WORLDWIDE wwPDB

PROTEIN DATA BANK

wwPDB EM Validation Summary Report (i)

Mar 20, 2024 – 04:42 AM JST

PDB ID	:	6KS8
EMDB ID	:	EMD-0760
Title	:	TRiC at 0.1 mM ADP-AlFx, Conformation 4, 0.1-C4
Authors	:	Jin, M.; Cong, Y.
Deposited on	:	2019-08-23
Resolution	:	4.69 Å(reported)

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 4.69 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.
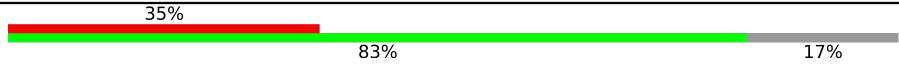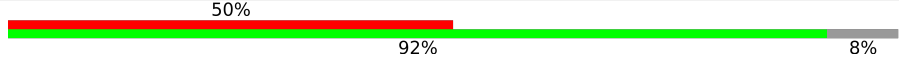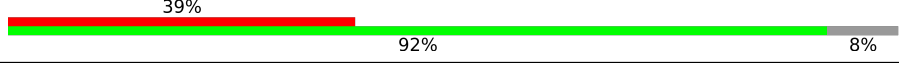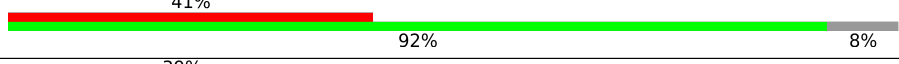
Metric	Percentile Ranks	Value
Ramachandran outliers		0.0%
Sidechain outliers		0.0%

Worse   *Better*

▌ Percentile relative to all structures
▐ Percentile relative to all EM structures
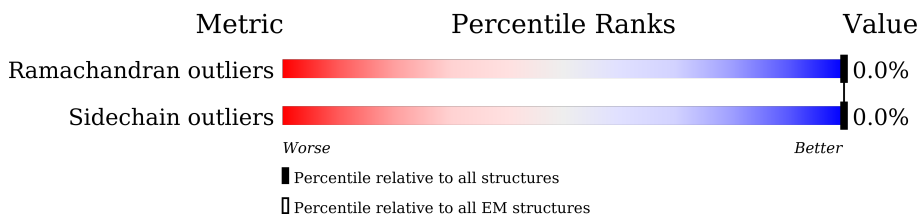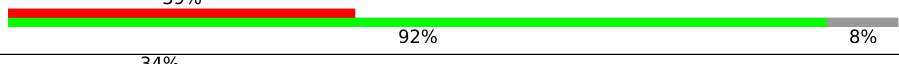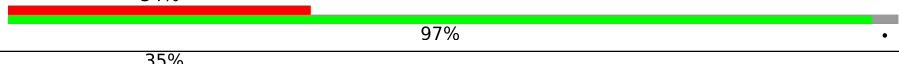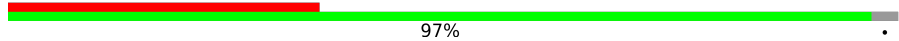
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	559	48% / 91% / 8%
1	a	559	44% / 93% / 7%
2	B	527	52% / 93% / 7%
2	b	527	40% / 95% / 5%
3	D	528	57% / 91% / 9%
3	d	528	52% / 94% / 5%
4	E	562	46% / 89% / 11%
4	e	562	41% / 92% / 8%
5	G	594	38% / 82% / 18%

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Mol	Chain	Length	Quality of chain
5	g	594	35% 83% 17%
6	H	550	50% 92% 8%
6	h	550	39% 92% 8%
7	Q	568	41% 92% 8%
7	q	568	39% 92% 8%
8	Z	546	34% 97% •
8	z	546	35% 97% •

2   Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 61943 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 alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	519	Total 3908	C 2447	N 682	O 759	S 20	0	0
1	A	512	Total 3859	C 2417	N 673	O 750	S 19	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	502	Total 3811	C 2385	N 658	O 754	S 14	0	0
2	B	489	Total 3708	C 2316	N 642	O 736	S 14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	499	Total 3816	C 2384	N 675	O 740	S 17	0	0
3	D	480	Total 3655	C 2284	N 647	O 708	S 16	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	518	Total 3982	C 2500	N 678	O 783	S 21	0	0
4	E	502	Total 3848	C 2416	N 656	O 755	S 21	0	0

- Molecule 5 is a protein called fusion protein of T-complex protein 1 subunit gamma, rep-His-CBP and T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	493	Total 3775	C 2374	N 661	O 715	S 25	0	0
5	G	485	Total 3709	C 2332	N 648	O 704	S 25	0	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	375	LEU	-	see sequence details	UNP P39077
g	376	GLU	-	see sequence details	UNP P39077
g	377	GLY	-	see sequence details	UNP P39077
g	378	SER	-	see sequence details	UNP P39077
g	379	GLY	-	see sequence details	UNP P39077
g	380	SER	-	see sequence details	UNP P39077
g	381	GLY	-	see sequence details	UNP P39077
g	382	TRP	-	see sequence details	UNP P39077
g	383	SER	-	see sequence details	UNP P39077
g	384	HIS	-	see sequence details	UNP P39077
g	385	PRO	-	see sequence details	UNP P39077
g	386	GLN	-	see sequence details	UNP P39077
g	387	PHE	-	see sequence details	UNP P39077
g	388	GLU	-	see sequence details	UNP P39077
g	389	LYS	-	see sequence details	UNP P39077
g	390	GLY	-	see sequence details	UNP P39077
g	391	SER	-	see sequence details	UNP P39077
g	392	GLY	-	see sequence details	UNP P39077
g	393	LYS	-	see sequence details	UNP P39077
g	394	ARG	-	see sequence details	UNP P39077
g	395	ARG	-	see sequence details	UNP P39077
g	396	TRP	-	see sequence details	UNP P39077
g	397	LYS	-	see sequence details	UNP P39077
g	398	LYS	-	see sequence details	UNP P39077
g	399	ASN	-	see sequence details	UNP P39077
g	400	PHE	-	see sequence details	UNP P39077
g	401	ILE	-	see sequence details	UNP P39077
g	402	ALA	-	see sequence details	UNP P39077
g	403	VAL	-	see sequence details	UNP P39077
g	404	SER	-	see sequence details	UNP P39077
g	405	ALA	-	see sequence details	UNP P39077
g	406	ALA	-	see sequence details	UNP P39077
g	407	ASN	-	see sequence details	UNP P39077
g	408	ARG	-	see sequence details	UNP P39077
g	409	PHE	-	see sequence details	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
g	410	LYS	-	see sequence details	UNP P39077
g	411	LYS	-	see sequence details	UNP P39077
g	412	ILE	-	see sequence details	UNP P39077
g	413	SER	-	see sequence details	UNP P39077
g	414	SER	-	see sequence details	UNP P39077
g	415	SER	-	see sequence details	UNP P39077
g	416	GLY	-	see sequence details	UNP P39077
g	417	ALA	-	see sequence details	UNP P39077
g	418	LEU	-	see sequence details	UNP P39077
g	419	GLY	-	see sequence details	UNP P39077
g	420	SER	-	see sequence details	UNP P39077
g	421	GLY	-	see sequence details	UNP P39077
g	422	HIS	-	see sequence details	UNP P39077
g	423	HIS	-	see sequence details	UNP P39077
g	424	HIS	-	see sequence details	UNP P39077
g	425	HIS	-	see sequence details	UNP P39077
g	426	HIS	-	see sequence details	UNP P39077
g	427	HIS	-	see sequence details	UNP P39077
g	428	HIS	-	see sequence details	UNP P39077
g	429	HIS	-	see sequence details	UNP P39077
g	430	GLY	-	see sequence details	UNP P39077
g	431	SER	-	see sequence details	UNP P39077
g	432	GLY	-	see sequence details	UNP P39077
g	433	LEU	-	see sequence details	UNP P39077
g	434	GLN	-	see sequence details	UNP P39077
G	375	LEU	-	see sequence details	UNP P39077
G	376	GLU	-	see sequence details	UNP P39077
G	377	GLY	-	see sequence details	UNP P39077
G	378	SER	-	see sequence details	UNP P39077
G	379	GLY	-	see sequence details	UNP P39077
G	380	SER	-	see sequence details	UNP P39077
G	381	GLY	-	see sequence details	UNP P39077
G	382	TRP	-	see sequence details	UNP P39077
G	383	SER	-	see sequence details	UNP P39077
G	384	HIS	-	see sequence details	UNP P39077
G	385	PRO	-	see sequence details	UNP P39077
G	386	GLN	-	see sequence details	UNP P39077
G	387	PHE	-	see sequence details	UNP P39077
G	388	GLU	-	see sequence details	UNP P39077
G	389	LYS	-	see sequence details	UNP P39077
G	390	GLY	-	see sequence details	UNP P39077
G	391	SER	-	see sequence details	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
G	392	GLY	-	see sequence details	UNP P39077
G	393	LYS	-	see sequence details	UNP P39077
G	394	ARG	-	see sequence details	UNP P39077
G	395	ARG	-	see sequence details	UNP P39077
G	396	TRP	-	see sequence details	UNP P39077
G	397	LYS	-	see sequence details	UNP P39077
G	398	LYS	-	see sequence details	UNP P39077
G	399	ASN	-	see sequence details	UNP P39077
G	400	PHE	-	see sequence details	UNP P39077
G	401	ILE	-	see sequence details	UNP P39077
G	402	ALA	-	see sequence details	UNP P39077
G	403	VAL	-	see sequence details	UNP P39077
G	404	SER	-	see sequence details	UNP P39077
G	405	ALA	-	see sequence details	UNP P39077
G	406	ALA	-	see sequence details	UNP P39077
G	407	ASN	-	see sequence details	UNP P39077
G	408	ARG	-	see sequence details	UNP P39077
G	409	PHE	-	see sequence details	UNP P39077
G	410	LYS	-	see sequence details	UNP P39077
G	411	LYS	-	see sequence details	UNP P39077
G	412	ILE	-	see sequence details	UNP P39077
G	413	SER	-	see sequence details	UNP P39077
G	414	SER	-	see sequence details	UNP P39077
G	415	SER	-	see sequence details	UNP P39077
G	416	GLY	-	see sequence details	UNP P39077
G	417	ALA	-	see sequence details	UNP P39077
G	418	LEU	-	see sequence details	UNP P39077
G	419	GLY	-	see sequence details	UNP P39077
G	420	SER	-	see sequence details	UNP P39077
G	421	GLY	-	see sequence details	UNP P39077
G	422	HIS	-	see sequence details	UNP P39077
G	423	HIS	-	see sequence details	UNP P39077
G	424	HIS	-	see sequence details	UNP P39077
G	425	HIS	-	see sequence details	UNP P39077
G	426	HIS	-	see sequence details	UNP P39077
G	427	HIS	-	see sequence details	UNP P39077
G	428	HIS	-	see sequence details	UNP P39077
G	429	HIS	-	see sequence details	UNP P39077
G	430	GLY	-	see sequence details	UNP P39077
G	431	SER	-	see sequence details	UNP P39077
G	432	GLY	-	see sequence details	UNP P39077
G	433	LEU	-	see sequence details	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
G	434	GLN	-	see sequence details	UNP P39077

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	507	Total	C	N	O	S	0	0
			3882	2447	664	752	19		
6	H	507	Total	C	N	O	S	0	0
			3882	2447	664	752	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	q	523	Total	C	N	O	S	0	0
			3974	2506	676	766	26		
7	Q	524	Total	C	N	O	S	0	0
			3978	2508	677	767	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	z	531	Total	C	N	O	S	0	0
			4086	2566	708	795	17		
8	Z	529	Total	C	N	O	S	0	0
			4070	2555	705	793	17		

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: T-complex protein 1 subunit alpha
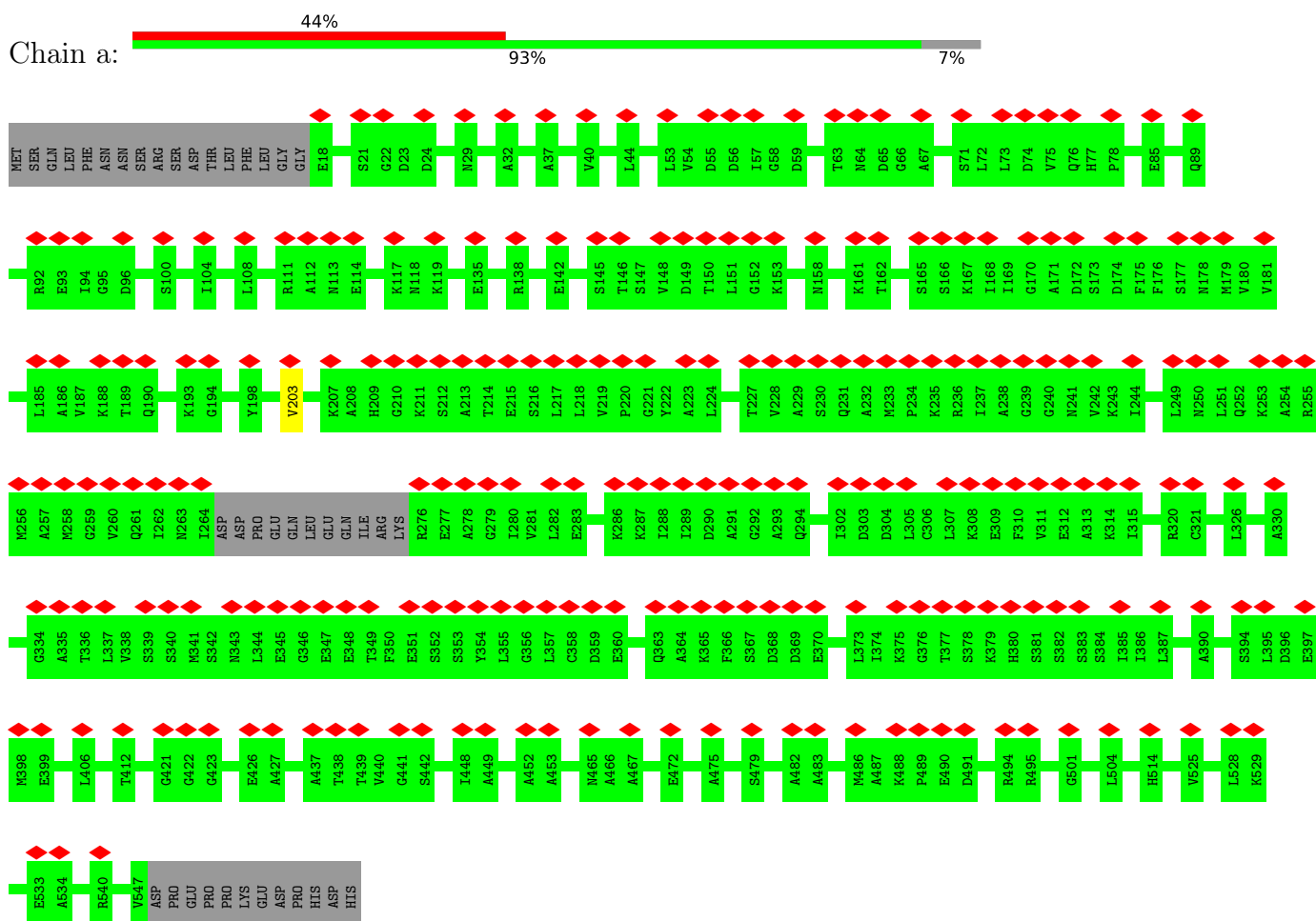
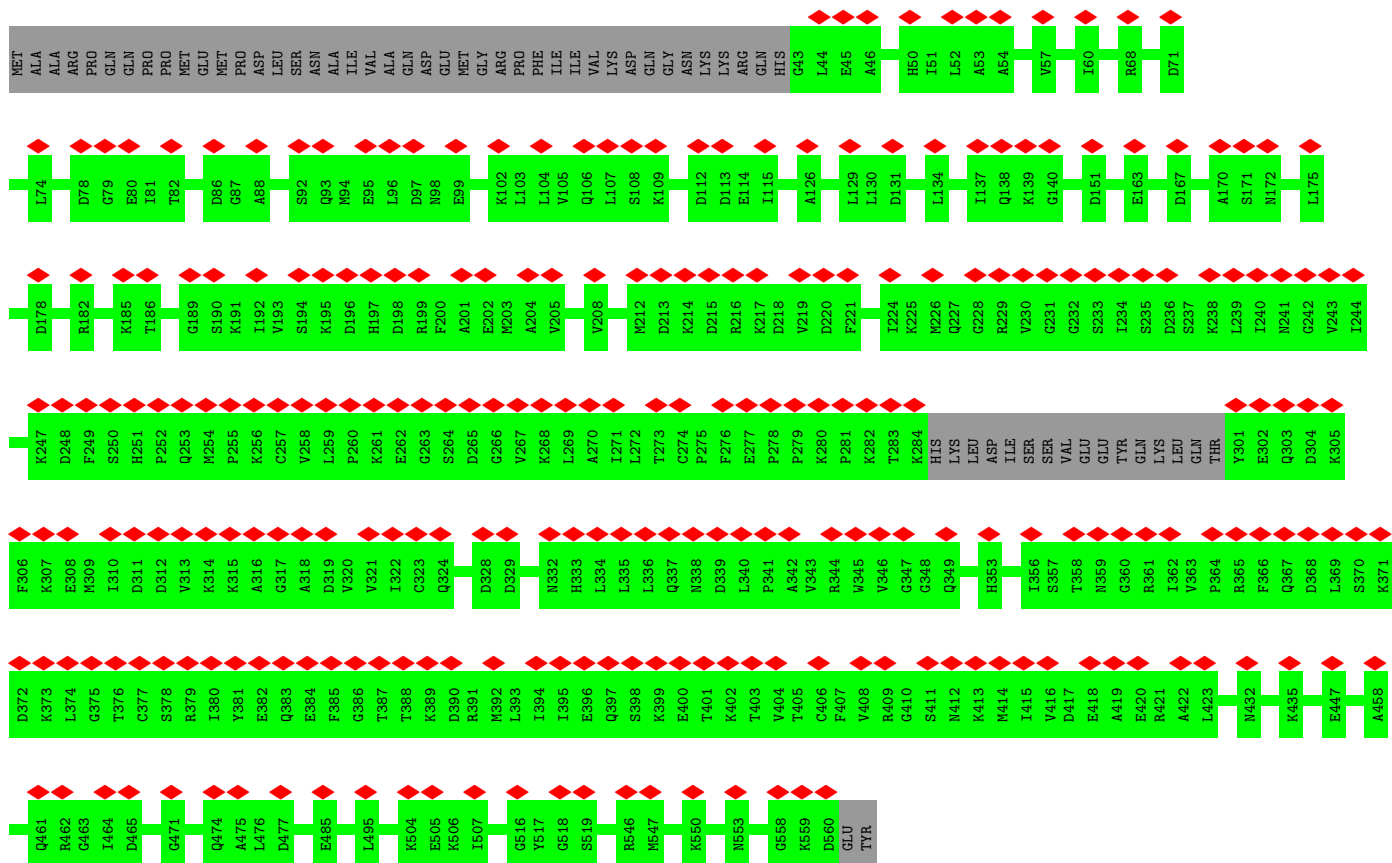- Molecule 1: T-complex protein 1 subunit alpha

• Molecule 2: T-complex protein 1 subunit beta
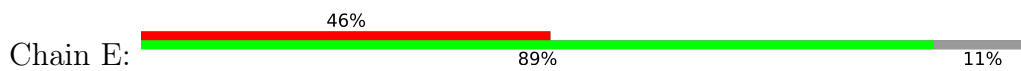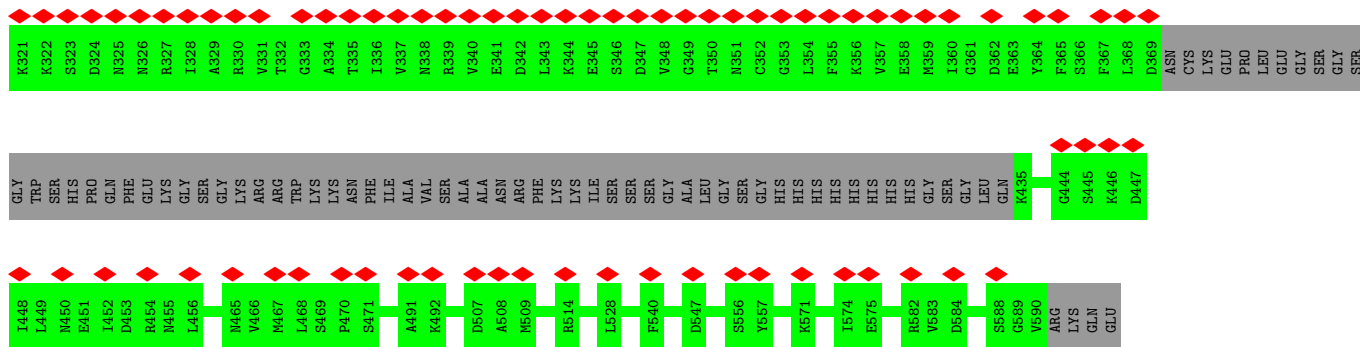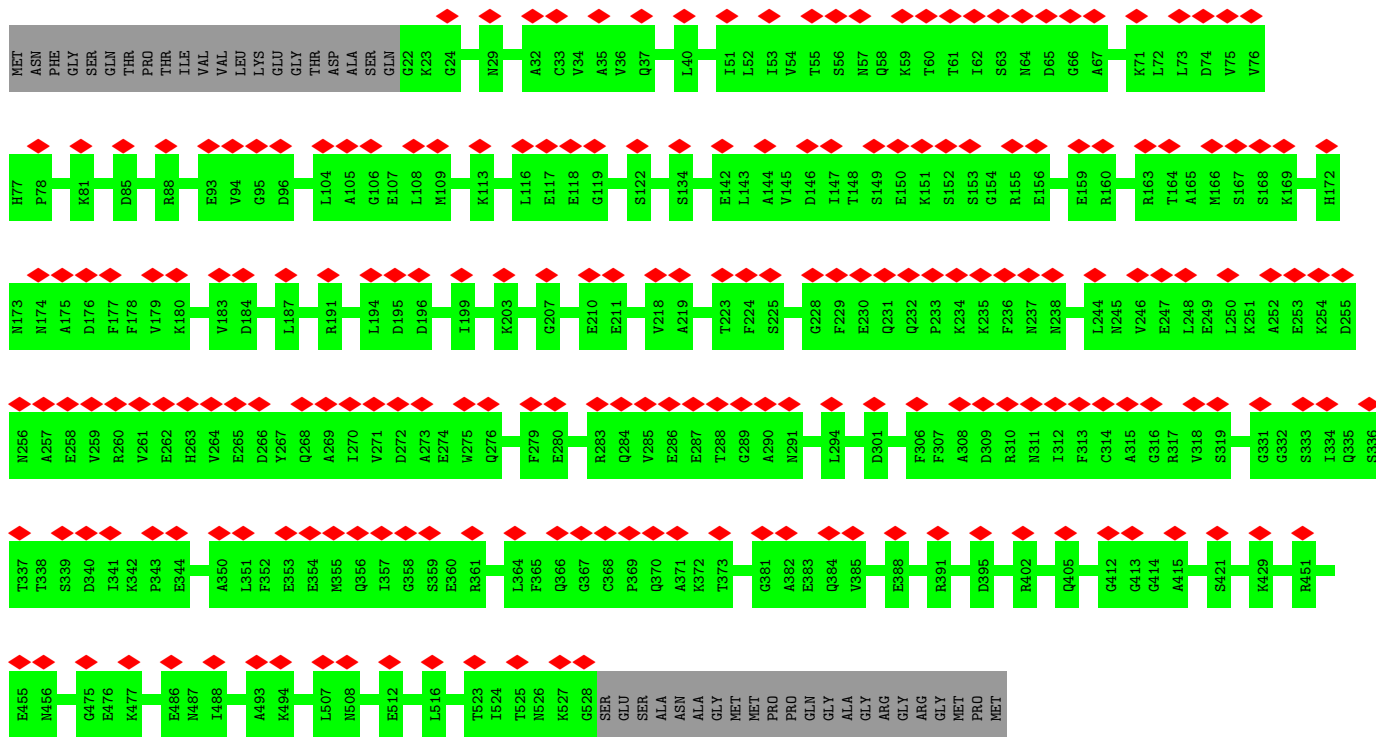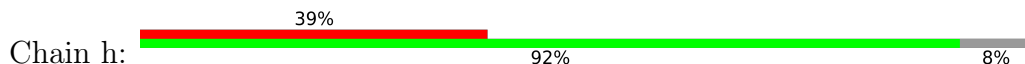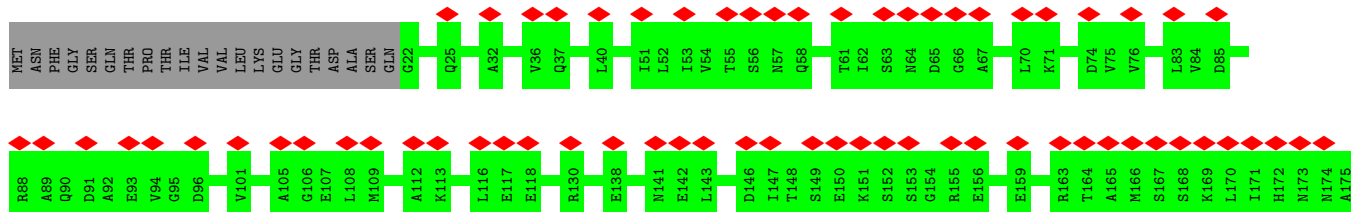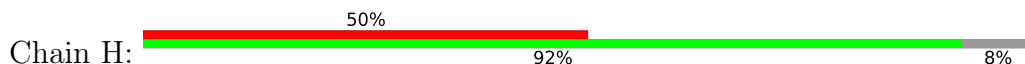
Chain b:

• Molecule 2: T-complex protein 1 subunit beta

Chain B:

52%

93%

7%

MET SER VAL GLN ILE PHE GLY ASP GLN VAL THR GLU GLU ARG ALA GLU ASN ALA R19 L20 S21 A22 F23 V24 G25 A26 I27 A28 V29 L32 V33 S50 S51 N52 T53 C54 M55 V56 D59 G60 A61 T62 K65 S66 L69 D70 N71 P72 K75 N79 K82 V83

Q84 D85 D86 E87 V88 G89 D90 A100 L103 R104 E107 D111 Q112 I121 A127 H144 D145 M148 F149 R150 E151 D152 L153 I154 H155 K158 T159 T160 L161 S162 S163 K164 I165 L166 S167 Q168 D169 K170 D171 H172 F173 A174 E175 L176 A177 T178 N179 A180 I181 L182 R183

L184 K185 G186 S187 T188 N189 L190 E191 H192 I193 Q194 I195 I196 K197 I198 L199 G200 G201 K202 L203 S204 D205 S206 F207 L208 D209 E210 G211 F212 I213 L214 A215 K216 K217 F218 G219 N220 N221 Q222 P223 K224 R225 I226 E227 N228 A229 K230 I231 L232 I233 A234 N235 T236 T237 L238 D239 T240 D241 K242 VAL

LYS ILE PHE GLY THR LYS PHE LYS VAL ASP SER THR A256 K257 L258 A259 Q260 L261 E262 K263 A264 E265 R266 E267 K268 M269 K270 N271 K272 I273 A274 K275 I276 S277 K278 F279 G280 I281 N282 N286 R287 Q288 L289 I290 Y291 P294 E295 Q296 L297 F298 T299 D300 L301 G302 I303 N304 S305 I306

E307 H308 A309 D310 F311 E312 G313 V314 E315 R316 L317 A318 L319 V320 T321 G322 G323 E324 V325 V326 S327 T328 F329 D330 E331 P332 S333 K334 C335 K336 L337 G338 E339 C340 D341 V342 I343 E344 A345 I346 M347 L348 G349 E350 Q351 P352 F353 L354 K355 F356 S357 G358 C359 K360 A361 G362 E363 A364 C365 T366

I367 V368 L369 R370 G371 A372 T373 D374 Q375 T376 L377 D378 E379 A380 E381 R382 S383 L384 H385 D386 A387 L391 S392 T395 K396 E408 S412 D416 D423 G424 K425 L428 A429 A432 R435 A436 Q439 L440 I443 D446 N447 A448 G449 S452 I467

L472 D473 L474 N475 N476 A480 D481 L485 A504 V507 L508 R518 P519 R520 THR ALA ASN GLN HIS MET

• Molecule 3: T-complex protein 1 subunit delta

Chain d:

52%

94%

5%

MET SER ALA LYS VAL PRO SER ASN ALA THR PHE LYS LYS ASN LYS GLU LYS P17 Q18 E19 V20 R21 K22 A23 N24 A27 A28 V31 A32 D33 A34 I35 R36 L39 K42 D45 R52 G53 E54 I55 I56 I57 S58 N59 D60 G61 H62 T63 K66 Q67 M68 A69 I70 L71

R76 E80 V81 S82 A83 S87 E88 A89 G90 D91 L104 E108 R109 L110 L111 N112 K113 G114 I115 H116 P117 T118 I119 I120 A121 F124 K129 E137 M138 K141 V142 S143 L144 S145 D146 R147 E148 R152 A153 A154 S155 T156 S157 L158 S159 S160 K161 I162 Q165

S168 F169 P172 L173 A174 V175 D176 L179 K180 D183 E184 N185 S186 K187 N188 V189 D190 L191 K199 T203 I204 D205 D206 T207 E208 M209 I210 D211 G212 V213 Q217 T218 A219 I220 K221 S222 A223 G224 G225 P226 T227 R228 K229 E230 K231 A232 K233 I234 G235 L236 I237 Q238 F239

Q240 I241 S242 P243 P244 K245 P246 D247 T248 E249 N250 N251 I252 I253 V254 N255 D256 Y257 R258 Q259 M260 D261 K262 I263 L264 K265 E266 E267 R268 A269 Y270 L271 L272 N273 I274 C275 K276 K277 I278 K279 K280 A281 R282 C283 N284 I287 I288 Q289 K290 S291 I292 L293 R294 D295 A296 V297 N298 D299 L300

A301 L302 H303 F304 L305 S306 K307 L308 N309 V313 K314 D315 I316 E317 R318 E319 L324 L328 P332 I333 A334 D335 I336 E337 L338 F339 T340 E341 D342 R343 L344 G345 S346 A347 D348 L349 V350 E351 E352 I353 D354 S355 D356 G357 S358 R362 V363 T364 G365 I366 R367 N368 N369 N370 A371

• Molecule 3: T-complex protein 1 subunit delta
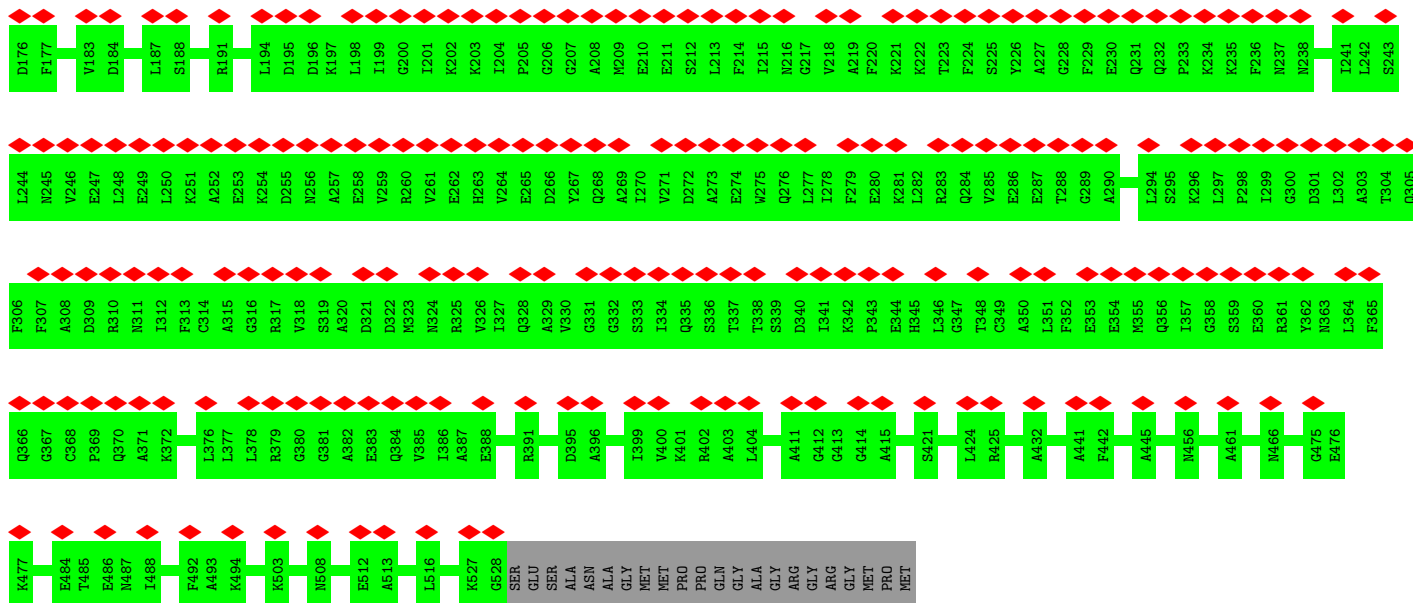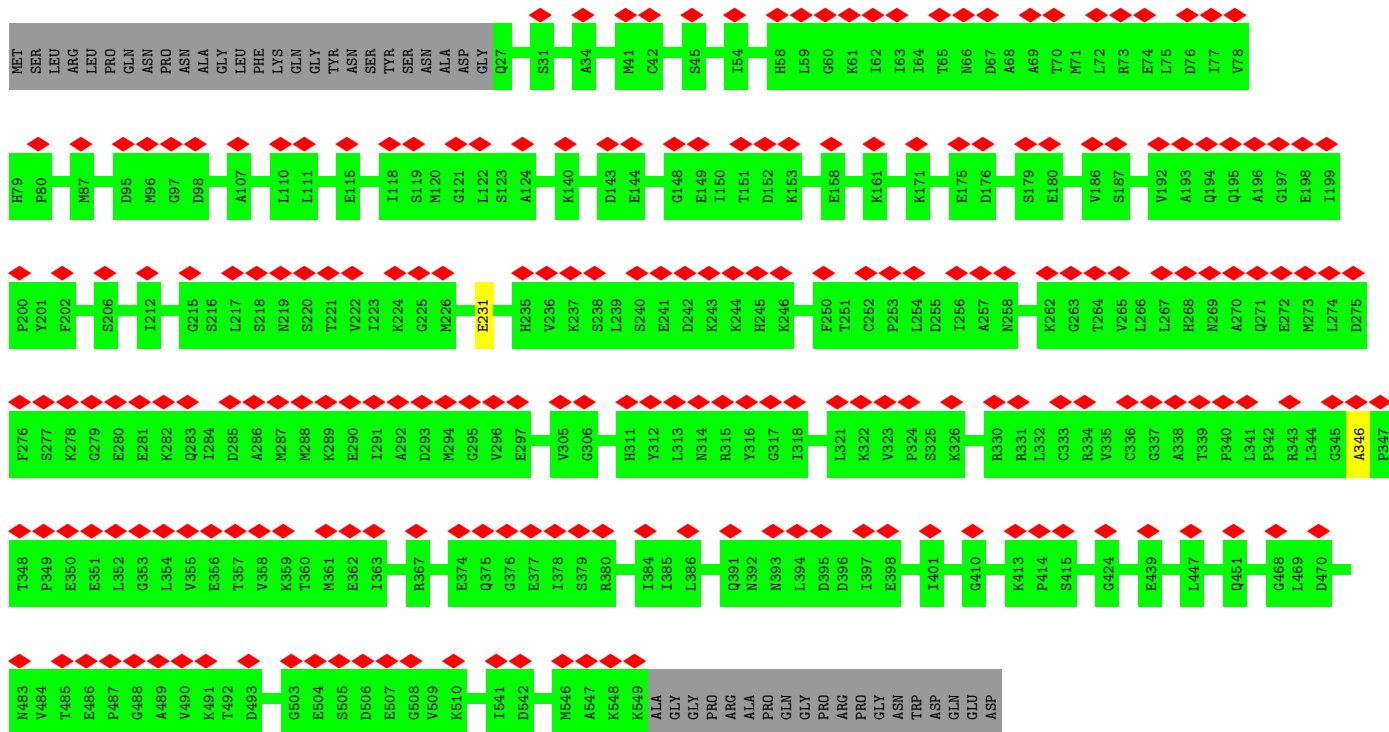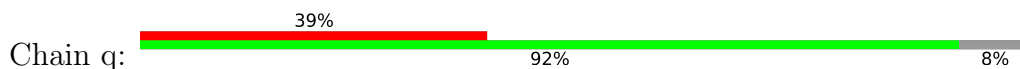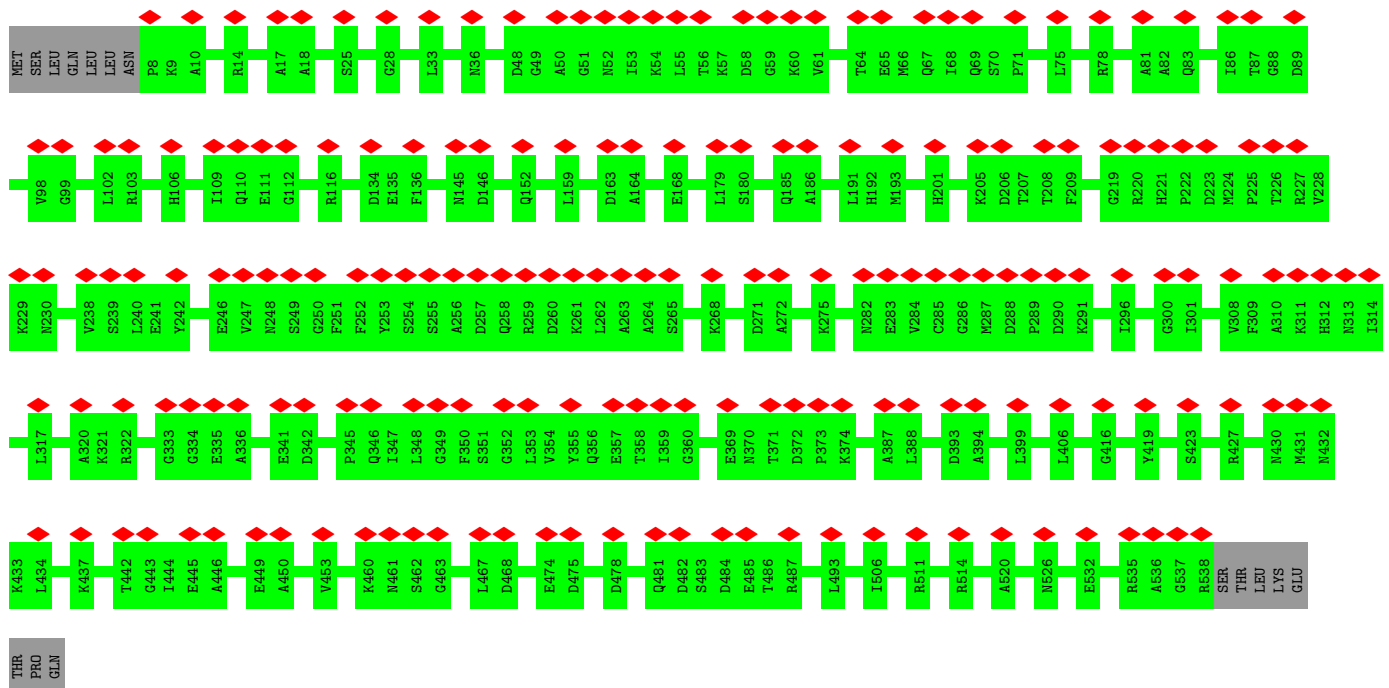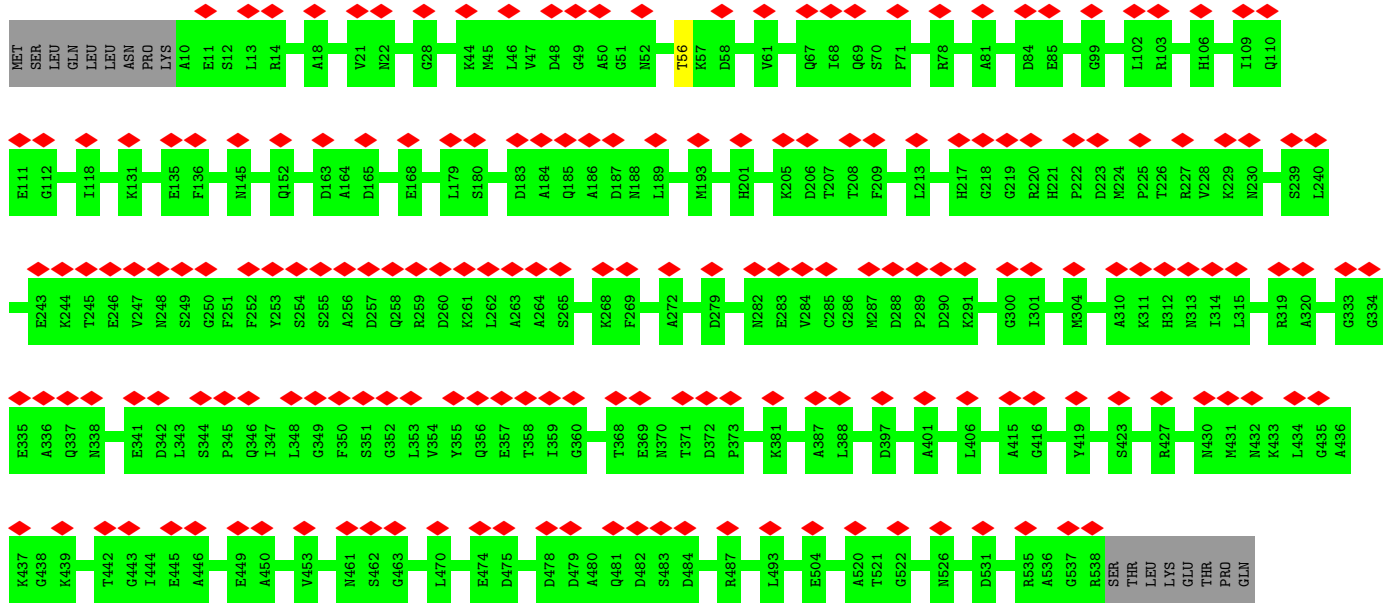
Chain D:

57%

91% 9%

• Molecule 4: T-complex protein 1 subunit epsilon

Chain e:

41%

92% 8%

• Molecule 4: T-complex protein 1 subunit epsilon

Chain E:

46%

89% 11%

• Molecule 5: fusion protein of T-complex protein 1 subunit gamma, rep-His-CBP and T-complex protein 1 subunit gamma

Chain g:

• Molecule 5: fusion protein of T-complex protein 1 subunit gamma, rep-His-CBP and T-complex protein 1 subunit gamma

Chain G:

• Molecule 6: T-complex protein 1 subunit eta

Chain h:

39%

92%

8%

• Molecule 6: T-complex protein 1 subunit eta

Chain H:

50%

92%

8%

D176 F177 V183 D184 L187 S188 R191 L194 D195 D196 K197 L198 I199 G200 I201 K202 K203 I204 P205 G206 G207 A208 M209 E210 E211 S212 L213 F214 I215 N216 G217 V218 A219 F220 K221 K222 T223 F224 S225 Y226 A227 G228 F229 E230 Q231 Q232 P233 K234 K235 F236 N237 N238 I241 L242 S243

L244 N245 V246 E247 L248 E249 L250 K251 A252 E253 K254 D255 N256 A257 E258 V259 R260 V261 E262 H263 V264 E265 D266 Y267 Q268 A269 I270 V271 D272 A273 E274 W275 Q276 L277 I278 F279 E280 K281 L282 R283 Q284 V285 E286 E287 T288 G289 A290 L294 S295 K296 L297 P298 I299 G300 D301 L302 A303 T304 Q305

F306 F307 A308 D309 R310 N311 I312 F313 C314 A315 G316 R317 V318 S319 A320 D321 D322 M323 N324 R325 V326 I327 Q328 A329 V330 G331 G332 S333 I334 Q335 S336 T337 T338 S339 D340 I341 K342 P343 E344 H345 L346 G347 T348 C349 A350 L351 F352 E353 E354 M355 Q356 I357 G358 S359 E360 R361 Y362 N363 L364 F365

Q366 G367 C368 P369 Q370 A371 K372 L376 L377 L378 R379 G380 G381 A382 E383 Q384 V385 I386 A387 E388 R391 D395 A396 I399 V400 K401 R402 A403 L404 A411 G412 G413 G414 A415 S421 L424 R425 A432 A441 F442 A445 A461 N466 G475 E476

K477 E484 T485 E486 N487 I488 F492 A493 K494 K503 N508 E512 A513 L516 K527 G528 SER GLU SER ALA ASN ALA GLY MET MET PRO PRO GLN GLY ALA GLY ARG GLY ARG GLY MET PRO MET

• Molecule 7: T-complex protein 1 subunit theta

39%

Chain q:

92% 8%

MET SER LEU ARG LEU PRO GLN ASN PRO ASN ALA GLY LEU PHE LYS GLN GLY TYR ASN SER TYR ASN ALA ASP GLY Q27 S31 A34 M41 C42 S45 I54 H58 L59 G60 K61 I62 I63 I64 T65 N66 D67 A68 A69 T70 M71 L72 R73 E74 L75 D76 I77 V78

H79 P80 M87 D95 M96 G97 D98 A107 L110 L111 E115 I118 S119 M120 G121 L122 S123 A124 K140 D143 E144 G148 E149 I150 T151 D152 K153 E158 K161 K171 E175 D176 S179 E180 V186 S187 V192 A193 Q194 A196 G197 E198 I199

P200 Y201 F202 S206 I212 G215 S216 L217 S218 N219 S220 T221 V222 I223 K224 G225 M226 E231 H235 V236 K237 S238 L239 S240 E241 D242 K243 K244 H245 K246 F250 T251 C252 P253 L254 D255 I256 A257 N258 K262 G263 T264 V265 L266 L267 H268 N269 A270 Q271 E272 M273 L274 D275

F276 S277 K278 G279 E280 E281 K282 Q283 I284 D285 A286 M287 M288 K289 E290 I291 A292 D293 N294 Q295 V296 E297 V305 G306 H311 Y312 L313 N314 R315 Y316 G317 I318 L321 K322 V323 P324 S325 K326 R330 R331 L332 C333 R334 V335 C336 G337 A338 T339 P340 L341 P342 R343 L344 G345 A346 P347

T348 P349 E350 E351 L352 G353 L354 V355 E356 T357 V358 K359 T360 M361 E362 I363 R367 E374 Q375 G376 E377 I378 S379 R380 I384 I385 L386 Q391 N392 N393 L394 D395 D396 I397 E398 I401 G410 K413 P414 S415 G424 E439 L447 Q451 G468 L469 D470

N483 V484 T485 E486 P487 G488 A489 V490 K491 T492 D493 G503 E504 S505 D506 E507 G508 V509 K510 I541 D542 M546 A547 K549 ALA GLY GLY PRO ARG ALA PRO GLN GLY PRO ARG PRO GLY ASN TRP ASP GLN GLU ASP

• Molecule 7: T-complex protein 1 subunit theta

41%

Chain Q:

92% 8%

• Molecule 8: T-complex protein 1 subunit zeta

Chain z:

35%

97%

• Molecule 8: T-complex protein 1 subunit zeta

Chain Z:

34%

97%

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53539	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 $(e^-/Å^2)$	38	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.268	Depositor
Minimum map value	-1.235	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.143	Depositor
Recommended contour level	0.85	Depositor
Map size (Å)	337.408, 337.408, 337.408	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.318, 1.318, 1.318	Depositor

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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	0/3891	0.40	0/5247
1	a	0.23	0/3941	0.40	0/5316
2	B	0.23	0/3743	0.38	0/5043
2	b	0.23	0/3849	0.39	0/5186
3	D	0.23	0/3687	0.38	0/4967
3	d	0.23	0/3851	0.38	0/5190
4	E	0.23	0/3893	0.39	0/5240
4	e	0.23	0/4030	0.39	0/5426
5	G	0.22	0/3751	0.39	0/5065
5	g	0.23	0/3817	0.39	0/5152
6	H	0.23	0/3931	0.38	0/5304
6	h	0.23	0/3931	0.39	0/5304
7	Q	0.23	0/4024	0.40	0/5431
7	q	0.26	2/4020 (0.0%)	0.40	0/5426
8	Z	0.23	0/4121	0.40	0/5568
8	z	0.23	0/4138	0.39	0/5590
All	All	0.23	2/62618 (0.0%)	0.39	0/84455

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	q	231	GLU	C-N	5.33	1.44	1.34
7	q	346	ALA	C-N	5.02	1.43	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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	507/559 (91%)	482 (95%)	24 (5%)	1 (0%)	47	81
1	a	515/559 (92%)	478 (93%)	36 (7%)	1 (0%)	47	81
2	B	485/527 (92%)	463 (96%)	21 (4%)	1 (0%)	47	81
2	b	500/527 (95%)	477 (95%)	23 (5%)	0	100	100
3	D	474/528 (90%)	452 (95%)	22 (5%)	0	100	100
3	d	495/528 (94%)	472 (95%)	22 (4%)	1 (0%)	47	81
4	E	498/562 (89%)	475 (95%)	23 (5%)	0	100	100
4	e	516/562 (92%)	492 (95%)	24 (5%)	0	100	100
5	G	479/594 (81%)	459 (96%)	20 (4%)	0	100	100
5	g	487/594 (82%)	466 (96%)	21 (4%)	0	100	100
6	H	505/550 (92%)	483 (96%)	22 (4%)	0	100	100
6	h	505/550 (92%)	485 (96%)	20 (4%)	0	100	100
7	Q	522/568 (92%)	505 (97%)	17 (3%)	0	100	100
7	q	521/568 (92%)	497 (95%)	24 (5%)	0	100	100
8	Z	527/546 (96%)	505 (96%)	22 (4%)	0	100	100
8	z	529/546 (97%)	514 (97%)	15 (3%)	0	100	100
All	All	8065/8868 (91%)	7705 (96%)	356 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	467	ILE
1	a	203	VAL
1	A	203	VAL
3	d	213	VAL

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	428/471 (91%)	428 (100%)	0	100	100
1	a	433/471 (92%)	433 (100%)	0	100	100
2	B	408/441 (92%)	408 (100%)	0	100	100
2	b	420/441 (95%)	420 (100%)	0	100	100
3	D	409/453 (90%)	409 (100%)	0	100	100
3	d	428/453 (94%)	428 (100%)	0	100	100
4	E	429/483 (89%)	429 (100%)	0	100	100
4	e	445/483 (92%)	445 (100%)	0	100	100
5	G	410/501 (82%)	410 (100%)	0	100	100
5	g	417/501 (83%)	417 (100%)	0	100	100
6	H	422/454 (93%)	422 (100%)	0	100	100
6	h	422/454 (93%)	422 (100%)	0	100	100
7	Q	439/473 (93%)	439 (100%)	0	100	100
7	q	439/473 (93%)	439 (100%)	0	100	100
8	Z	446/463 (96%)	445 (100%)	1 (0%)	93	96
8	z	448/463 (97%)	448 (100%)	0	100	100
All	All	6843/7478 (92%)	6842 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	Z	56	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
6	H	231	GLN
8	z	69	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	q	66	ASN
7	Q	91	GLN
8	z	356	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0760. 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 |
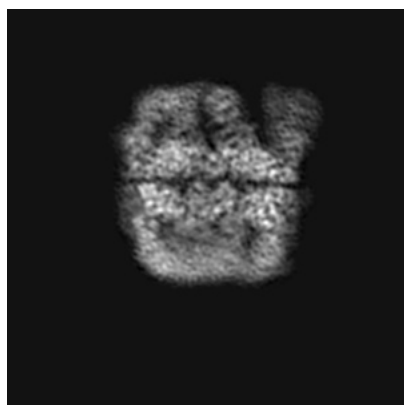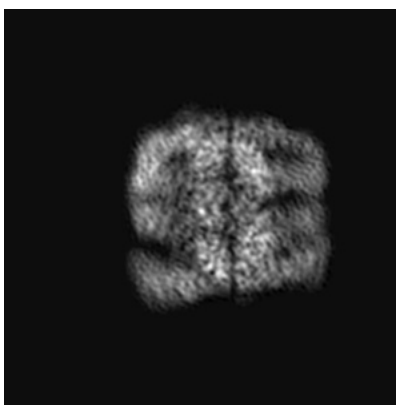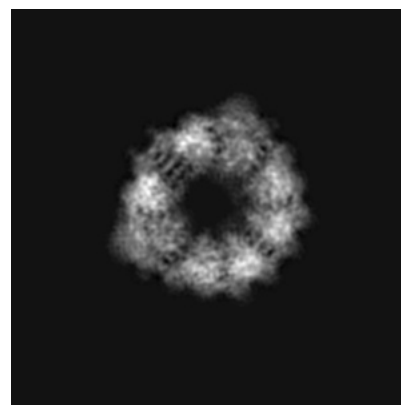
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map
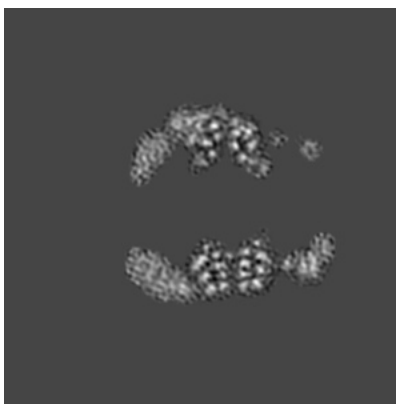
| X Index: 128 | Y Index: 128 | Z Index: 128 |
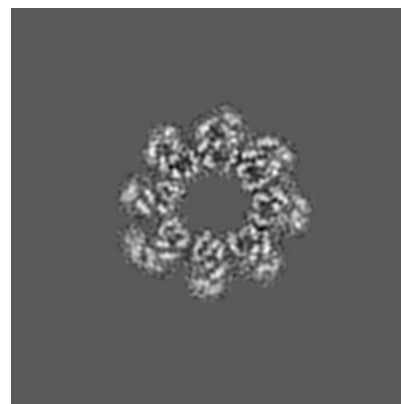
The images above show central slices of the map in three orthogonal directions.

6.3   Largest variance slices ⓘ
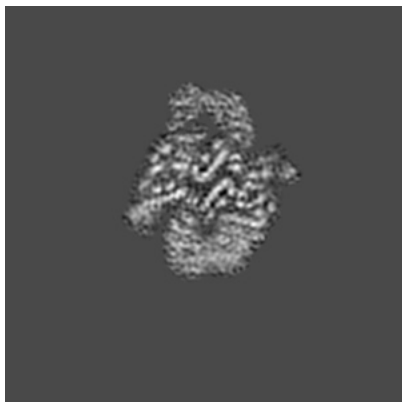
6.3.1   Primary map
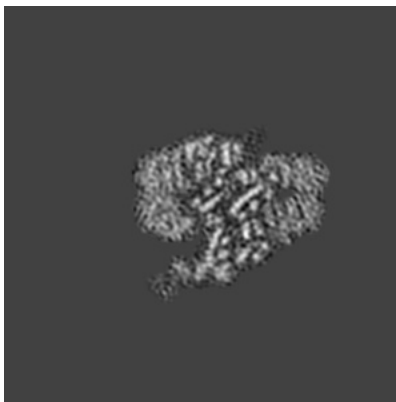
| X Index: 168 | Y Index: 91 | Z Index: 126 |

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

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

6.4.1   Primary map

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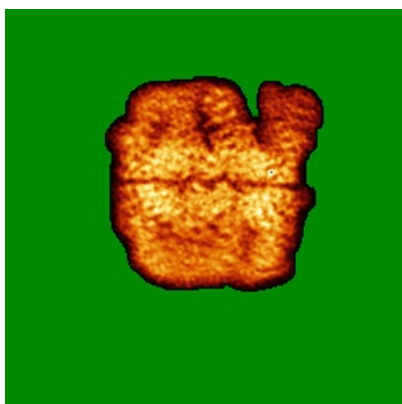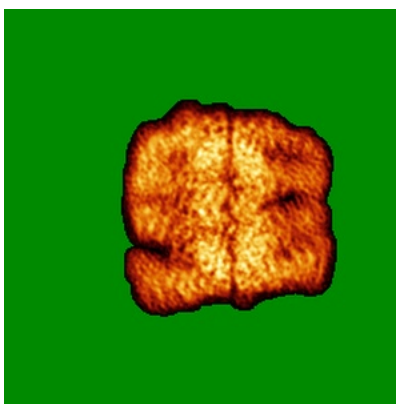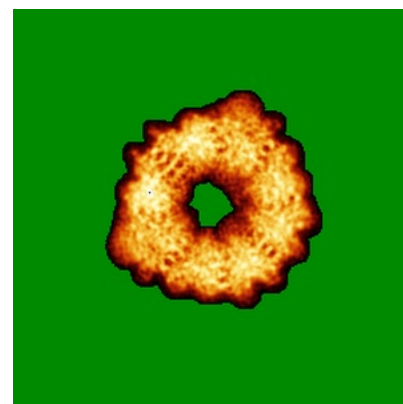
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

| X | Y | Z |
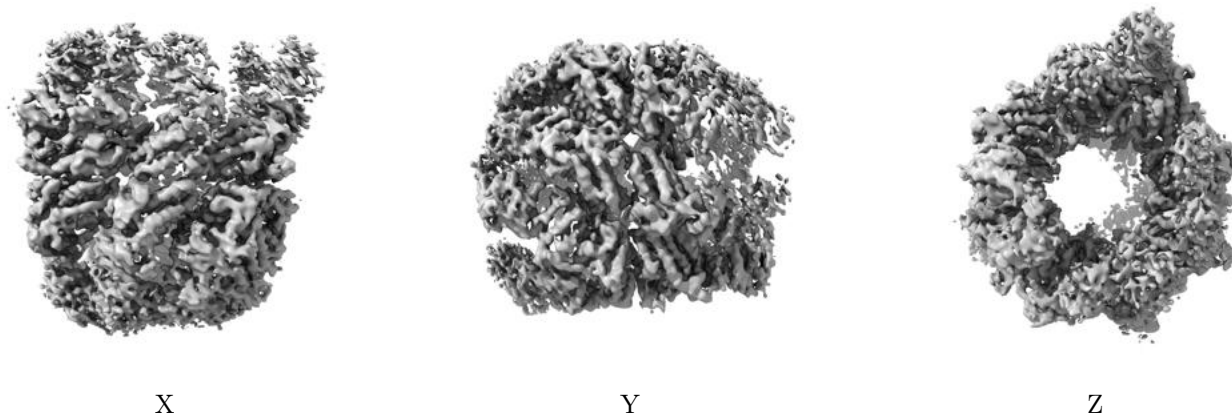
The images above show the 3D surface view of the map at the recommended contour level 0.85. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 Mask visualisation (i)

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

7　Map analysis ⓘ

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

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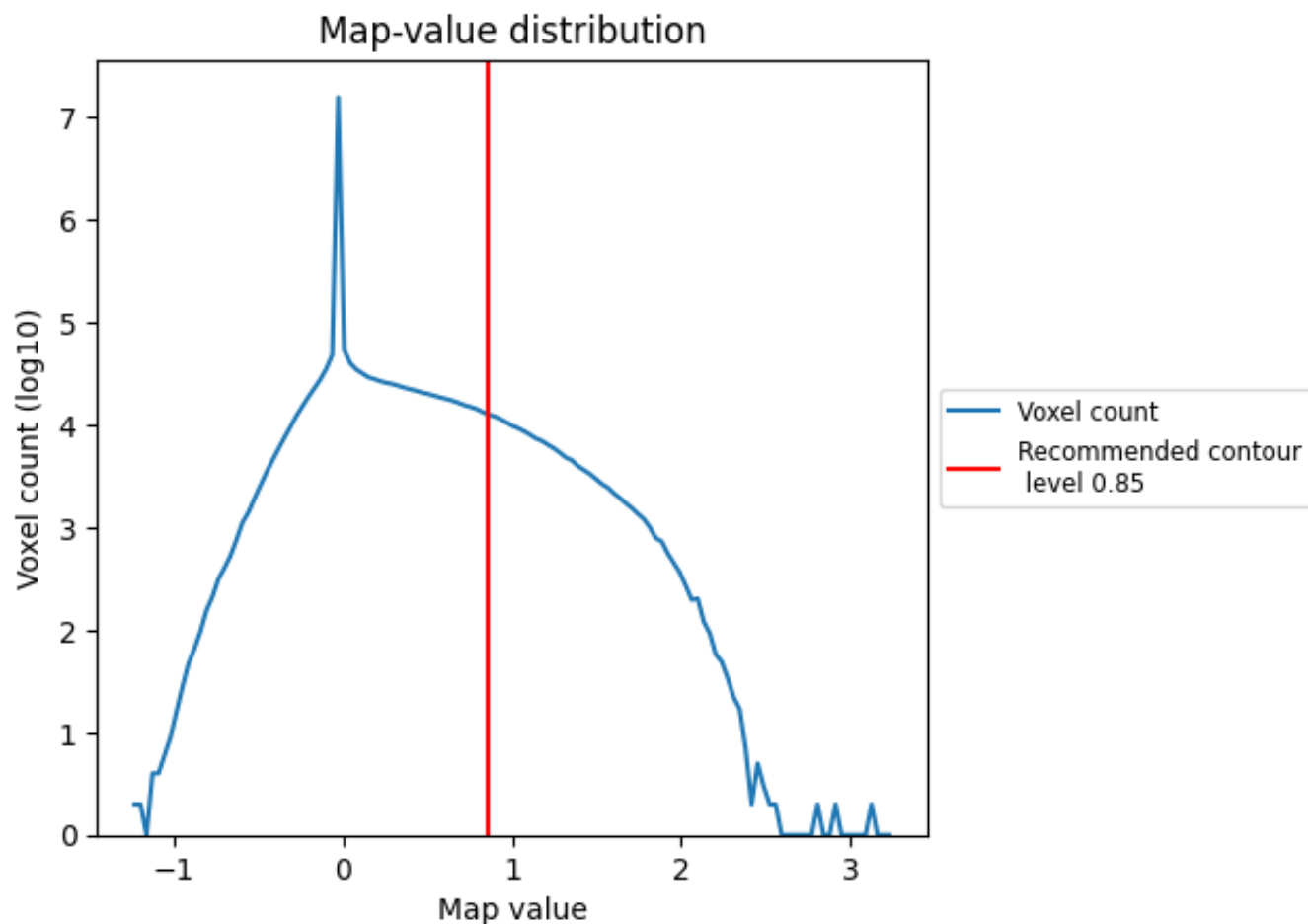
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
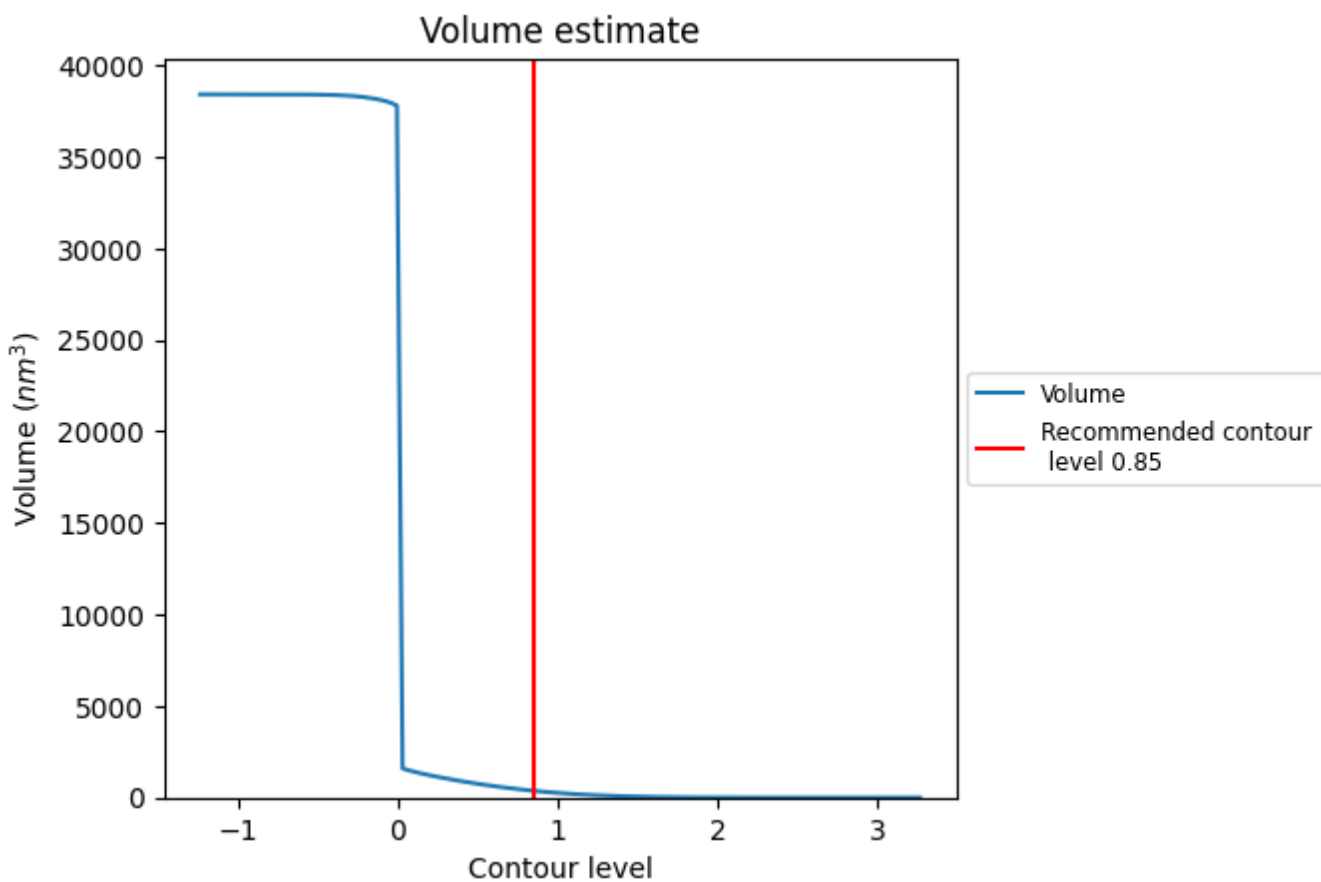
The volume at the recommended contour level is 369 nm^3; this corresponds to an approximate mass of 333 kDa.

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   ⓘ
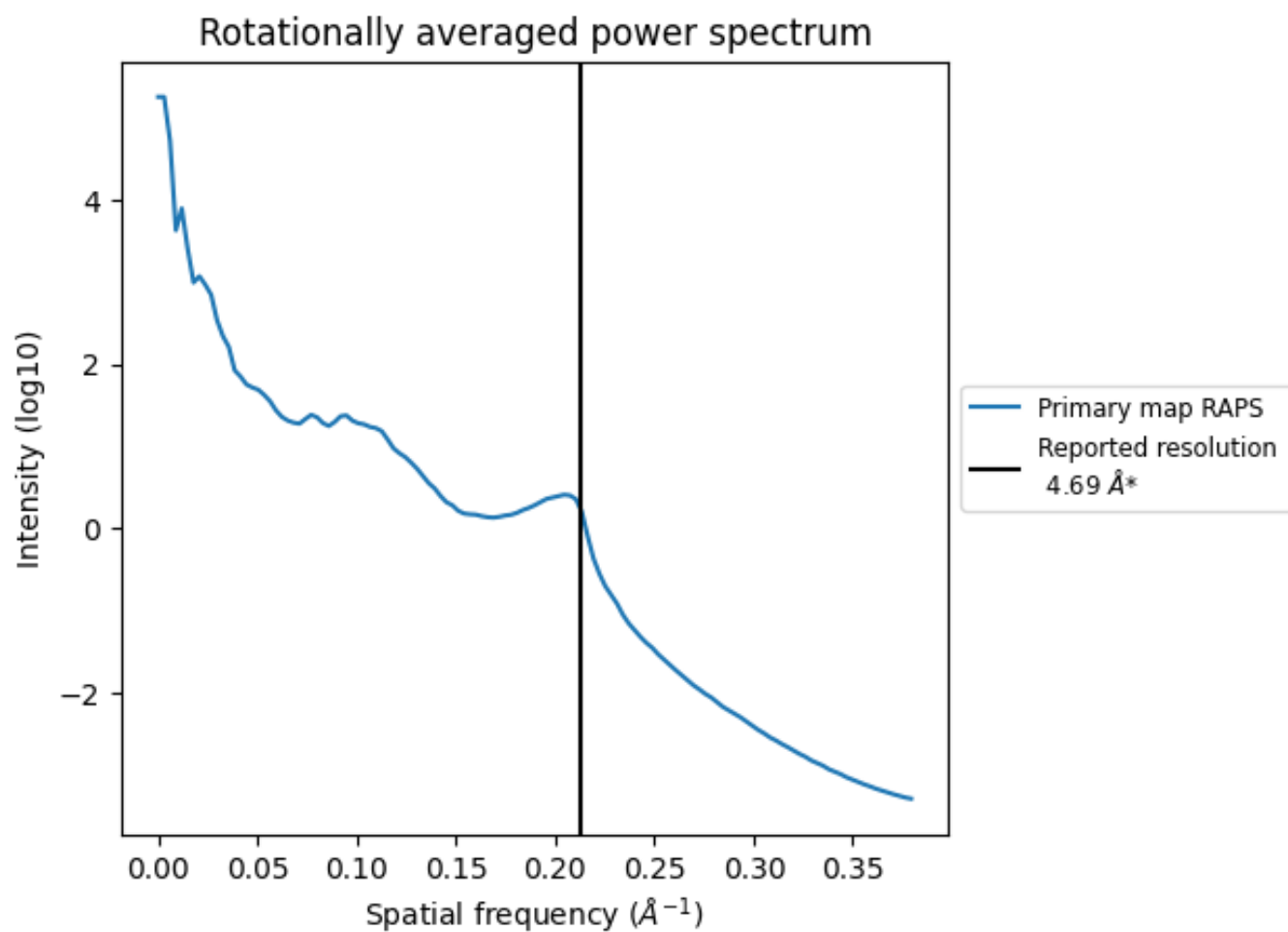
*Reported resolution corresponds to spatial frequency of 0.213 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

9　Map-model fit　ⓘ

This section contains information regarding the fit between EMDB map EMD-0760 and PDB model 6KS8. Per-residue inclusion information can be found in section 3 on page 9.

9.1　Map-model overlay　ⓘ

| X | Y | Z |
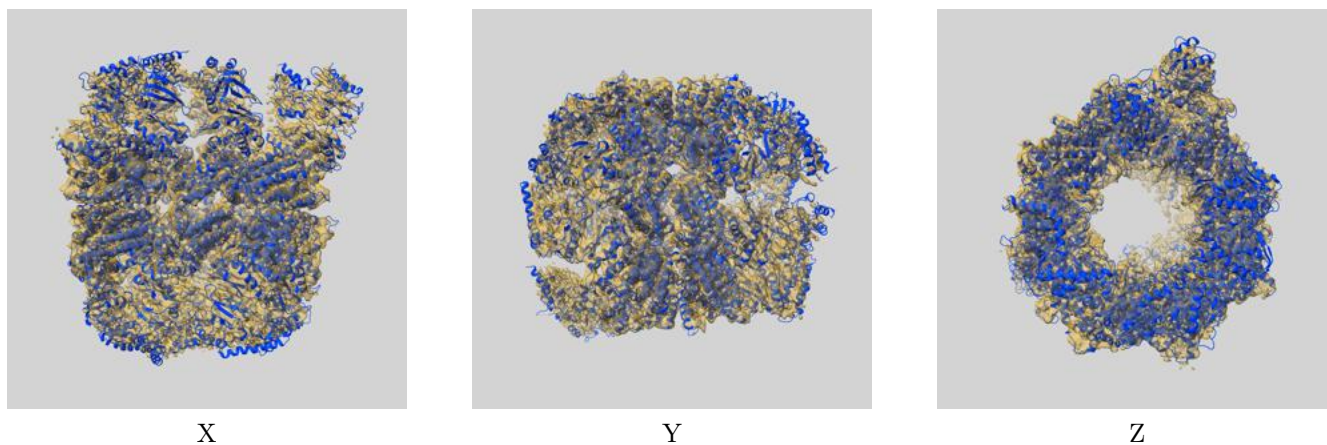
The images above show the 3D surface view of the map at the recommended contour level 0.85 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ
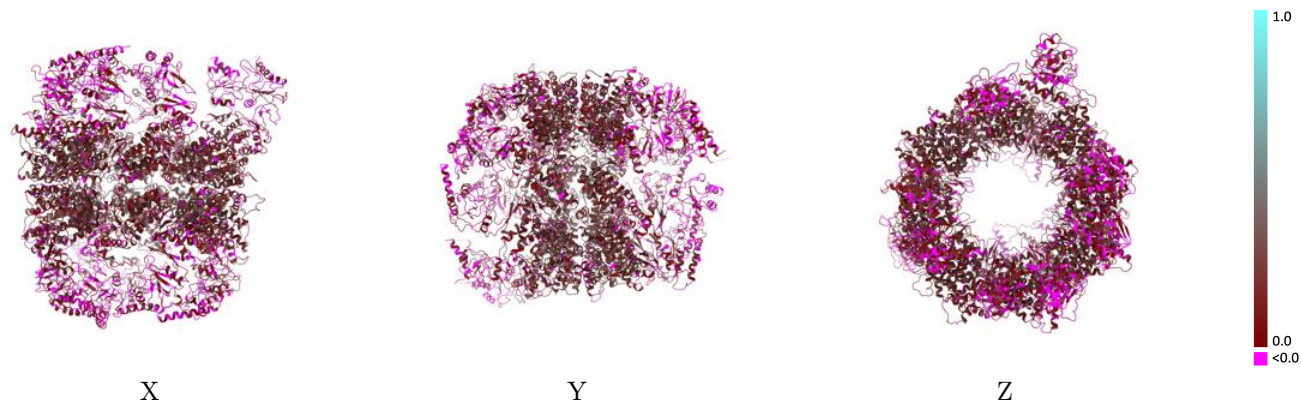
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ
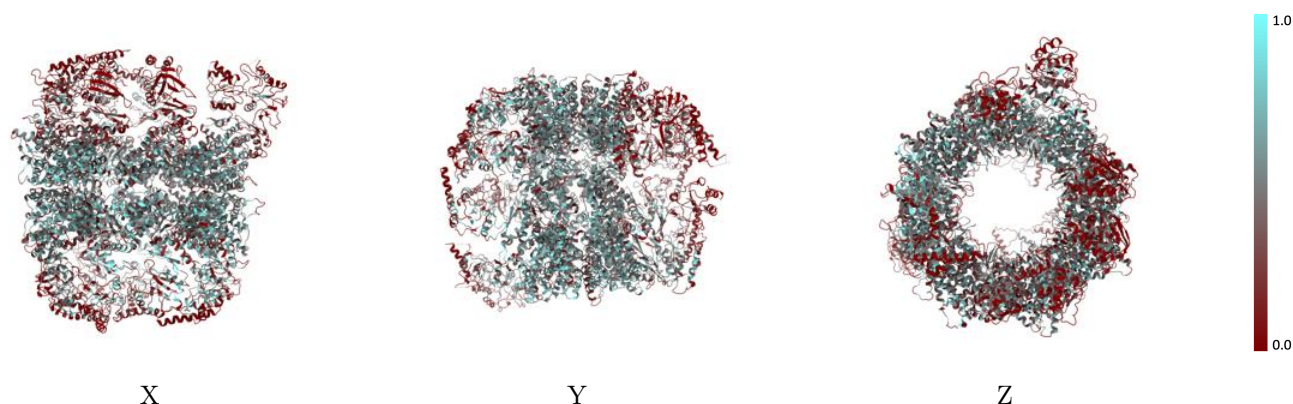
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.85).

9.4 Atom inclusion ⓘ
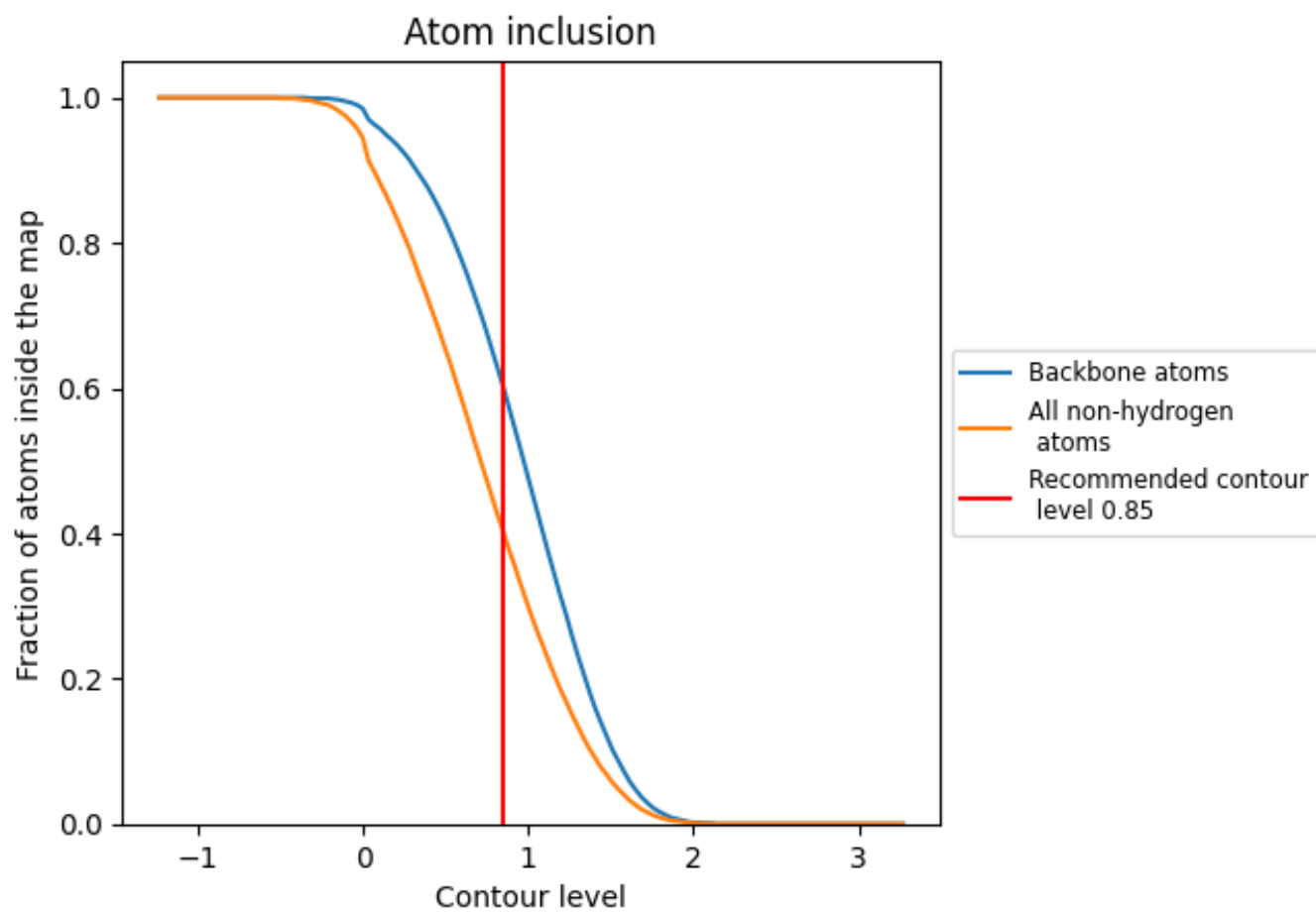
At the recommended contour level, 60% of all backbone atoms, 40% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.85) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4010	0.1340
A	0.3540	0.1310
B	0.3390	0.1300
D	0.2860	0.1030
E	0.3710	0.1140
G	0.3900	0.1390
H	0.3660	0.1270
Q	0.4040	0.1360
Z	0.4720	0.1730
a	0.4020	0.1280
b	0.4390	0.1390
d	0.3550	0.1160
e	0.4220	0.1170
g	0.4500	0.1440
h	0.4550	0.1360
q	0.4120	0.1340
z	0.4790	0.1750

1.0

0.0
<0.0