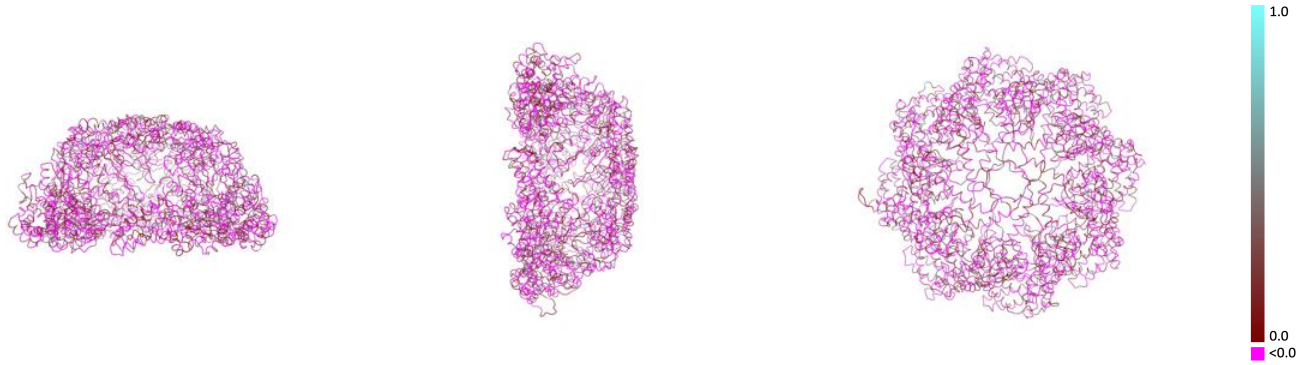
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.5 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.

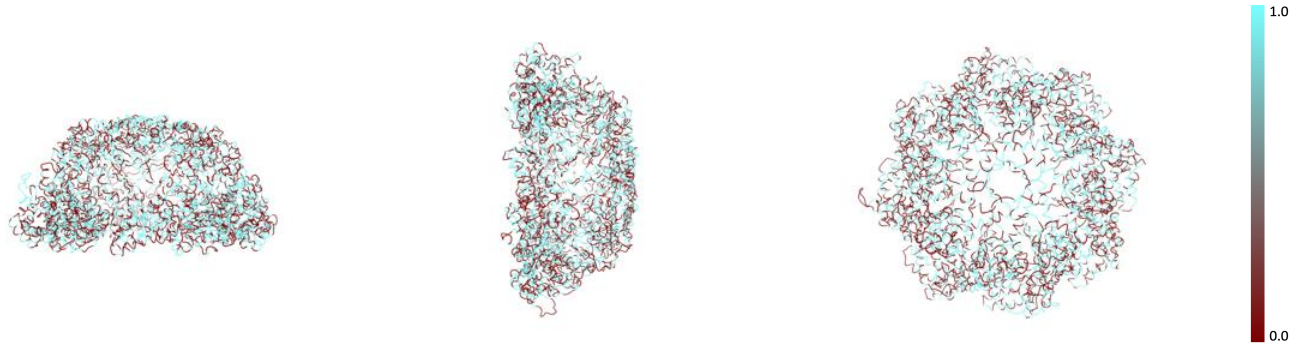
9.2 Q-score mapped to coordinate model (i)



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.

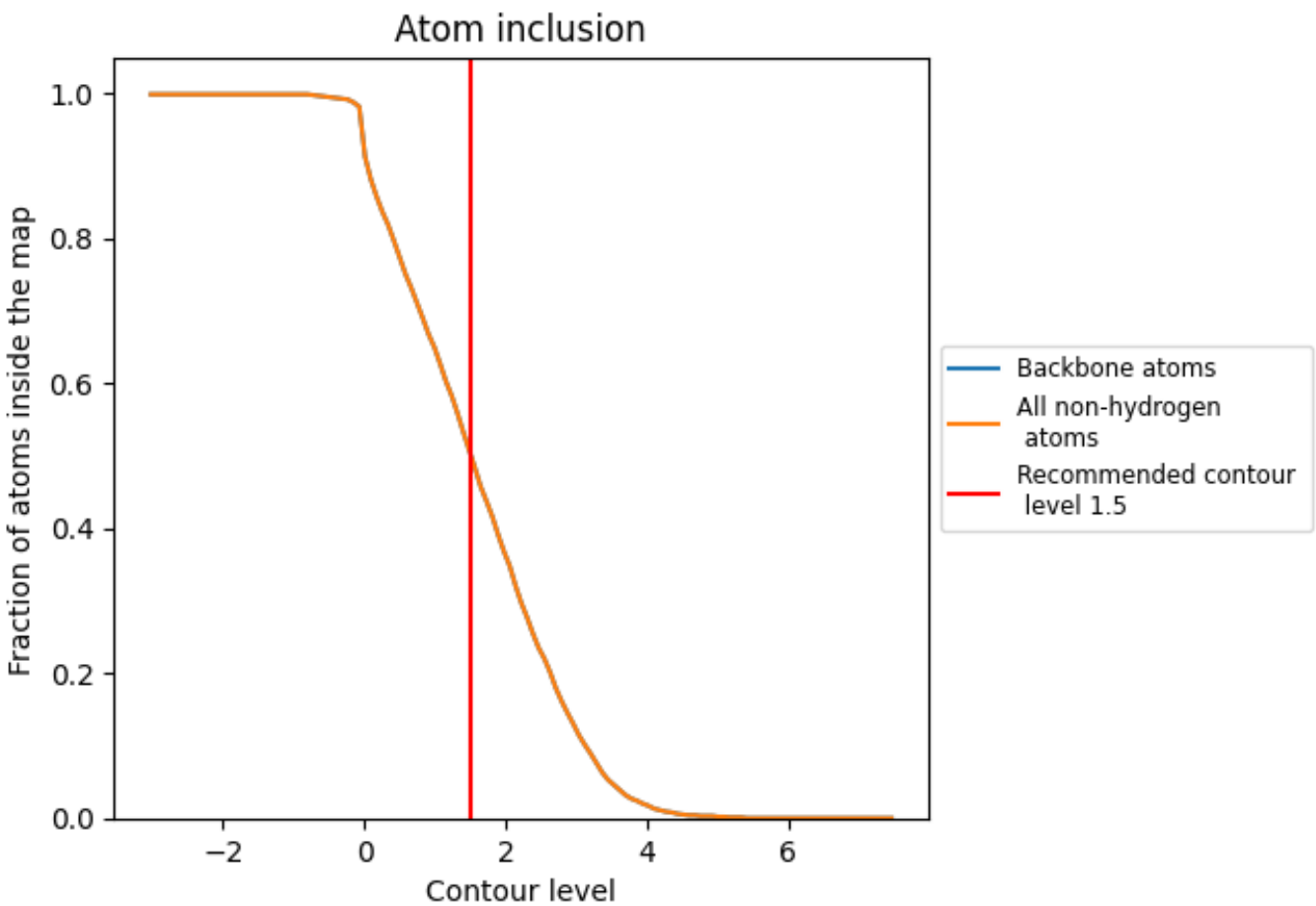
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.5).

9.4 Atom inclusion (i)



At the recommended contour level, 50% of all backbone atoms, 50% 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 (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5020	0.0390
A	0.4520	0.0230
B	0.5200	0.0450
D	0.5250	0.0480
E	0.4970	0.0200
G	0.5050	0.0330
H	0.5050	0.0570
Q	0.5270	0.0390
Z	0.4850	0.0440