Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 10:43 am GMT

PDB ID	:	6QG0
EMDB ID	:	EMD-4543
Title	:	Structure of eIF2B-eIF2 (phosphorylated at Ser51) complex (model 1)
Authors	:	Llacer, J.L.; Gordiyenko, Y.; Ramakrishnan, V.
Deposited on	:	2019-01-10
Resolution	:	4.20 Å(reported)

This is a Full wwPDB EM Validation 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:

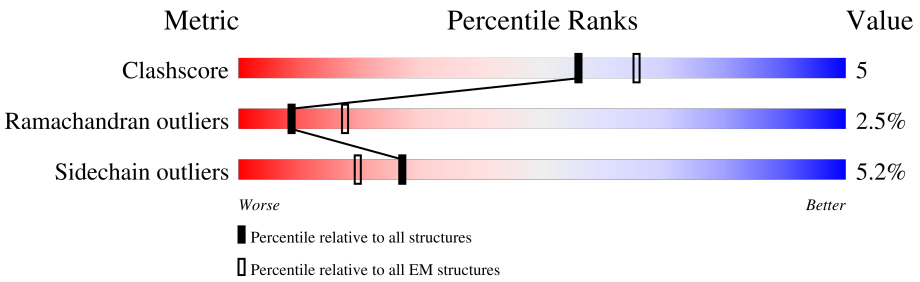
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	305	37%, 74%, 23%, • •
1	B	305	38%, 73%, 24%, • •
2	C	381	19%, 73%, 16%, •, 9%
2	D	381	19%, 74%, 15%, •, 9%
3	E	578	35%, 41%, 5%, •, 54%
3	F	578	35%, 42%, • •, 54%
4	G	651	12%, 43%, 10%, •, 45%
4	H	651	12%, 43%, 10%, •, 45%

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Mol	Chain	Length	Quality of chain
5	I	712	10% 50% 10% 39%
5	J	712	11% 52% 9% 39%
6	K	304	77% 62% 14% • 19%
6	L	304	79% 63% 14% • 19%
7	M	527	77% 69% 8% 23%
7	N	527	77% 70% 7% 23%
8	O	285	6% 6% 94%
8	P	285	6% 6% 94%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 36980 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 Translation initiation factor eIF-2B subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	302	2351	1504	394	443	10	0	0
1	B	302	2351	1504	394	443	10	0	0

- Molecule 2 is a protein called Translation initiation factor eIF-2B subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	345	2665	1694	463	502	6	0	0
2	C	345	2665	1694	463	502	6	0	0

- Molecule 3 is a protein called Translation initiation factor eIF-2B subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	267	2164	1391	363	400	10	0	0
3	F	267	2164	1391	363	400	10	0	0

- Molecule 4 is a protein called Translation initiation factor eIF-2B subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	355	2744	1738	474	521	11	0	0
4	H	355	2744	1738	474	521	11	0	0

- Molecule 5 is a protein called Translation initiation factor eIF-2B subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	431	3406	2147	573	666	20	0	0
5	J	431	3406	2147	573	666	20	0	0

- Molecule 6 is a protein called Eukaryotic translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
6	L	246	1973	1259	324	381	1	8	0	0
6	K	246	1973	1259	324	381	1	8	0	0

- Molecule 7 is a protein called Eukaryotic translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	M	408	3044	1934	546	548	16	0	0
7	N	408	3044	1934	546	548	16	0	0

- Molecule 8 is a protein called Eukaryotic translation initiation factor 2 subunit beta.

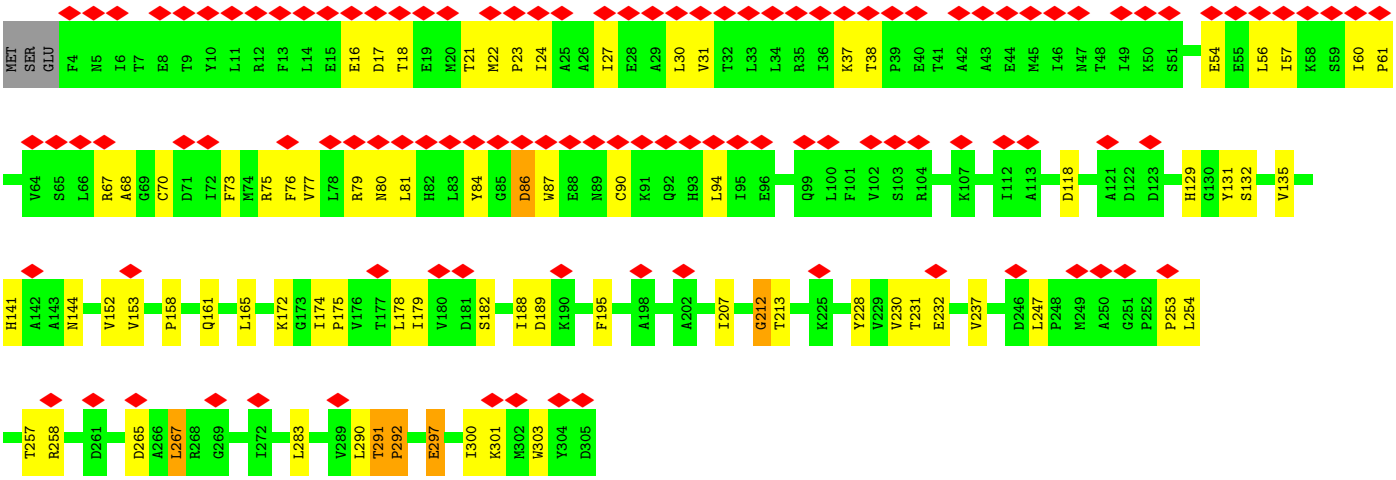
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	O	17	143	96	24	23	0	0
8	P	17	143	96	24	23	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

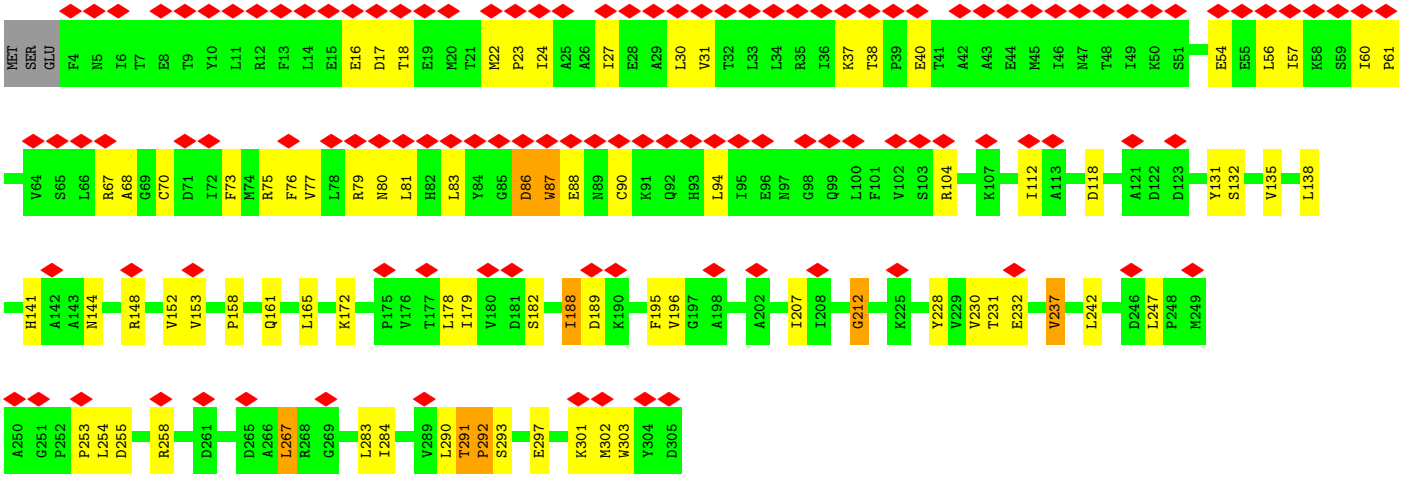
• Molecule 1: Translation initiation factor eIF-2B subunit alpha

Chain A: 37% 74% 23%



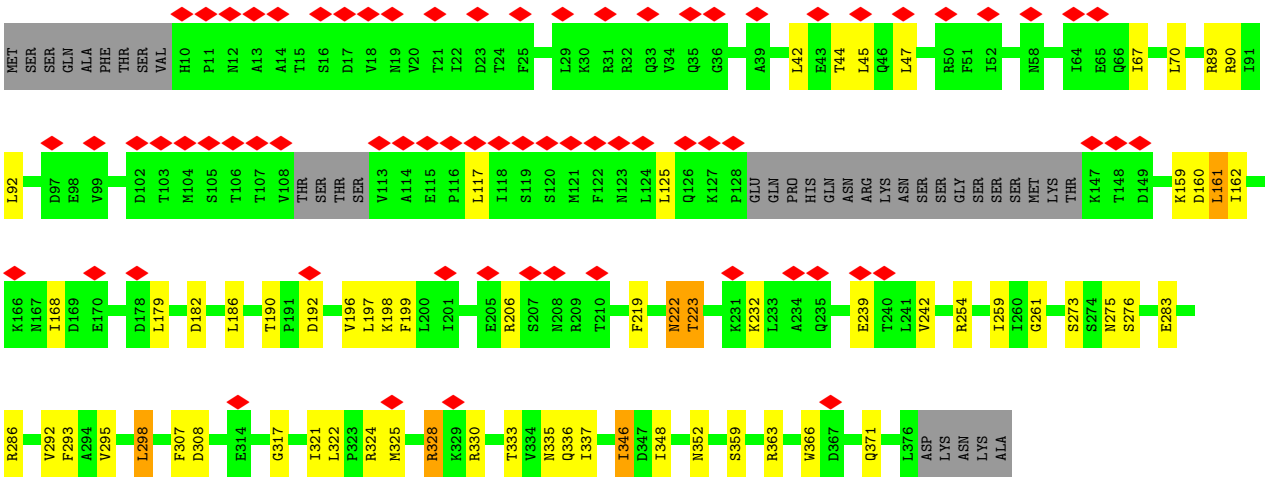
• Molecule 1: Translation initiation factor eIF-2B subunit alpha

Chain B: 38% 73% 24%



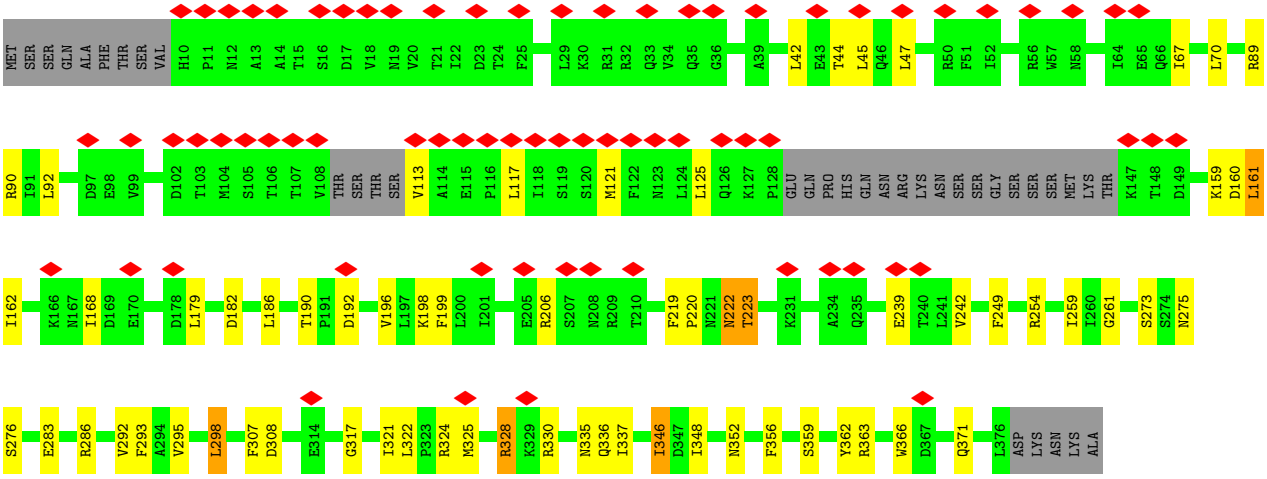
• Molecule 2: Translation initiation factor eIF-2B subunit beta

Chain D:



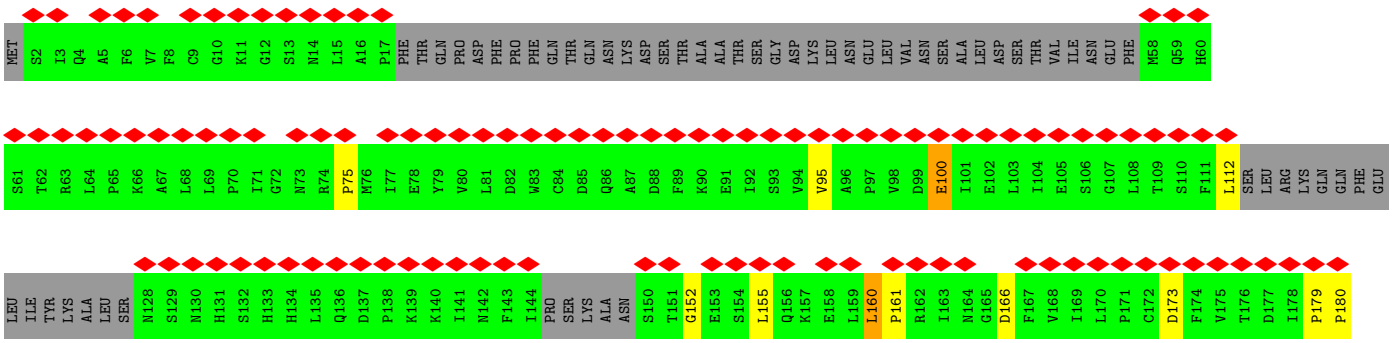
- Molecule 2: Translation initiation factor eIF-2B subunit beta

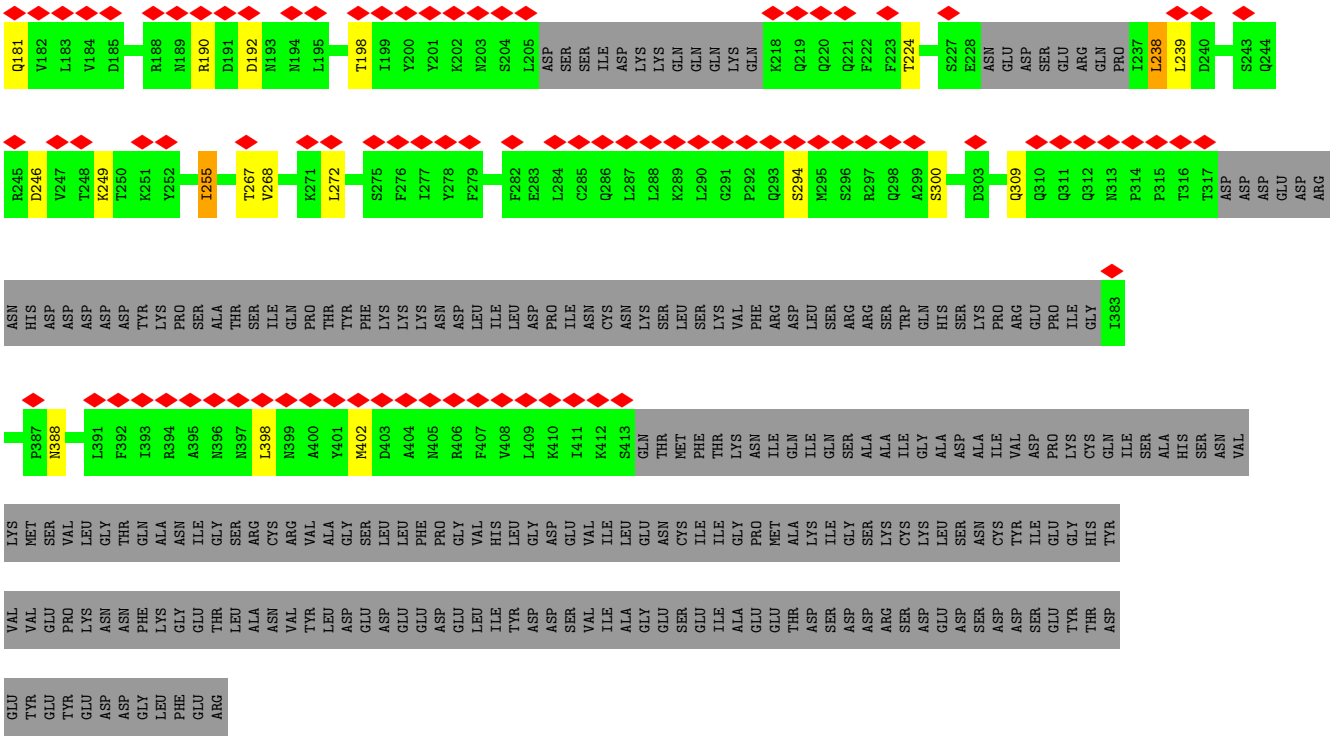
Chain C:



- Molecule 3: Translation initiation factor eIF-2B subunit gamma

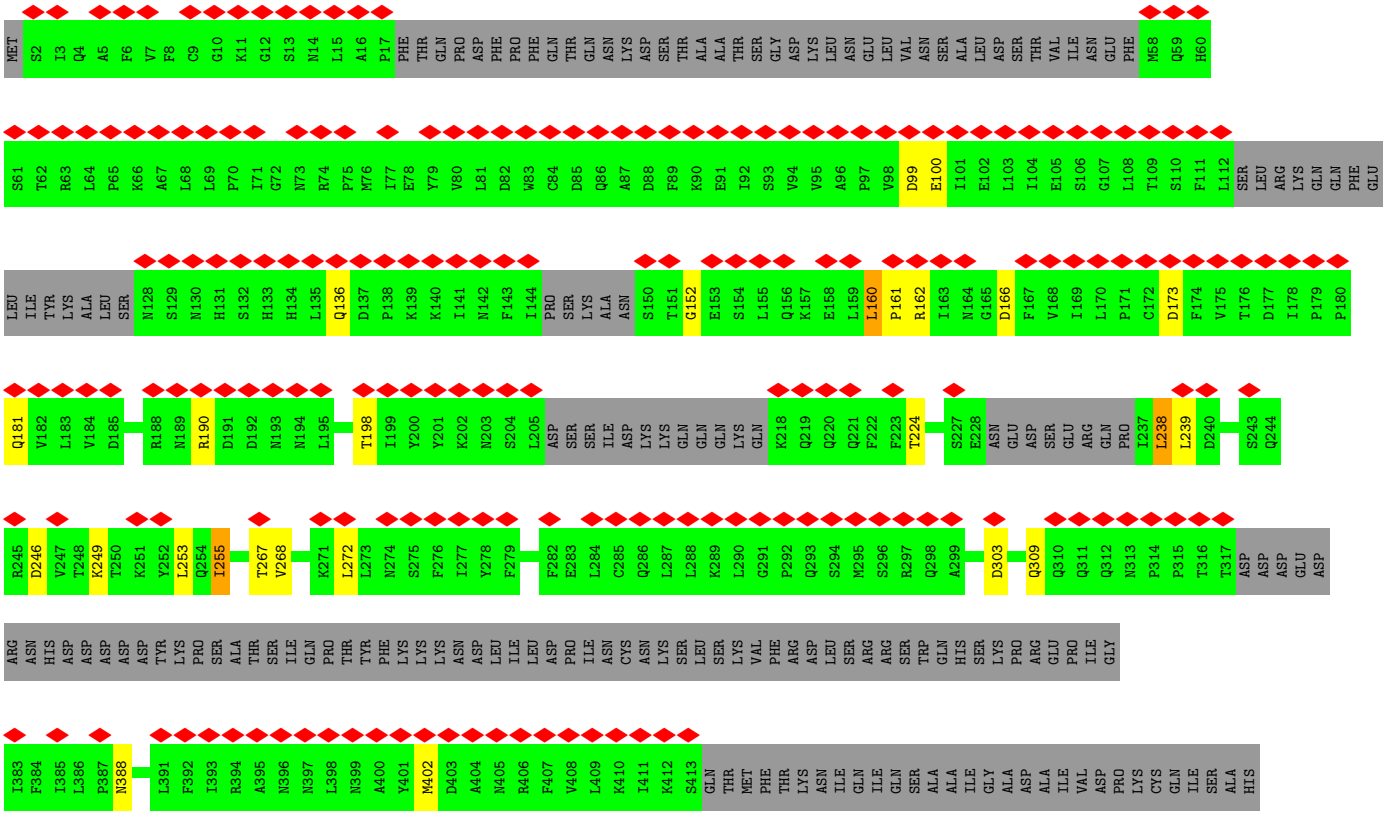
Chain E:

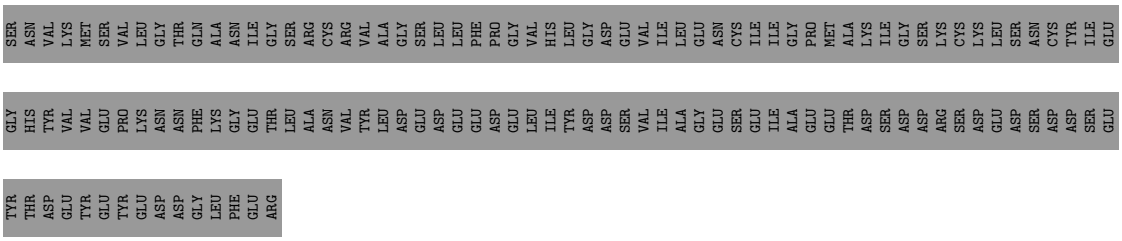




- Molecule 3: Translation initiation factor eIF-2B subunit gamma

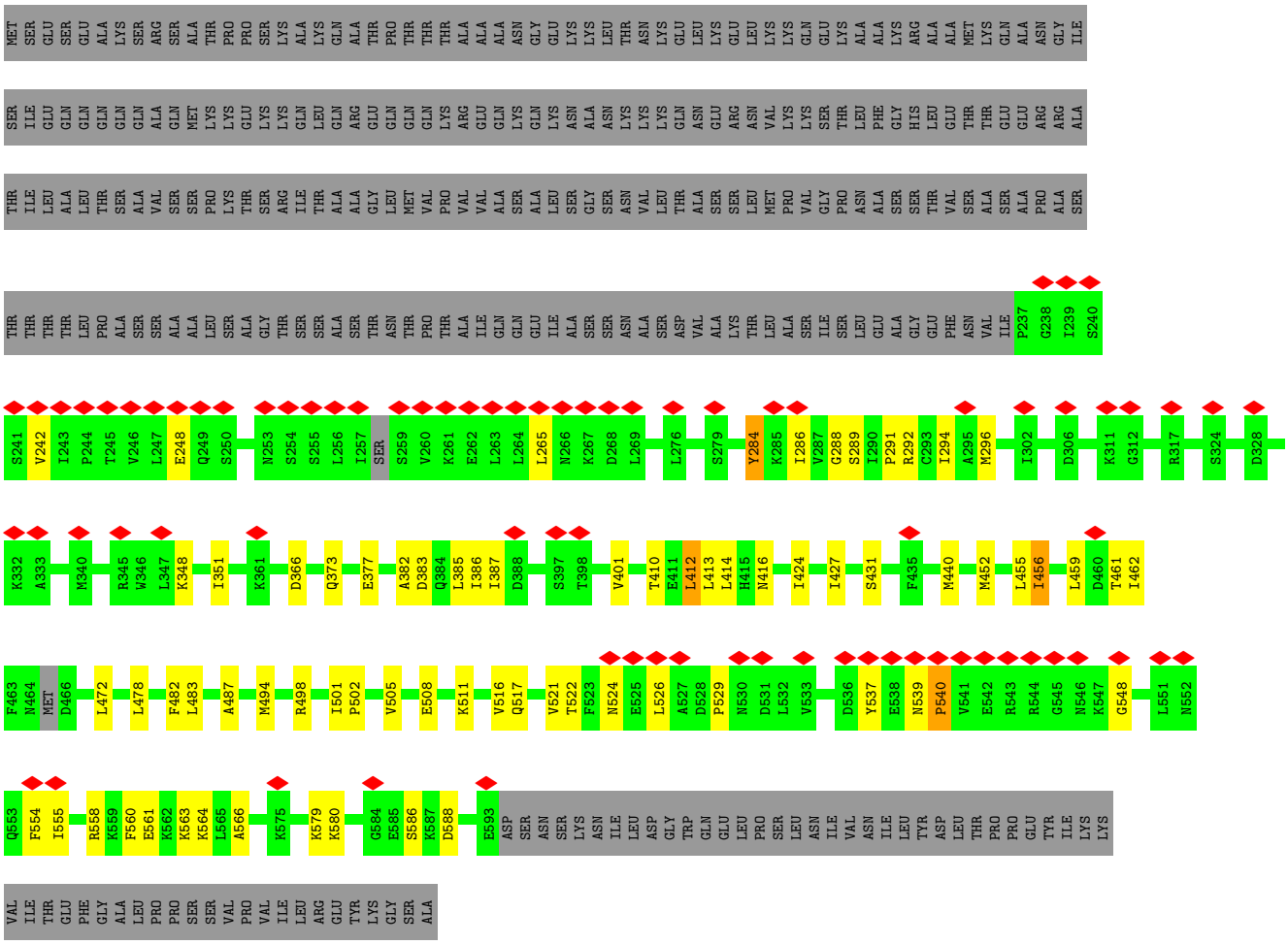
Chain F:





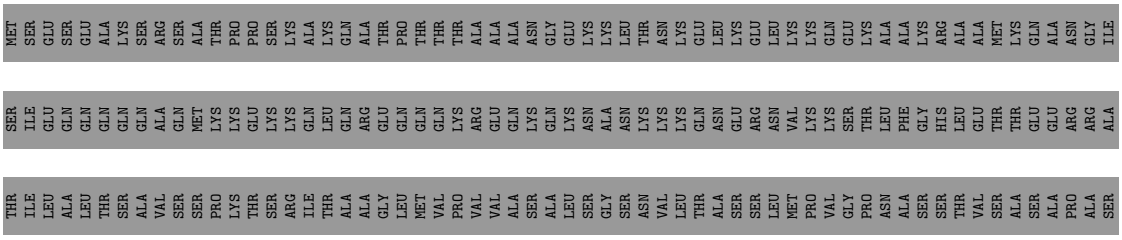
• Molecule 4: Translation initiation factor eIF-2B subunit delta

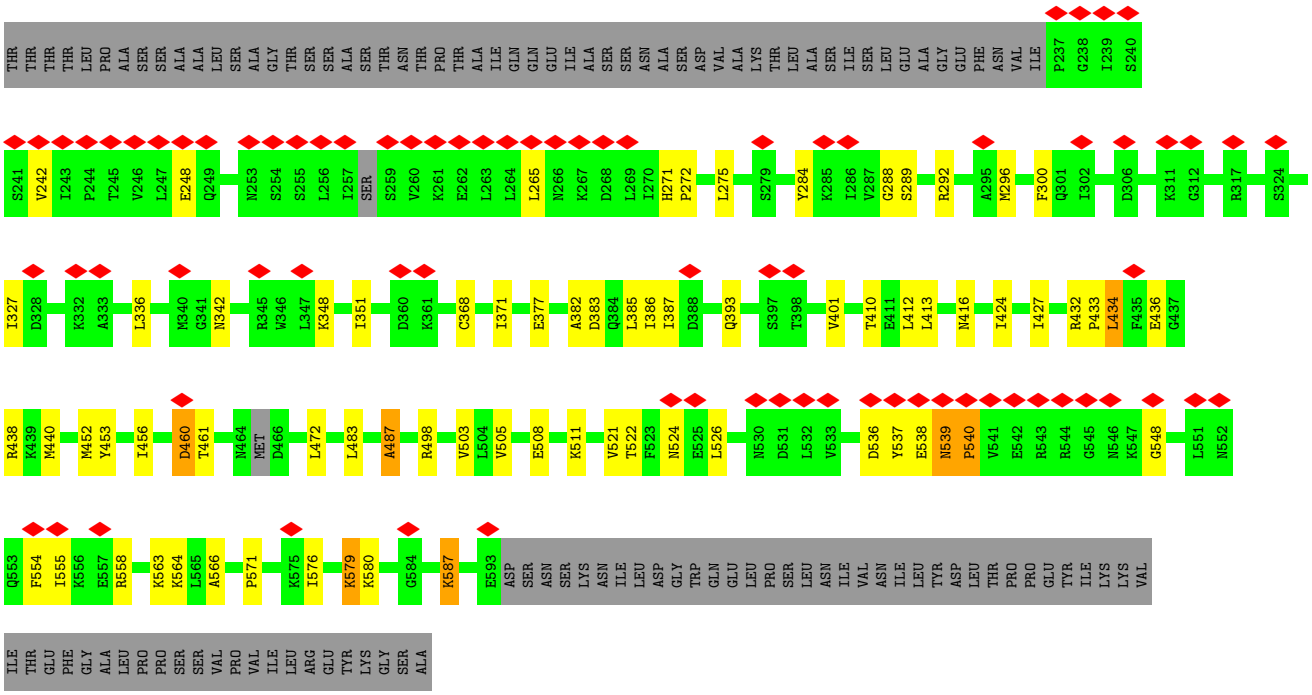
Chain G: 12% 43% 10% • 45%



• Molecule 4: Translation initiation factor eIF-2B subunit delta

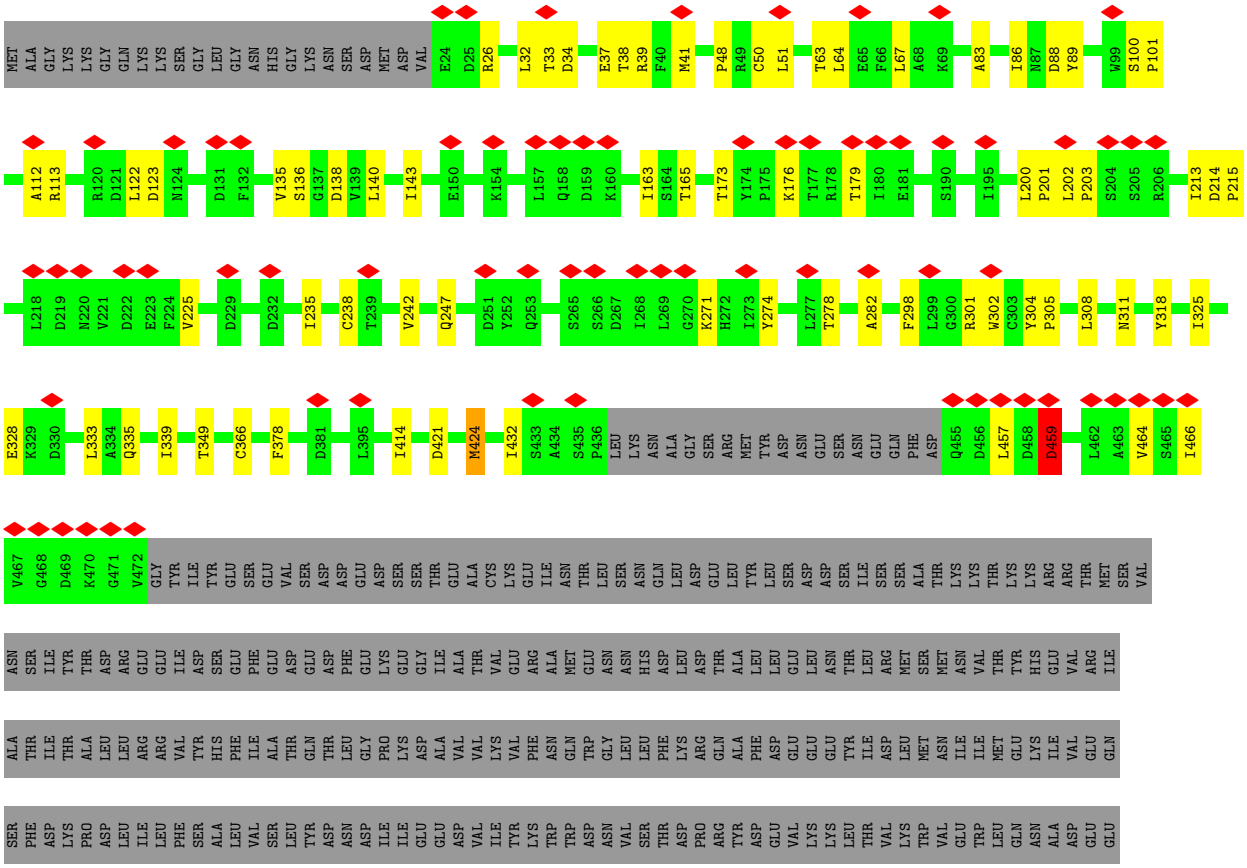
Chain H: 12% 43% 10% • 45%



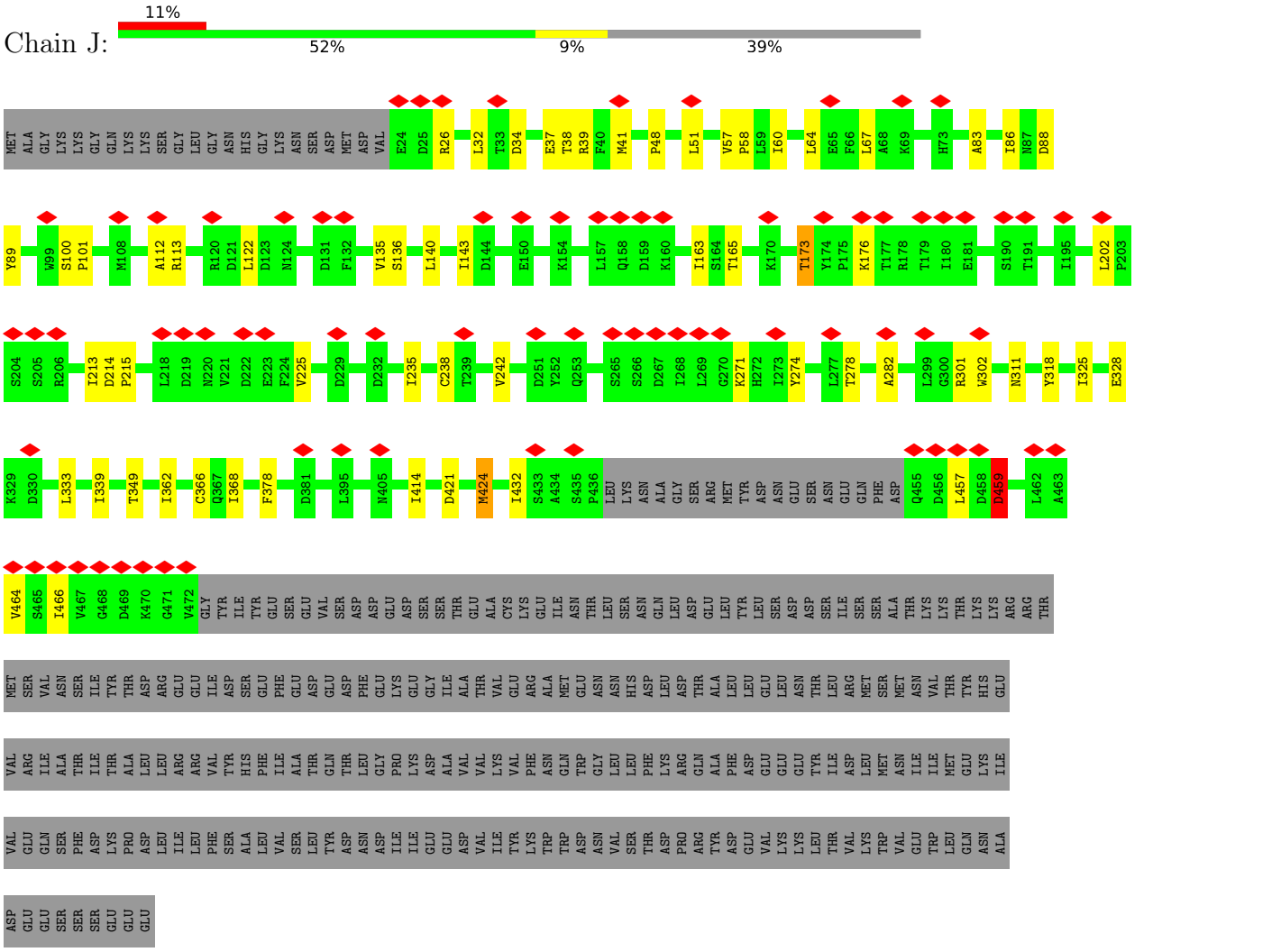


• Molecule 5: Translation initiation factor eIF-2B subunit epsilon

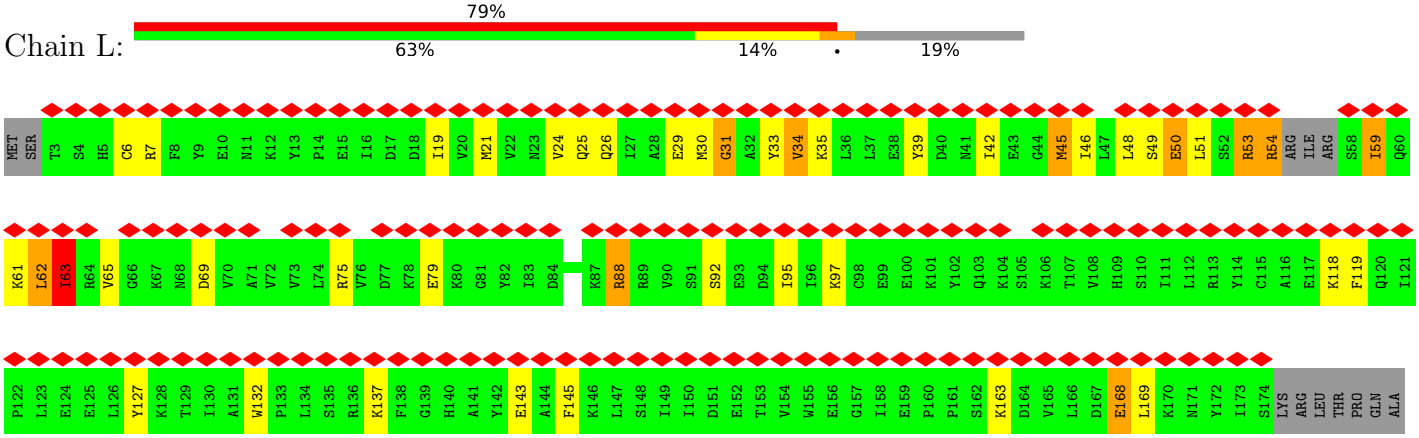
Chain I: 10% 50% 10% 39%

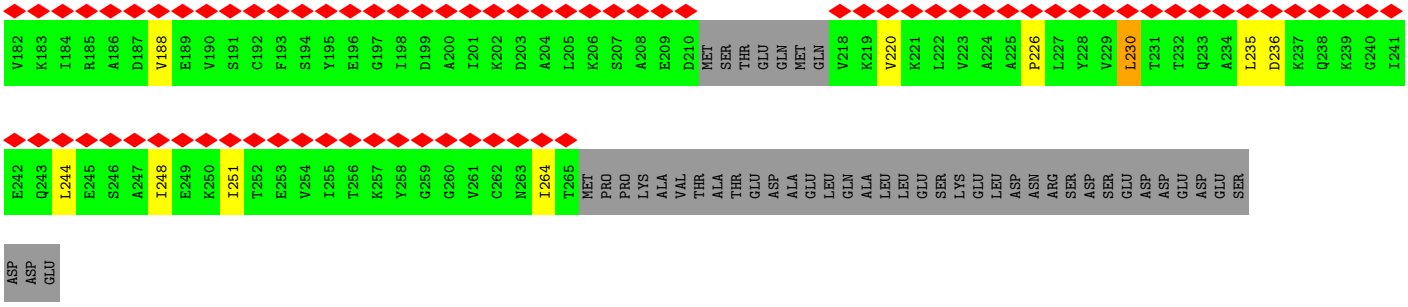


• Molecule 5: Translation initiation factor eIF-2B subunit epsilon



• Molecule 6: Eukaryotic translation initiation factor 2 subunit alpha



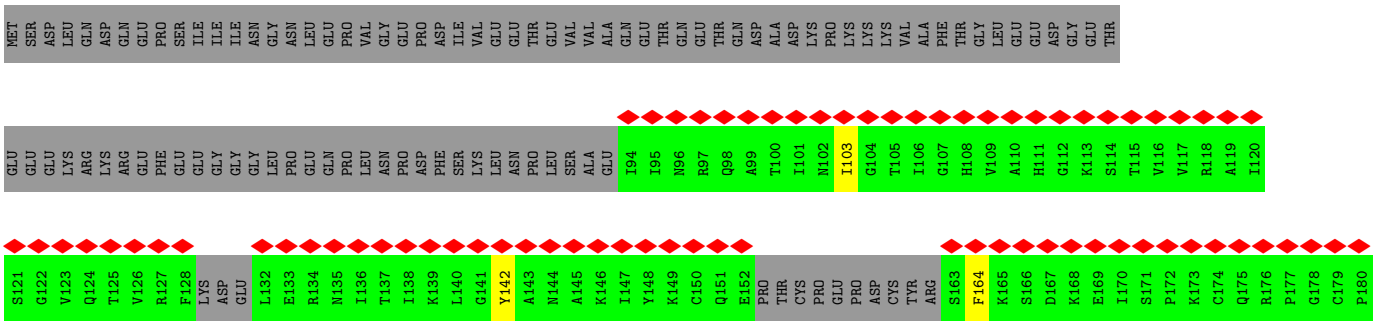


• Molecule 6: Eukaryotic translation initiation factor 2 subunit alpha

Chain K:

• Molecule 7: Eukaryotic translation initiation factor 2 subunit gamma

Chain M:



G181 R182 Y183 K184 L185 V186 R187 H188 V189 S190 F191 V192 D193 C194 P195 G196 H197 D198 I199 L200 M201 S202 T203 M204 L205 S206 G207 A208 A209 V210 M211 D212 A213 A214 L215 L216 L217 I218 A219 G220 N221 E222 S223 C224 P225 Q226 P227 Q228 T229 S230 E231 H232 L233 A234 A235 I236 E237 I238 M239 K240

L241 K242 H243 V244 I245 I246 L247 Q248 N249 K250 V251 D252 L253 M254 R255 E256 E257 S258 A259 L260 E261 H262 Q263 K264 S265 I266 L267 K268 F269 I270 R271 G272 T273 I274 A275 D276 G277 A278 P279 I280 V281 P282 I283 S284 A285 Q286 L287 K288 Y289 N290 I291 D292 A293 V294 N295 E296 F297 I298 V299 K300

T301 I302 P303 V304 P305 P306 R307 D308 F309 M310 I311 S312 P313 R314 L315 I316 V317 I318 R319 S320 F321 D322 V323 N324 K325 P326 G327 A328 E329 I330 E331 D332 L333 K334 G335 G336 V337 A338 G339 G340 S341 I342 L343 N344 G345 V346 F347 K348 L349 G350 D351 E352 I353 E354 I355 R356 P357 G358 I359 V360

T361 K362 D363 ASP K365 G366 K367 I368 Q369 C370 K371 P372 I373 F374 S375 N376 I377 V378 S379 L380 F381 A382 E383 Q384 N385 D386 L387 K388 F389 A390 V391 P392 G393 G394 L395 I396 G397 V398 G399 T400 K401 V402 D403 P404 T405 L406 C407 R408 A409 D410 R411 L412 V413 G414 Q415 V416 V417 G418 A419 K420

G421 H422 L423 P424 M425 I426 Y427 T428 D429 I430 E431 I432 M433 Y434 F435 L436 L437 R438 R439 L440 L441 G442 V443 K444 THR ASP GLY GLN K449 Q450 A451 K452 V453 R454 K455 L456 E457 P458 M459 E460 V461 L462 M463 V464 M465 I466 G467 S468 T469 A470 T471 G472 A473 R474 V475 V476 A477 V478 K479 A480

D481 M482 A483 R484 L485 Q486 L487 T488 S489 P490 A491 C492 T493 E494 I495 N496 E497 K498 I499 A500 L501 S502 R503 R504 I505 E506 K507 H508 W509 R510 L511 I512 G513 W514 A515 T516 I517 K518 K519 GLY THR THR LEU GLU PRO ILE ALA

- Molecule 7: Eukaryotic translation initiation factor 2 subunit gamma

Chain N: 77% 70% 7% 23%

MET SER ASP LEU GLN ASP GLN GLU PRO SER ILE ILE ILE ASN GLY ASN LEU GLU PRO VAL GLY GLU PRO ASP ILE VAL GLU GLU THR GLU VAL VAL ALA GLN GLU THR GLN GLU THR GLN ASP ALA ASP LYS PRO LYS LYS LYS VAL ALA PHE THR GLY LEU GLU GLU ASP GLY GLU THR

GLU GLU GLU LYS ARG LYS ARG GLU PHE GLU GLU GLY GLY GLY LEU PRO GLU GLN PRO LEU ASN PRO ASP PHE SER LYS LEU ASN PRO LEU SER ALA GLU I94 I95 N96 R97 Q98 A99 T100 I101 N102 I103 G104 T105 I106 G107 H108 V109 A110 H111 G112 K113 S114 T115 V116 V117 R118 A119 I120

S121 G122 V123 Q124 T125 V126 R127 F128 LYS ASP GLU L132 E133 R134 N135 I136 T137 I138 K139 L140 G141 Y142 A143 N144 A145 K146 I147 Y148 K149 C150 Q151 E152 PRO THR CYS PRO GLU PRO ASP CYS TYR ARG S163 F164 K165 S166 D167 K168 E169 I170 S171 P172 K173 C174 Q175 R176 P177 G178 C179 P180

G181 R182 Y183 K184 L185 V186 R187 H188 V189 S190 F191 V192 D193 C194 P195 G196 H197 D198 I199 L200 M201 S202 T203 M204 L205 S206 G207 A208 A209 V210 M211 D212 A213 A214 L215 L216 L217 I218 A219 G220 N221 E222 S223 C224 P225 Q226 P227 Q228 T229 S230 E231 H232 L233 A234 A235 I236 E237 I238 M239 K240

L241 K242 H243 V244 I245 I246 L247 Q248 N249 K250 V251 D252 L253 M254 R255 E256 E257 S258 A259 L260 E261 H262 Q263 K264 S265 I266 L267 K268 F269 I270 R271 G272 T273 I274 A275 D276 G277 A278 P279 I280 V281 P282 I283 S284 A285 Q286 L287 K288 Y289 N290 I291 D292 A293 V294 N295 E296 F297 I298 V299 K300

T301 I302 P303 V304 P305 P306 R307 D308 F309 M310 I311 S312 P313 R314 L315 I316 V317 I318 R319 S320 F321 D322 V323 N324 K325 P326 G327 A328 E329 I330 E331 D332 L333 K334 G335 G336 V337 A338 G339 G340 S341 I342 L343 N344 G345 V346 F347 K348 L349 G350 D351 E352 I353 E354 I355 R356 P357 G358 I359 V360

T361 K362 D363 ASP K365 G366 K367 I368 Q369 C370 K371 P372 I373 F374 S375 N376 I377 V378 S379 L380 F381 A382 E383 Q384 N385 D386 L387 K388 F389 A390 V391 P392 G393 G394 L395 I396 G397 V398 G399 T400 K401 V402 D403 P404 T405 L406 C407 R408 A409 D410 R411 L412 V413 G414 Q415 V416 V417 G418 A419 K420

G421 H422 L423 P424 N425 I426 Y427 T428 D429 I430 E431 I432 N433 Y434 F435 L436 L437 R438 R439 L440 L441 G442 V443 K444 THR ASP GLY GLN K449 Q450 A451 K452 V453 R454 K455 L456 E457 P458 N459 E460 V461 L462 M463 V464 N465 I466 G467 S468 T469 A470 T471 G472 A473 R474 V475 V476 A477 V478 K479 A480

D481 M482 A483 R484 L485 Q486 L487 T488 S489 P490 A491 C492 T493 E494 I495 N496 E497 K498 I499 A500 L501 S502 R503 R504 I505 E506 K507 H508 W509 R510 L511 I512 G513 W514 A515 T516 I517 K518 K519 GLY THR THR LEU GLU PRO ILE ALA

- Molecule 8: Eukaryotic translation initiation factor 2 subunit beta

Chain O: 6% 6% 94%

MET SER SER ASP LEU ALA ALA GLU LEU GLY PHE ASP PRO ALA LEU LYS LYS LYS LYS LYS THR LYS LYS VAL ILE PRO ASP ASP PHE ASP ALA ALA VAL ASN GLY LYS GLU ASN GLY SER GLY ASP ASP LEU PHE ALA GLY LEU LYS LYS LYS LYS LYS SER LYS SER VAL SER ALA

ASP ALA GLU ALA GLU LYS GLU PRO THR ASP ASP ILE ALA GLU ALA LEU GLY GLU LEU SER LEU LYS LYS LYS LYS LYS THR LYS ASP SER SER VAL ASP ALA PHE GLU LYS GLU LEU ALA LYS ALA GLY LEU ASP ASN VAL ASP ALA GLU SER LYS GLU GLY THR PRO SER ALA ASN

SER SER ILE GLN GLN GLU V127 G128 L129 P130 Y131 S132 E133 L134 L135 S136 R137 F138 F139 N140 I141 L142 R143 THR ASN ASN PRO GLU LEU ALA GLY ASP ARG SER GLY PRO LYS PHE ARG ILE PRO PRO PRO VAL CYS LEU ARG ASP GLY LYS LYS THR ILE PHE SER ASN ILE GLN ASP ILE

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

SER ILE ASN THR GLU LEU LYS ARG GLU GLN GLN SER ASN ARG LEU PHE PHE MET VAL CYS LYS SER CYS GLY SER THR ARG SER VAL SER SER ILE LYS THR GLY PHE GLN ALA THR VAL GLY LYS ARG ARG ARG MET

- Molecule 8: Eukaryotic translation initiation factor 2 subunit beta

Chain P: 6% 6% 94%

MET SER SER ASP LEU ALA ALA GLU LEU GLY PHE ASP PRO ALA LEU LYS LYS LYS LYS LYS THR LYS LYS VAL ILE PRO ASP ASP PHE ASP ALA ALA VAL ASN GLY LYS GLU ASN GLY SER GLY ASP ASP LEU PHE ALA GLY LEU LYS LYS LYS LYS LYS SER LYS SER VAL SER ALA

ASP ALA GLU ALA GLU LYS GLU PRO THR ASP ASP ILE ALA GLU ALA LEU GLY GLU LEU SER LEU LYS LYS LYS LYS LYS THR LYS ASP SER SER VAL ASP ALA PHE GLU LYS GLU LEU ALA LYS ALA GLY LEU ASP ASN VAL ASP ALA GLU SER LYS GLU GLY THR PRO SER ALA ASN

SER SER ILE GLN GLN GLU V127 G128 L129 P130 Y131 S132 E133 L134 L135 S136 R137 F138 F139 N140 I141 L142 R143 THR ASN ASN PRO GLU LEU ALA GLY ASP ARG SER GLY PRO LYS PHE ARG ILE PRO PRO PRO VAL CYS LEU ARG ASP GLY LYS LYS THR ILE PHE SER ASN ILE GLN ASP ILE

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

SER ILE ASN THR GLU LEU LYS ARG GLU GLN GLN SER ASN ARG LEU PHE PHE MET VAL CYS LYS SER CYS GLY SER THR ARG SER VAL SER SER ILE LYS THR GLY PHE GLN ALA THR VAL GLY LYS ARG ARG ARG MET

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	131663	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 ($e^-/Å^2$)	21	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.579	Depositor
Minimum map value	-0.341	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	375.2, 375.2, 375.2	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SEP

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	0.47	0/2395	0.66	0/3251
1	B	0.48	0/2395	0.65	0/3251
2	C	0.41	0/2714	0.64	0/3693
2	D	0.41	0/2714	0.64	0/3693
3	E	0.45	0/2209	0.59	0/2989
3	F	0.45	0/2209	0.59	0/2989
4	G	0.43	0/2781	0.66	1/3747 (0.0%)
4	H	0.43	0/2781	0.66	0/3747
5	I	0.41	0/3468	0.63	0/4704
5	J	0.41	0/3468	0.63	0/4704
6	K	0.46	0/1988	0.64	0/2674
6	L	0.47	0/1988	0.62	0/2674
7	M	0.42	0/3087	0.58	0/4173
7	N	0.42	0/3087	0.58	0/4173
8	O	0.51	0/146	0.62	0/196
8	P	0.51	0/146	0.63	0/196
All	All	0.43	0/37576	0.63	1/50854 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	412	LEU	CA-CB-CG	5.01	126.83	115.30

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	A	2351	0	2365	46	0
1	B	2351	0	2365	55	0
2	C	2665	0	2626	38	0
2	D	2665	0	2626	32	0
3	E	2164	0	2154	12	0
3	F	2164	0	2154	10	0
4	G	2744	0	2819	34	0
4	H	2744	0	2819	35	0
5	I	3406	0	3359	31	0
5	J	3406	0	3359	26	0
6	K	1973	0	2016	40	0
6	L	1973	0	2014	49	0
7	M	3044	0	3126	18	0
7	N	3044	0	3126	16	0
8	O	143	0	148	0	0
8	P	143	0	148	0	0
All	All	36980	0	37224	388	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 5.

All (388) 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)
6:L:25:GLN:OE1	6:L:35:LYS:HE2	1.34	1.21
6:L:25:GLN:OE1	6:L:35:LYS:CE	1.98	1.11
6:L:26:GLN:HG2	6:L:33:TYR:N	1.34	1.10
6:L:26:GLN:CG	6:L:33:TYR:N	2.18	1.06
1:A:31:VAL:HG22	1:A:73:PHE:CE2	1.89	1.06
1:B:81:LEU:HG	1:B:90:CYS:SG	1.95	1.05
1:A:31:VAL:CG2	1:A:73:PHE:HE2	1.70	1.03
6:L:30:MET:O	6:L:48:LEU:HD12	1.58	1.00
1:A:31:VAL:CG2	1:A:73:PHE:CE2	2.46	0.98
6:K:24:VAL:O	6:K:65:VAL:HG23	1.66	0.95
1:B:31:VAL:CG2	1:B:73:PHE:HE2	1.81	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:25:GLN:OE1	6:L:35:LYS:CD	2.16	0.93
1:B:31:VAL:HG22	1:B:73:PHE:CE2	2.04	0.92
6:K:21:MET:SD	6:K:69:ASP:O	2.28	0.91
1:A:77:VAL:HA	1:A:94:LEU:HD21	1.53	0.91
6:L:21:MET:SD	6:L:69:ASP:O	2.29	0.90
6:K:54:ARG:HB3	6:K:54:ARG:HH11	1.34	0.90
1:B:31:VAL:CG2	1:B:73:PHE:CE2	2.58	0.86
1:B:77:VAL:HA	1:B:94:LEU:HD21	1.56	0.86
1:A:31:VAL:HG22	1:A:73:PHE:HE2	1.31	0.85
6:K:88:ARG:HH21	6:K:88:ARG:HG2	1.43	0.84
1:B:80:ASN:HB3	1:B:90:CYS:SG	2.19	0.83
1:A:80:ASN:HB3	1:A:90:CYS:SG	2.20	0.82
6:L:26:GLN:HG2	6:L:33:TYR:H	1.45	0.81
1:B:75:ARG:NH1	1:B:303:TRP:HA	1.96	0.81
1:A:31:VAL:HG22	1:A:73:PHE:CZ	2.16	0.80
6:K:27:ILE:HG21	6:K:64:ARG:NH2	1.98	0.79
1:A:77:VAL:HA	1:A:94:LEU:CD2	2.13	0.79
6:L:25:GLN:H	6:L:34:VAL:HG12	1.49	0.77
1:B:31:VAL:HG22	1:B:73:PHE:HE2	1.43	0.77
6:K:25:GLN:H	6:K:34:VAL:HG12	1.49	0.76
3:E:160:LEU:H	3:E:161:PRO:HD2	1.49	0.76
3:F:160:LEU:H	3:F:161:PRO:HD2	1.50	0.76
6:K:54:ARG:HH11	6:K:54:ARG:CB	1.98	0.76
6:L:88:ARG:HG2	6:L:88:ARG:HH21	1.49	0.75
1:A:84:TYR:CE1	6:L:88:ARG:HD2	2.23	0.74
6:K:24:VAL:HB	6:K:65:VAL:HA	1.69	0.74
6:L:26:GLN:HG2	6:L:33:TYR:CA	2.18	0.73
1:A:267:LEU:HA	1:B:178:LEU:HD23	1.73	0.71
6:K:50:GLU:HA	6:K:50:GLU:OE1	1.89	0.71
6:L:53:ARG:HD2	6:L:88:ARG:CG	2.21	0.70
6:K:25:GLN:HB2	6:K:34:VAL:HA	1.73	0.70
6:K:27:ILE:CG2	6:K:64:ARG:NH2	2.56	0.69
1:A:75:ARG:NH1	1:A:303:TRP:HA	2.08	0.68
1:B:31:VAL:HG22	1:B:73:PHE:CZ	2.28	0.68
1:A:31:VAL:HG23	1:A:73:PHE:CE2	2.29	0.67
1:B:75:ARG:HH11	1:B:303:TRP:HA	1.60	0.66
1:B:77:VAL:HA	1:B:94:LEU:CD2	2.24	0.66
6:K:88:ARG:HG2	6:K:88:ARG:NH2	2.11	0.65
2:D:321:ILE:HD11	2:D:335:ASN:HB2	1.79	0.65
1:A:297:GLU:O	1:A:301:LYS:HG3	1.97	0.65
1:A:178:LEU:HD23	1:B:267:LEU:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:255:ILE:HD11	5:I:213:ILE:HD11	1.79	0.64
5:J:349:THR:HG22	5:J:366:CYS:H	1.63	0.63
6:K:27:ILE:HG21	6:K:64:ARG:HH21	1.62	0.63
1:A:84:TYR:CE1	6:L:50:GLU:OE1	2.53	0.62
3:E:255:ILE:HD11	5:J:213:ILE:HD11	1.81	0.62
6:L:25:GLN:OE1	6:L:35:LYS:HD3	1.99	0.62
5:I:349:THR:HG22	5:I:366:CYS:H	1.63	0.62
1:B:40:GLU:O	6:K:75:ARG:NE	2.33	0.61
4:G:373:GLN:O	4:G:377:GLU:HG3	2.01	0.60
1:A:84:TYR:HE1	6:L:50:GLU:OE1	1.83	0.60
6:L:24:VAL:HB	6:L:65:VAL:HA	1.84	0.60
6:L:65:VAL:HG23	6:L:65:VAL:O	2.02	0.60
4:H:587:LYS:HZ3	2:C:356:PHE:HD1	1.50	0.59
2:C:321:ILE:HD11	2:C:335:ASN:HB2	1.84	0.59
1:B:68:ALA:HB2	1:B:237:VAL:HG22	1.83	0.59
4:H:377:GLU:OE1	6:K:61:LYS:HB3	2.03	0.59
1:B:67:ARG:O	1:B:70:CYS:SG	2.56	0.58
7:N:142:TYR:HB2	7:N:319:ARG:HH12	1.68	0.58
6:K:54:ARG:HH11	6:K:54:ARG:CG	2.16	0.58
1:A:68:ALA:HB2	1:A:237:VAL:HG22	1.85	0.58
6:L:50:GLU:OE1	6:L:50:GLU:HA	2.03	0.58
5:I:163:ILE:HD11	5:I:271:LYS:HB3	1.86	0.58
5:J:163:ILE:HD11	5:J:271:LYS:HB3	1.85	0.58
2:D:292:VAL:HB	2:D:346:ILE:HA	1.85	0.58
2:C:90:ARG:HG2	2:C:161:LEU:HD21	1.85	0.58
1:B:301:LYS:HD3	2:C:121:MET:H	1.69	0.57
4:G:461:THR:HG21	2:C:336:GLN:HG2	1.84	0.57
2:C:292:VAL:HB	2:C:346:ILE:HA	1.86	0.57
6:L:26:GLN:HG2	6:L:33:TYR:C	2.24	0.57
6:L:25:GLN:CD	6:L:35:LYS:HG2	2.25	0.57
2:D:90:ARG:HG2	2:D:161:LEU:HD21	1.87	0.57
4:H:383:ASP:HA	4:H:386:ILE:HD12	1.86	0.57
6:K:220:VAL:HG13	6:K:230:LEU:HB3	1.86	0.57
2:C:196:VAL:HG21	2:C:261:GLY:HA2	1.86	0.57
1:B:31:VAL:HG23	1:B:73:PHE:CE2	2.37	0.56
3:E:267:THR:HG23	5:J:225:VAL:HG22	1.86	0.56
1:A:135:VAL:HG22	1:A:230:VAL:HB	1.88	0.56
1:B:75:ARG:HD3	1:B:302:MET:O	2.06	0.56
6:L:26:GLN:HG3	6:L:34:VAL:HG13	1.87	0.56
6:K:24:VAL:C	6:K:65:VAL:HG23	2.27	0.55
2:D:298:LEU:HG	2:D:352:ASN:HD21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:196:VAL:HG21	2:D:261:GLY:HA2	1.88	0.55
6:L:53:ARG:HD2	6:L:88:ARG:HG3	1.88	0.54
7:M:307:ARG:HD3	7:M:392:PRO:HB2	1.89	0.54
1:A:283:LEU:HB3	1:A:291:THR:HA	1.89	0.54
1:B:292:PRO:HB2	2:C:359:SER:OG	2.07	0.54
4:G:498:ARG:HD2	2:C:283:GLU:OE1	2.07	0.54
7:N:307:ARG:HD3	7:N:392:PRO:HB2	1.90	0.54
6:L:26:GLN:CG	6:L:33:TYR:O	2.55	0.54
6:L:220:VAL:HG13	6:L:230:LEU:HB3	1.89	0.54
1:B:132:SER:HB3	1:B:135:VAL:HG23	1.90	0.54
2:C:298:LEU:HG	2:C:352:ASN:HD21	1.71	0.54
2:D:168:ILE:HG23	2:D:352:ASN:HD22	1.73	0.53
4:G:483:LEU:HB3	4:G:566:ALA:HB3	1.90	0.53
4:H:438:ARG:HH12	4:H:538:GLU:HA	1.74	0.53
1:A:67:ARG:O	1:A:70:CYS:SG	2.62	0.53
3:F:198:THR:HB	3:F:272:LEU:HB3	1.90	0.53
2:C:168:ILE:HG23	2:C:352:ASN:HD22	1.74	0.53
4:G:579:LYS:HG2	4:G:580:LYS:HG3	1.89	0.53
6:L:88:ARG:HG2	6:L:88:ARG:NH2	2.22	0.53
4:G:382:ALA:HA	4:G:385:LEU:HD12	1.91	0.53
6:L:25:GLN:OE1	6:L:35:LYS:CG	2.55	0.53
1:A:76:PHE:CE2	2:D:125:LEU:HA	2.44	0.53
1:A:132:SER:HB3	1:A:135:VAL:HG23	1.91	0.53
4:G:383:ASP:HA	4:G:386:ILE:HD12	1.91	0.53
4:H:483:LEU:HB3	4:H:566:ALA:HB3	1.91	0.53
7:M:375:SER:HB3	7:M:402:VAL:HG23	1.91	0.53
2:D:336:GLN:HG2	4:H:461:THR:HG21	1.90	0.53
6:K:46:ILE:HB	6:K:51:LEU:HD11	1.89	0.53
1:A:152:VAL:HG13	1:A:179:ILE:HD13	1.91	0.53
1:A:195:PHE:HA	1:A:228:TYR:HB2	1.91	0.53
4:G:524:ASN:HD22	4:G:526:LEU:HG	1.73	0.52
7:N:462:LEU:HD22	7:N:503:ARG:HG2	1.91	0.52
7:M:462:LEU:HD22	7:M:503:ARG:HG2	1.91	0.52
6:L:26:GLN:OE1	6:L:31:GLY:O	2.27	0.52
3:F:246:ASP:HA	3:F:249:LYS:HB3	1.91	0.52
4:H:539:ASN:HB2	4:H:540:PRO:HD3	1.92	0.52
6:L:24:VAL:HG12	6:L:65:VAL:HG12	1.91	0.52
6:L:118:LYS:HE3	6:L:168:GLU:HG2	1.91	0.52
4:H:472:LEU:HB2	4:H:505:VAL:HG22	1.92	0.52
1:B:79:ARG:NE	1:B:79:ARG:HA	2.25	0.52
1:B:135:VAL:HG22	1:B:230:VAL:HB	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:VAL:HG13	1:B:179:ILE:HD13	1.92	0.51
7:N:103:ILE:HG12	7:N:213:ALA:HB3	1.92	0.51
3:F:267:THR:HG23	5:I:225:VAL:HG22	1.91	0.51
6:L:26:GLN:HG2	6:L:33:TYR:O	2.11	0.51
7:M:238:ILE:HG12	7:M:514:TRP:HB3	1.92	0.51
4:H:410:THR:HG22	4:H:440:MET:HG3	1.92	0.51
7:N:238:ILE:HG12	7:N:514:TRP:HB3	1.92	0.51
7:N:375:SER:HB3	7:N:402:VAL:HG23	1.92	0.51
1:A:79:ARG:HA	1:A:79:ARG:NE	2.26	0.51
6:L:25:GLN:OE1	6:L:35:LYS:HG2	2.11	0.51
7:N:354:GLU:HB2	7:N:372:PRO:HB2	1.92	0.51
4:G:508:GLU:H	4:G:511:LYS:HD2	1.76	0.51
3:E:190:ARG:HH12	3:E:238:LEU:HD12	1.76	0.51
4:H:434:LEU:HD13	4:H:436:GLU:HG3	1.93	0.51
4:G:288:GLY:HA2	4:G:292:ARG:HH21	1.76	0.51
4:H:579:LYS:HG2	4:H:580:LYS:HG3	1.93	0.50
5:J:414:ILE:HG12	5:J:432:ILE:HD12	1.92	0.50
2:D:196:VAL:HG22	2:D:295:VAL:HB	1.94	0.50
4:G:410:THR:HG22	4:G:440:MET:HG3	1.94	0.50
7:M:103:ILE:HG12	7:M:213:ALA:HB3	1.94	0.50
4:H:487:ALA:HA	4:H:564:LYS:HE3	1.93	0.50
6:K:26:GLN:HE21	6:K:32:ALA:HA	1.76	0.50
1:A:27:ILE:HG23	1:A:73:PHE:HD2	1.77	0.50
4:G:558:ARG:HA	2:C:242:VAL:HB	1.92	0.50
1:A:292:PRO:HB2	2:D:359:SER:OG	2.12	0.50
4:H:587:LYS:NZ	2:C:356:PHE:HB3	2.27	0.50
2:D:254:ARG:HH12	4:H:521:VAL:HG11	1.77	0.49
3:E:198:THR:HB	3:E:272:LEU:HB3	1.94	0.49
3:E:246:ASP:HA	3:E:249:LYS:HB3	1.94	0.49
6:L:24:VAL:HG21	6:L:63:ILE:HD11	1.94	0.49
6:K:118:LYS:HE3	6:K:168:GLU:HG2	1.93	0.49
3:E:294:SER:HA	3:E:300:SER:HB3	1.95	0.49
4:H:524:ASN:HD22	4:H:526:LEU:HG	1.77	0.49
5:I:301:ARG:HB3	2:C:317:GLY:HA2	1.93	0.49
1:A:57:ILE:HA	1:A:60:ILE:HD12	1.94	0.49
1:A:267:LEU:HA	1:B:178:LEU:HB3	1.94	0.49
4:H:432:ARG:H	4:H:433:PRO:HD2	1.78	0.49
1:B:80:ASN:C	1:B:90:CYS:SG	2.91	0.49
6:K:27:ILE:HG13	6:K:28:ALA:H	1.77	0.48
2:C:196:VAL:HG22	2:C:295:VAL:HB	1.95	0.48
4:H:348:LYS:HA	4:H:351:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:302:TRP:CZ2	2:C:328:ARG:HG3	2.49	0.48
6:L:53:ARG:HD2	6:L:88:ARG:HG2	1.94	0.48
6:K:54:ARG:CG	6:K:54:ARG:NH1	2.75	0.48
1:B:83:LEU:HD23	2:C:113:VAL:N	2.29	0.48
1:B:118:ASP:HB3	2:C:307:PHE:CD1	2.48	0.48
1:B:76:PHE:CE2	2:C:125:LEU:HA	2.48	0.48
3:E:224:THR:HG22	3:E:268:VAL:HG22	1.95	0.48
4:G:401:VAL:HG22	4:G:427:ILE:HB	1.96	0.48
4:G:427:ILE:HG12	4:G:452:MET:HB2	1.96	0.48
1:B:112:ILE:HG22	1:B:138:LEU:HD21	1.96	0.48
2:D:44:THR:HA	2:D:47:LEU:HD12	1.95	0.48
5:I:325:ILE:HD13	5:I:339:ILE:HD13	1.94	0.48
7:N:215:LEU:HD23	7:N:245:ILE:HB	1.96	0.48
1:B:57:ILE:HA	1:B:60:ILE:HD12	1.96	0.48
5:I:165:THR:HA	5:I:274:TYR:HB2	1.96	0.48
4:G:348:LYS:HA	4:G:351:ILE:HD12	1.95	0.47
4:H:288:GLY:HA2	4:H:292:ARG:HH21	1.78	0.47
4:H:401:VAL:HG22	4:H:427:ILE:HB	1.96	0.47
5:J:325:ILE:HD13	5:J:339:ILE:HD13	1.95	0.47
1:B:195:PHE:HA	1:B:228:TYR:HB2	1.95	0.47
5:J:83:ALA:HA	5:J:86:ILE:HD12	1.96	0.47
1:A:178:LEU:HB3	1:B:267:LEU:HA	1.95	0.47
1:B:131:TYR:HB3	1:B:161:GLN:HE22	1.79	0.47
4:G:383:ASP:O	4:G:387:ILE:HG12	2.14	0.47
7:M:424:PRO:HB3	7:M:494:GLU:HG3	1.97	0.47
7:N:337:VAL:HA	7:N:399:GLY:HA2	1.96	0.47
1:A:182:SER:HB2	1:B:212:GLY:HA3	1.97	0.47
5:J:64:LEU:HA	5:J:67:LEU:HD12	1.97	0.47
1:A:212:GLY:HA3	1:B:182:SER:HB2	1.97	0.47
1:B:87:TRP:CE3	6:K:75:ARG:NH2	2.83	0.47
4:G:539:ASN:HB2	4:G:540:PRO:HD3	1.97	0.47
4:G:561:GLU:HB2	4:G:564:LYS:HE2	1.97	0.47
4:H:383:ASP:O	4:H:387:ILE:HG12	2.14	0.47
5:I:32:LEU:HB2	5:I:136:SER:HA	1.97	0.47
3:F:190:ARG:HH12	3:F:238:LEU:HD12	1.79	0.47
6:K:92:SER:HA	6:K:95:ILE:HD12	1.97	0.47
2:C:44:THR:HA	2:C:47:LEU:HD12	1.96	0.47
4:H:427:ILE:HG12	4:H:452:MET:HB2	1.97	0.47
6:L:59:ILE:HD13	6:L:62:LEU:HB2	1.95	0.47
7:M:330:ILE:HB	6:K:205:LEU:HG	1.97	0.47
7:N:424:PRO:HB3	7:N:494:GLU:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:317:GLY:HA2	5:J:301:ARG:HB3	1.97	0.46
4:G:472:LEU:HB2	4:G:505:VAL:HG22	1.96	0.46
5:I:64:LEU:HA	5:I:67:LEU:HD12	1.97	0.46
5:J:432:ILE:HG12	5:J:459:ASP:HB2	1.97	0.46
6:K:46:ILE:HG21	6:K:51:LEU:HD21	1.97	0.46
6:K:248:ILE:HG12	6:K:264:ILE:HG21	1.97	0.46
3:F:136:GLN:HG3	3:F:162:ARG:HH12	1.80	0.46
6:L:30:MET:O	6:L:48:LEU:CD1	2.47	0.46
5:J:165:THR:HA	5:J:274:TYR:HB2	1.98	0.46
6:K:53:ARG:HD2	6:K:88:ARG:CG	2.45	0.46
2:D:283:GLU:O	4:H:498:ARG:NH2	2.49	0.46
2:D:328:ARG:HG3	5:J:302:TRP:CZ2	2.50	0.46
5:I:83:ALA:HA	5:I:86:ILE:HD12	1.97	0.46
7:M:215:LEU:HD23	7:M:245:ILE:HB	1.97	0.46
7:M:337:VAL:HA	7:M:399:GLY:HA2	1.98	0.46
2:D:328:ARG:HG3	5:J:302:TRP:HZ2	1.81	0.46
2:D:197:LEU:HD21	2:D:232:LYS:HD2	1.98	0.46
5:I:48:PRO:HG2	5:I:51:LEU:HB2	1.97	0.46
2:C:90:ARG:HH12	2:C:298:LEU:HD22	1.81	0.46
1:B:301:LYS:HD3	2:C:121:MET:N	2.31	0.45
5:I:302:TRP:HZ2	2:C:328:ARG:HG3	1.81	0.45
5:J:135:VAL:HG22	5:J:235:ILE:HG23	1.98	0.45
2:C:192:ASP:HB2	2:C:222:ASN:HD21	1.81	0.45
1:A:80:ASN:C	1:A:90:CYS:SG	2.95	0.45
2:D:67:ILE:HA	2:D:70:LEU:HD12	1.97	0.45
5:J:32:LEU:HB2	5:J:136:SER:HA	1.98	0.45
6:L:59:ILE:HG12	6:L:62:LEU:HD12	1.97	0.45
6:K:31:GLY:HA2	6:K:48:LEU:HD23	1.98	0.45
2:C:67:ILE:HA	2:C:70:LEU:HD12	1.98	0.45
4:G:494:MET:HE3	2:C:249:PHE:HE2	1.82	0.45
4:H:413:LEU:HA	4:H:416:ASN:HD22	1.82	0.45
1:A:22:MET:HB2	1:A:23:PRO:HD3	1.99	0.45
1:B:27:ILE:HA	1:B:30:LEU:HD12	1.99	0.45
5:J:48:PRO:HG2	5:J:51:LEU:HB2	1.98	0.45
6:L:92:SER:HA	6:L:95:ILE:HD12	1.98	0.45
3:F:224:THR:HG22	3:F:268:VAL:HG22	1.97	0.45
6:K:53:ARG:HD2	6:K:88:ARG:HG2	1.97	0.45
2:C:219:PHE:HA	2:C:223:THR:HG23	1.98	0.45
2:D:219:PHE:HA	2:D:223:THR:HG23	1.97	0.45
6:K:45:MET:CE	6:K:45:MET:H	2.29	0.45
1:B:242:LEU:HD13	4:H:393:GLN:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:291:PRO:HA	4:G:294:ILE:HD12	1.99	0.45
6:L:248:ILE:HG12	6:L:264:ILE:HG21	1.99	0.45
1:B:86:ASP:C	1:B:88:GLU:H	2.21	0.44
4:G:377:GLU:HB3	6:L:61:LYS:HB3	1.99	0.44
5:I:414:ILE:HG12	5:I:432:ILE:HD12	1.98	0.44
4:G:561:GLU:CB	4:G:564:LYS:HE2	2.47	0.44
2:D:90:ARG:HH12	2:D:298:LEU:HD22	1.81	0.44
4:G:413:LEU:HA	4:G:416:ASN:HD22	1.83	0.44
6:L:45:MET:H	6:L:45:MET:CE	2.30	0.44
6:K:8:PHE:HE2	6:K:109:HIS:HB2	1.82	0.44
2:C:89:ARG:HA	2:C:92:LEU:HD12	2.00	0.44
3:E:75:PRO:HG2	3:E:112:LEU:HD21	1.99	0.44
1:A:131:TYR:HB2	1:A:165:LEU:HD13	1.99	0.44
4:G:284:TYR:HD1	4:G:286:ILE:H	1.66	0.44
1:B:22:MET:HB2	1:B:23:PRO:HD3	1.99	0.44
2:D:192:ASP:HB2	2:D:222:ASN:HD21	1.81	0.44
2:D:89:ARG:HA	2:D:92:LEU:HD12	2.00	0.44
5:I:135:VAL:HG22	5:I:235:ILE:HG23	2.00	0.44
1:B:27:ILE:HG23	1:B:73:PHE:HD2	1.83	0.43
2:D:159:LYS:HA	2:D:162:ILE:HD12	2.00	0.43
4:H:503:VAL:HB	4:H:571:PRO:HA	2.00	0.43
6:L:88:ARG:CG	6:L:88:ARG:NH2	2.78	0.43
7:M:142:TYR:HB2	7:M:319:ARG:HH12	1.83	0.43
1:B:283:LEU:HB3	1:B:291:THR:HA	1.99	0.43
5:I:459:ASP:H	5:I:466:ILE:HD12	1.84	0.43
2:C:42:LEU:HA	2:C:45:LEU:HD12	1.99	0.43
4:H:271:HIS:HA	4:H:272:PRO:HD3	1.87	0.43
7:M:216:LEU:HD23	7:M:246:ILE:HG12	2.01	0.43
3:F:239:LEU:HA	3:F:388:ASN:HA	2.01	0.43
4:G:517:GLN:HB2	4:G:522:THR:HG21	1.99	0.43
3:E:239:LEU:HA	3:E:388:ASN:HA	2.00	0.43
5:I:33:THR:HG22	5:I:50:CYS:SG	2.59	0.43
1:A:27:ILE:HA	1:A:30:LEU:HD12	2.00	0.43
1:B:86:ASP:OD1	1:B:86:ASP:N	2.47	0.43
1:A:300:ILE:HD13	4:G:588:ASP:HB3	2.01	0.43
5:J:57:VAL:HA	5:J:58:PRO:HD2	1.86	0.43
1:B:153:VAL:HG13	1:B:165:LEU:HD23	2.01	0.43
5:I:179:THR:HG22	5:I:203:PRO:HG2	2.01	0.43
7:N:216:LEU:HD23	7:N:246:ILE:HG12	2.01	0.43
1:B:188:ILE:H	1:B:188:ILE:HG13	1.71	0.42
2:D:242:VAL:HB	4:H:558:ARG:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:188:VAL:HG22	6:L:264:ILE:HG23	2.00	0.42
2:D:42:LEU:HA	2:D:45:LEU:HD12	2.00	0.42
4:H:432:ARG:N	4:H:433:PRO:HD2	2.34	0.42
5:I:37:GLU:C	5:I:39:ARG:H	2.23	0.42
5:I:318:TYR:HA	5:I:328:GLU:HA	2.01	0.42
5:I:100:SER:HA	5:I:101:PRO:HD3	1.93	0.42
5:J:318:TYR:HA	5:J:328:GLU:HA	2.01	0.42
5:J:459:ASP:H	5:J:466:ILE:HD12	1.84	0.42
2:C:159:LYS:HA	2:C:162:ILE:HD12	2.00	0.42
1:A:75:ARG:HH11	1:A:303:TRP:HA	1.83	0.42
1:A:174:ILE:HA	1:A:175:PRO:HD3	1.94	0.42
1:B:230:VAL:HG22	1:B:284:ILE:HD12	2.01	0.42
6:L:59:ILE:HD13	6:L:59:ILE:O	2.19	0.42
2:C:179:LEU:HD13	2:C:293:PHE:HE2	1.84	0.42
1:B:141:HIS:HA	1:B:144:ASN:HB2	2.01	0.42
5:I:200:LEU:HA	5:I:201:PRO:HD3	1.93	0.42
5:I:238:CYS:HB3	5:I:242:VAL:HG21	2.01	0.42
5:J:214:ASP:HA	5:J:215:PRO:HD3	1.90	0.42
2:C:186:LEU:HD22	2:C:259:ILE:HD11	2.00	0.42
1:B:242:LEU:HD23	1:B:242:LEU:H	1.85	0.42
2:D:186:LEU:HD22	2:D:259:ILE:HD11	2.01	0.42
4:H:508:GLU:H	4:H:511:LYS:HD2	1.85	0.42
2:D:190:THR:HG21	2:D:273:SER:HB3	2.02	0.42
4:G:459:LEU:HA	4:G:462:ILE:HG22	2.02	0.42
5:I:123:ASP:HB3	5:I:247:GLN:HE21	1.85	0.42
5:J:143:ILE:HD12	5:J:282:ALA:HB2	2.00	0.42
7:N:356:ARG:HB2	7:N:416:VAL:HG23	2.02	0.42
2:C:90:ARG:HH22	2:C:298:LEU:HB2	1.84	0.42
1:A:141:HIS:HA	1:A:144:ASN:HB2	2.01	0.42
3:F:253:LEU:HB2	5:I:213:ILE:HB	2.02	0.42
5:I:143:ILE:HD12	5:I:282:ALA:HB2	2.01	0.42
7:N:473:ALA:HB2	7:N:487:LEU:HD23	2.02	0.42
4:H:272:PRO:HA	4:H:275:LEU:HD12	2.01	0.42
5:J:37:GLU:C	5:J:39:ARG:H	2.22	0.42
1:A:87:TRP:CE3	6:L:75:ARG:NH2	2.87	0.41
1:B:75:ARG:NH1	1:B:303:TRP:CA	2.76	0.41
1:B:293:SER:HB3	2:C:362:TYR:HE1	1.85	0.41
5:I:214:ASP:HA	5:I:215:PRO:HD3	1.90	0.41
5:I:304:TYR:HB3	5:I:305:PRO:HD3	2.02	0.41
2:D:179:LEU:HD13	2:D:293:PHE:HE2	1.84	0.41
4:G:455:LEU:HD13	2:C:220:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:54:ARG:HD3	6:L:54:ARG:HA	1.77	0.41
6:K:30:MET:O	6:K:48:LEU:HG	2.20	0.41
1:A:118:ASP:HB3	2:D:307:PHE:CD1	2.55	0.41
1:A:129:HIS:HD2	1:A:213:THR:HG22	1.86	0.41
2:D:333:THR:HG22	4:H:453:TYR:HB3	2.03	0.41
4:H:377:GLU:CD	6:K:61:LYS:HB3	2.41	0.41
2:C:190:THR:HG21	2:C:273:SER:HB3	2.01	0.41
3:E:95:VAL:HB	3:E:155:LEU:HD22	2.02	0.41
4:G:529:PRO:HA	4:G:560:PHE:HE1	1.86	0.41
5:I:298:PHE:HE2	5:I:308:LEU:HG	1.85	0.41
5:J:238:CYS:HB3	5:J:242:VAL:HG21	2.02	0.41
7:M:312:SER:HA	7:M:313:PRO:HD3	1.93	0.41
7:M:473:ALA:HB2	7:M:487:LEU:HD23	2.01	0.41
7:N:226:GLN:HA	7:N:227:PRO:HD3	1.92	0.41
5:J:362:ILE:HG21	5:J:368:ILE:HD11	2.02	0.41
7:M:226:GLN:HA	7:M:227:PRO:HD3	1.91	0.41
2:D:325:MET:HA	2:D:328:ARG:HB2	2.01	0.41
7:M:503:ARG:HD3	7:M:512:ILE:HG21	2.01	0.41
1:A:86:ASP:OD1	1:A:86:ASP:N	2.51	0.41
3:E:179:PRO:HA	3:E:180:PRO:HD3	1.75	0.41
5:J:421:ASP:HB3	5:J:424:MET:HE1	2.02	0.41
7:N:503:ARG:HD3	7:N:512:ILE:HG21	2.01	0.41
1:A:257:THR:HG21	1:A:265:ASP:HB3	2.02	0.41
2:D:90:ARG:HH22	2:D:298:LEU:HB2	1.85	0.41
4:G:478:LEU:HD12	4:G:482:PHE:HB2	2.01	0.41
4:H:382:ALA:HA	4:H:385:LEU:HD12	2.03	0.41
6:L:34:VAL:HB	6:L:35:LYS:H	1.64	0.41
7:N:390:ALA:HB1	7:N:396:ILE:HD13	2.02	0.41
6:K:26:GLN:HG2	6:K:33:TYR:CD1	2.55	0.41
6:K:54:ARG:HD2	6:K:54:ARG:HA	1.71	0.41
1:B:87:TRP:HE3	6:K:75:ARG:NH2	2.19	0.41
1:B:148:ARG:HG3	5:I:335:GLN:HG3	2.01	0.41
4:G:431:SER:HA	4:G:456:ILE:HD11	2.02	0.41
4:G:521:VAL:HG11	2:C:254:ARG:HH12	1.84	0.41
6:L:63:ILE:HD12	6:L:63:ILE:C	2.42	0.41
1:B:81:LEU:CG	1:B:90:CYS:SG	2.87	0.40
4:H:327:ILE:HG23	4:H:336:LEU:HD11	2.02	0.40
6:L:24:VAL:CG1	6:L:65:VAL:HA	2.51	0.40
7:M:187:ARG:HH21	7:M:299:VAL:HA	1.85	0.40
6:K:27:ILE:HG23	6:K:64:ARG:NH2	2.33	0.40
7:M:390:ALA:HB1	7:M:396:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:45:MET:H	6:K:45:MET:HE3	1.87	0.40
1:A:153:VAL:HG13	1:A:165:LEU:HD23	2.03	0.40
5:I:421:ASP:HB3	5:I:424:MET:HE1	2.03	0.40
7:M:356:ARG:HB2	7:M:416:VAL:HG23	2.03	0.40
2:C:325:MET:HA	2:C:328:ARG:HB2	2.03	0.40
4:G:501:ILE:HA	4:G:502:PRO:HD3	1.89	0.40
4:H:368:CYS:HA	4:H:371:ILE:HD12	2.04	0.40
5:J:100:SER:HA	5:J:101:PRO:HD3	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	300/305 (98%)	260 (87%)	28 (9%)	12 (4%)	3	26
1	B	300/305 (98%)	261 (87%)	26 (9%)	13 (4%)	2	25
2	C	339/381 (89%)	302 (89%)	31 (9%)	6 (2%)	8	42
2	D	339/381 (89%)	302 (89%)	31 (9%)	6 (2%)	8	42
3	E	253/578 (44%)	218 (86%)	30 (12%)	5 (2%)	7	40
3	F	253/578 (44%)	222 (88%)	26 (10%)	5 (2%)	7	40
4	G	349/651 (54%)	298 (85%)	41 (12%)	10 (3%)	4	32
4	H	349/651 (54%)	300 (86%)	35 (10%)	14 (4%)	3	26
5	I	427/712 (60%)	388 (91%)	31 (7%)	8 (2%)	8	41
5	J	427/712 (60%)	387 (91%)	32 (8%)	8 (2%)	8	41
6	K	237/304 (78%)	199 (84%)	30 (13%)	8 (3%)	3	30
6	L	237/304 (78%)	199 (84%)	29 (12%)	9 (4%)	3	27
7	M	398/527 (76%)	347 (87%)	47 (12%)	4 (1%)	15	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	N	398/527 (76%)	351 (88%)	43 (11%)	4 (1%)	15	54
8	O	15/285 (5%)	12 (80%)	2 (13%)	1 (7%)	1	18
8	P	15/285 (5%)	12 (80%)	2 (13%)	1 (7%)	1	18
All	All	4636/7486 (62%)	4058 (88%)	464 (10%)	114 (2%)	9	35

All (114) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	PRO
1	B	158	PRO
1	B	292	PRO
4	H	487	ALA
5	I	202	LEU
5	J	202	LEU
6	L	62	LEU
1	A	16	GLU
1	A	18	THR
1	A	158	PRO
1	B	16	GLU
2	D	276	SER
3	E	100	GLU
3	F	100	GLU
4	G	487	ALA
4	G	586	SER
4	H	536	ASP
4	H	537	TYR
5	I	173	THR
5	J	173	THR
7	M	164	PHE
7	M	507	LYS
7	N	164	PHE
7	N	507	LYS
6	K	62	LEU
2	C	276	SER
1	A	38	THR
1	A	61	PRO
1	A	189	ASP
1	A	291	THR
1	B	38	THR
1	B	61	PRO
1	B	267	LEU

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Mol	Chain	Res	Type
1	B	291	THR
3	E	309	GLN
3	F	160	LEU
4	G	537	TYR
4	G	548	GLY
4	H	548	GLY
5	I	112	ALA
5	I	459	ASP
5	I	464	VAL
5	J	112	ALA
5	J	459	ASP
6	L	53	ARG
6	L	132	TRP
7	M	383	GLU
7	M	497	GLU
7	N	383	GLU
7	N	497	GLU
6	K	132	TRP
1	A	267	LEU
1	B	18	THR
1	B	189	ASP
1	B	254	LEU
2	D	239	GLU
2	D	275	ASN
2	D	324	ARG
2	D	337	ILE
3	E	160	LEU
3	E	238	LEU
3	F	238	LEU
3	F	309	GLN
4	G	289	SER
4	H	248	GLU
4	H	265	LEU
4	H	289	SER
4	H	460	ASP
4	H	539	ASN
4	H	579	LYS
5	I	26	ARG
5	I	38	THR
5	I	311	ASN
5	J	26	ARG
5	J	38	THR

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Mol	Chain	Res	Type
5	J	311	ASN
5	J	464	VAL
6	K	64	ARG
2	C	117	LEU
2	C	239	GLU
2	C	275	ASN
2	C	324	ARG
2	C	337	ILE
1	A	254	LEU
1	B	87	TRP
2	D	117	LEU
4	G	242	VAL
4	G	248	GLU
4	G	265	LEU
4	G	555	ILE
4	H	242	VAL
4	H	522	THR
4	H	555	ILE
6	L	6	CYS
6	L	29	GLU
6	K	6	CYS
6	K	29	GLU
3	E	152	GLY
4	G	540	PRO
1	A	253	PRO
1	B	253	PRO
4	H	540	PRO
6	K	65	VAL
6	L	34	VAL
6	L	226	PRO
8	O	129	LEU
6	K	34	VAL
1	A	212	GLY
3	F	152	GLY
6	L	63	ILE
8	P	129	LEU
1	B	212	GLY
6	L	31	GLY
6	K	31	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	257/265 (97%)	239 (93%)	18 (7%)	15	42
1	B	257/265 (97%)	238 (93%)	19 (7%)	13	40
2	C	286/338 (85%)	267 (93%)	19 (7%)	16	44
2	D	286/338 (85%)	267 (93%)	19 (7%)	16	44
3	E	249/529 (47%)	241 (97%)	8 (3%)	39	62
3	F	249/529 (47%)	242 (97%)	7 (3%)	43	65
4	G	305/561 (54%)	295 (97%)	10 (3%)	38	61
4	H	305/561 (54%)	292 (96%)	13 (4%)	29	55
5	I	389/649 (60%)	373 (96%)	16 (4%)	30	56
5	J	389/649 (60%)	373 (96%)	16 (4%)	30	56
6	K	218/273 (80%)	191 (88%)	27 (12%)	4	22
6	L	218/273 (80%)	190 (87%)	28 (13%)	4	21
7	M	319/449 (71%)	312 (98%)	7 (2%)	52	70
7	N	319/449 (71%)	313 (98%)	6 (2%)	57	74
8	O	16/246 (6%)	16 (100%)	0	100	100
8	P	16/246 (6%)	16 (100%)	0	100	100
All	All	4078/6620 (62%)	3865 (95%)	213 (5%)	27	50

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	21	THR
1	A	24	ILE
1	A	37	LYS
1	A	54	GLU
1	A	56	LEU
1	A	81	LEU
1	A	86	ASP

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Mol	Chain	Res	Type
1	A	161	GLN
1	A	172	LYS
1	A	188	ILE
1	A	207	ILE
1	A	231	THR
1	A	232	GLU
1	A	247	LEU
1	A	258	ARG
1	A	290	LEU
1	A	297	GLU
1	B	17	ASP
1	B	24	ILE
1	B	37	LYS
1	B	54	GLU
1	B	56	LEU
1	B	86	ASP
1	B	104	ARG
1	B	172	LYS
1	B	188	ILE
1	B	196	VAL
1	B	207	ILE
1	B	231	THR
1	B	232	GLU
1	B	237	VAL
1	B	247	LEU
1	B	255	ASP
1	B	258	ARG
1	B	290	LEU
1	B	297	GLU
2	D	160	ASP
2	D	161	LEU
2	D	182	ASP
2	D	198	LYS
2	D	199	PHE
2	D	206	ARG
2	D	222	ASN
2	D	223	THR
2	D	286	ARG
2	D	298	LEU
2	D	308	ASP
2	D	322	LEU
2	D	328	ARG

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Mol	Chain	Res	Type
2	D	330	ARG
2	D	346	ILE
2	D	348	ILE
2	D	363	ARG
2	D	366	TRP
2	D	371	GLN
3	E	100	GLU
3	E	166	ASP
3	E	173	ASP
3	E	181	GLN
3	E	192	ASP
3	E	255	ILE
3	E	398	LEU
3	E	402	MET
3	F	99	ASP
3	F	166	ASP
3	F	173	ASP
3	F	181	GLN
3	F	255	ILE
3	F	303	ASP
3	F	402	MET
4	G	284	TYR
4	G	296	MET
4	G	366	ASP
4	G	412	LEU
4	G	414	LEU
4	G	424	ILE
4	G	456	ILE
4	G	516	VAL
4	G	554	PHE
4	G	563	LYS
4	H	284	TYR
4	H	296	MET
4	H	300	PHE
4	H	342	ASN
4	H	412	LEU
4	H	424	ILE
4	H	434	LEU
4	H	456	ILE
4	H	460	ASP
4	H	554	PHE
4	H	563	LYS

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Mol	Chain	Res	Type
4	H	576	ILE
4	H	587	LYS
5	I	34	ASP
5	I	41	MET
5	I	63	THR
5	I	88	ASP
5	I	89	TYR
5	I	113	ARG
5	I	122	LEU
5	I	138	ASP
5	I	140	LEU
5	I	176	LYS
5	I	278	THR
5	I	333	LEU
5	I	378	PHE
5	I	424	MET
5	I	457	LEU
5	I	459	ASP
5	J	34	ASP
5	J	41	MET
5	J	60	ILE
5	J	88	ASP
5	J	89	TYR
5	J	113	ARG
5	J	122	LEU
5	J	140	LEU
5	J	173	THR
5	J	176	LYS
5	J	278	THR
5	J	333	LEU
5	J	378	PHE
5	J	424	MET
5	J	457	LEU
5	J	459	ASP
6	L	7	ARG
6	L	19	ILE
6	L	39	TYR
6	L	42	ILE
6	L	45	MET
6	L	46	ILE
6	L	49	SER
6	L	50	GLU

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Mol	Chain	Res	Type
6	L	51	LEU
6	L	54	ARG
6	L	59	ILE
6	L	63	ILE
6	L	79	GLU
6	L	88	ARG
6	L	97	LYS
6	L	119	PHE
6	L	127	TYR
6	L	137	LYS
6	L	143	GLU
6	L	145	PHE
6	L	163	LYS
6	L	168	GLU
6	L	169	LEU
6	L	230	LEU
6	L	235	LEU
6	L	236	ASP
6	L	244	LEU
6	L	251	ILE
7	M	228	GLN
7	M	318	ILE
7	M	371	LYS
7	M	395	LEU
7	M	432	ILE
7	M	462	LEU
7	M	508	HIS
7	N	318	ILE
7	N	371	LYS
7	N	395	LEU
7	N	432	ILE
7	N	462	LEU
7	N	508	HIS
6	K	7	ARG
6	K	19	ILE
6	K	39	TYR
6	K	42	ILE
6	K	45	MET
6	K	46	ILE
6	K	49	SER
6	K	50	GLU
6	K	51	LEU

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Mol	Chain	Res	Type
6	K	53	ARG
6	K	54	ARG
6	K	79	GLU
6	K	88	ARG
6	K	97	LYS
6	K	119	PHE
6	K	127	TYR
6	K	137	LYS
6	K	143	GLU
6	K	145	PHE
6	K	163	LYS
6	K	168	GLU
6	K	169	LEU
6	K	230	LEU
6	K	235	LEU
6	K	236	ASP
6	K	244	LEU
6	K	251	ILE
2	C	160	ASP
2	C	161	LEU
2	C	182	ASP
2	C	198	LYS
2	C	199	PHE
2	C	206	ARG
2	C	222	ASN
2	C	223	THR
2	C	286	ARG
2	C	298	LEU
2	C	308	ASP
2	C	322	LEU
2	C	328	ARG
2	C	330	ARG
2	C	346	ILE
2	C	348	ILE
2	C	363	ARG
2	C	366	TRP
2	C	371	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	161	GLN

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Mol	Chain	Res	Type
2	D	61	ASN
2	D	222	ASN
2	D	352	ASN
3	E	156	GLN
3	E	274	ASN
3	E	309	GLN
3	F	59	GLN
3	F	156	GLN
3	F	274	ASN
3	F	309	GLN
4	G	271	HIS
4	G	416	ASN
4	H	271	HIS
4	H	416	ASN
4	H	480	ASN
4	H	574	ASN
5	I	28	GLN
5	I	73	HIS
5	I	247	GLN
5	I	296	GLN
5	I	359	ASN
5	J	28	GLN
5	J	73	HIS
5	J	247	GLN
5	J	296	GLN
5	J	359	ASN
6	L	11	ASN
6	L	60	GLN
7	M	98	GLN
7	M	197	HIS
7	N	98	GLN
7	N	197	HIS
7	N	465	ASN
6	K	11	ASN
6	K	60	GLN
6	K	103	GLN
2	C	61	ASN
2	C	222	ASN
2	C	352	ASN
2	C	357	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	SEP	L	52	6	8,9,10	0.78	0	8,12,14	1.13	0
6	SEP	K	52	6	8,9,10	0.86	0	8,12,14	1.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SEP	L	52	6	-	5/5/8/10	-
6	SEP	K	52	6	-	5/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	52	SEP	CA-CB-OG-P
6	L	52	SEP	CB-OG-P-O2P
6	L	52	SEP	CB-OG-P-O3P
6	K	52	SEP	CB-OG-P-O2P
6	K	52	SEP	CB-OG-P-O3P
6	L	52	SEP	CB-OG-P-O1P

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Mol	Chain	Res	Type	Atoms
6	K	52	SEP	CB-OG-P-O1P
6	L	52	SEP	N-CA-CB-OG
6	K	52	SEP	N-CA-CB-OG
6	K	52	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

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)

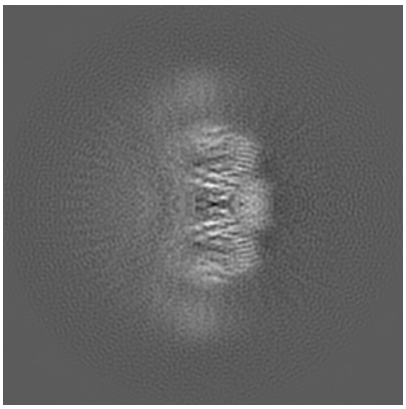
This section contains visualisations of the EMDB entry EMD-4543. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

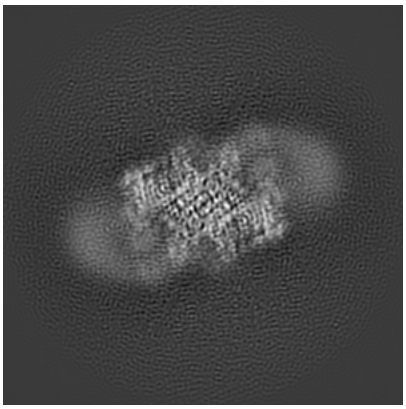
6.1 Orthogonal projections (i)

6.1.1 Primary map

X

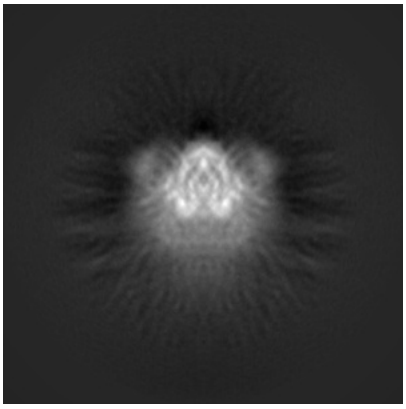


Y

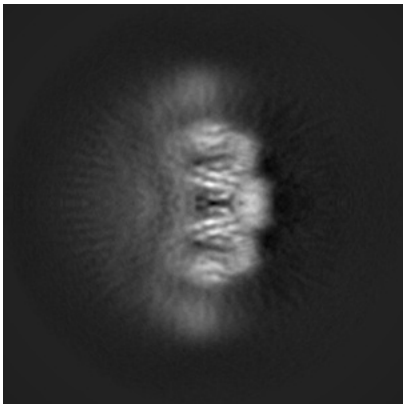


Z

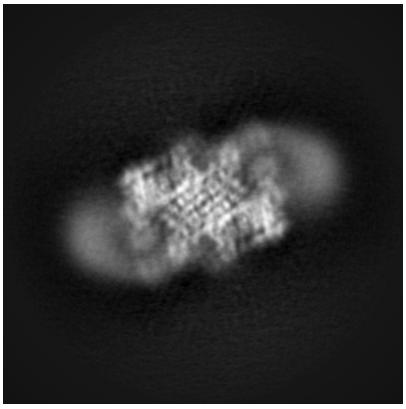
6.1.2 Raw map



X



Y

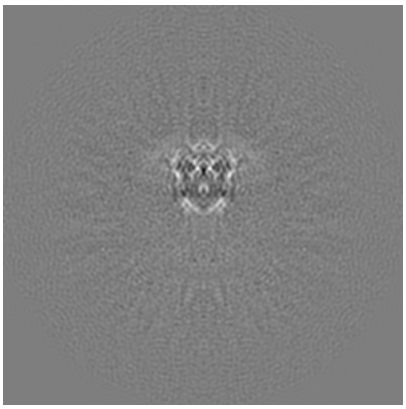


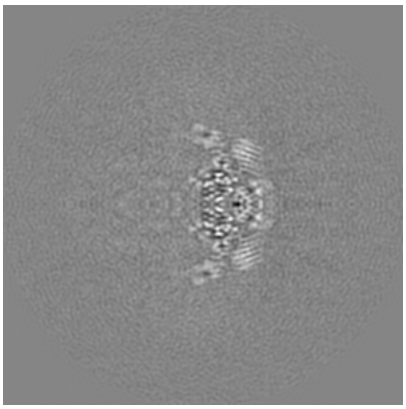
Z

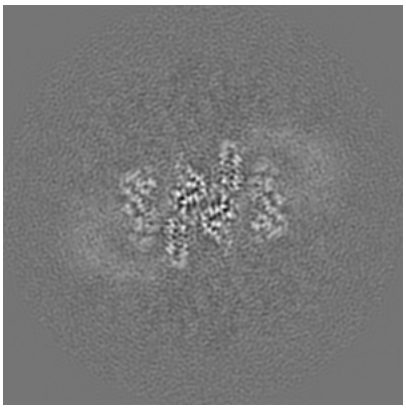
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

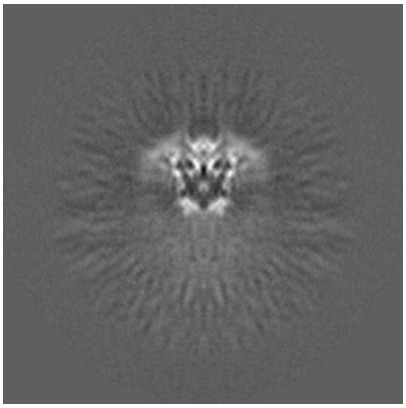
6.2.1 Primary map

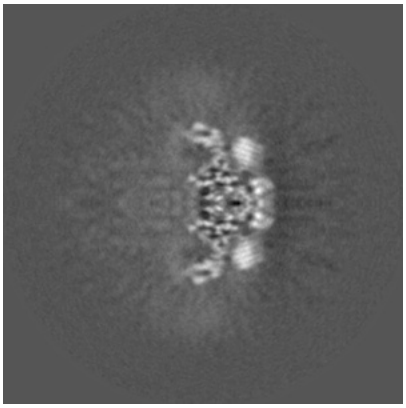

X Index: 140

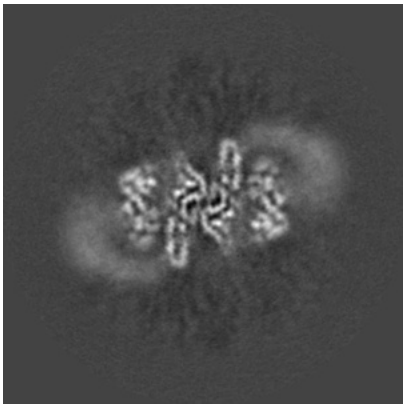

Y Index: 140


Z Index: 140

6.2.2 Raw map


X Index: 140

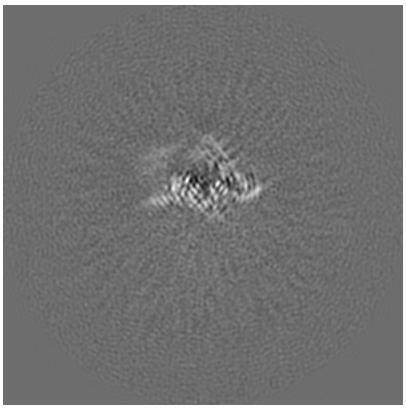

Y Index: 140

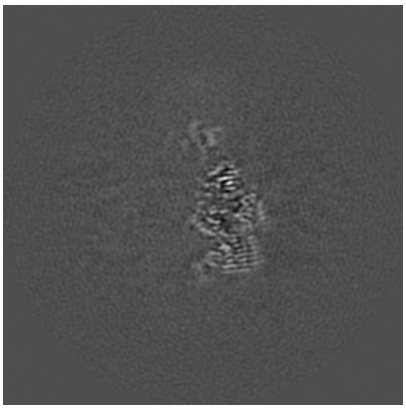

Z Index: 140

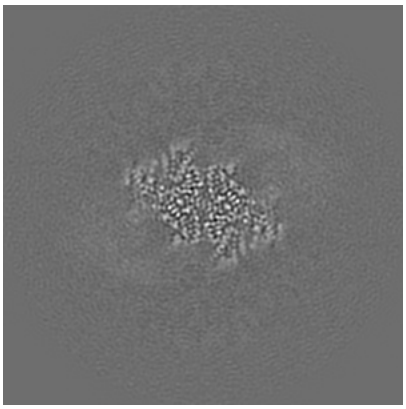
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

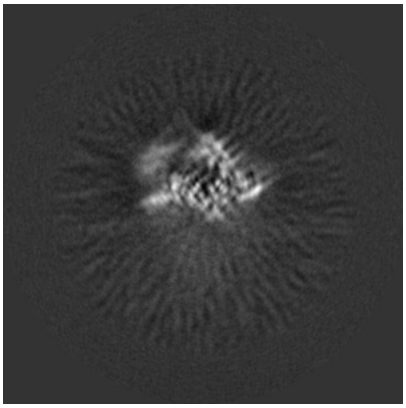
6.3.1 Primary map

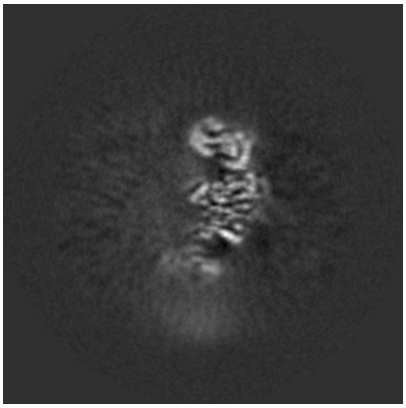

X Index: 127

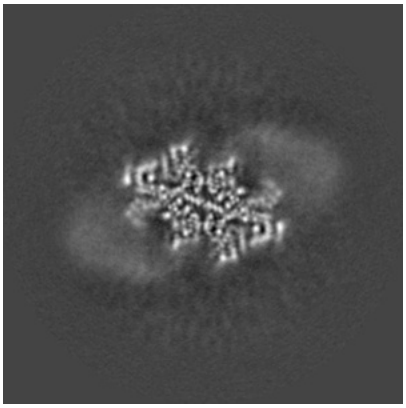

Y Index: 147


Z Index: 153

6.3.2 Raw map


X Index: 127


Y Index: 126


Z Index: 151

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

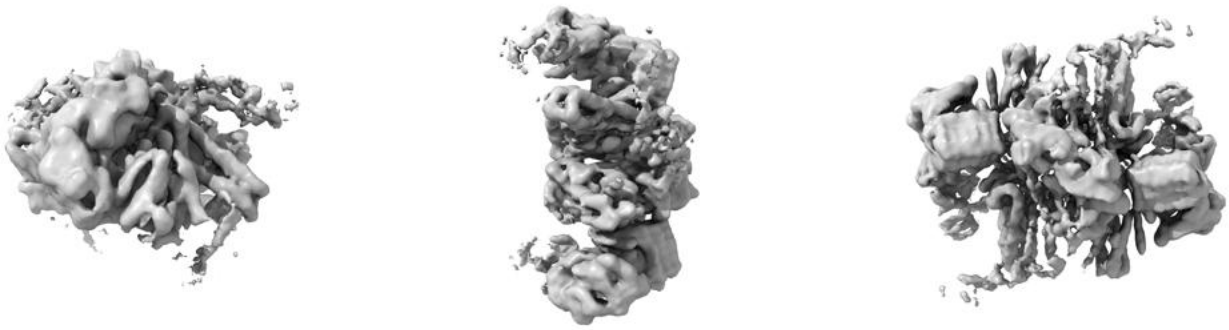
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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.

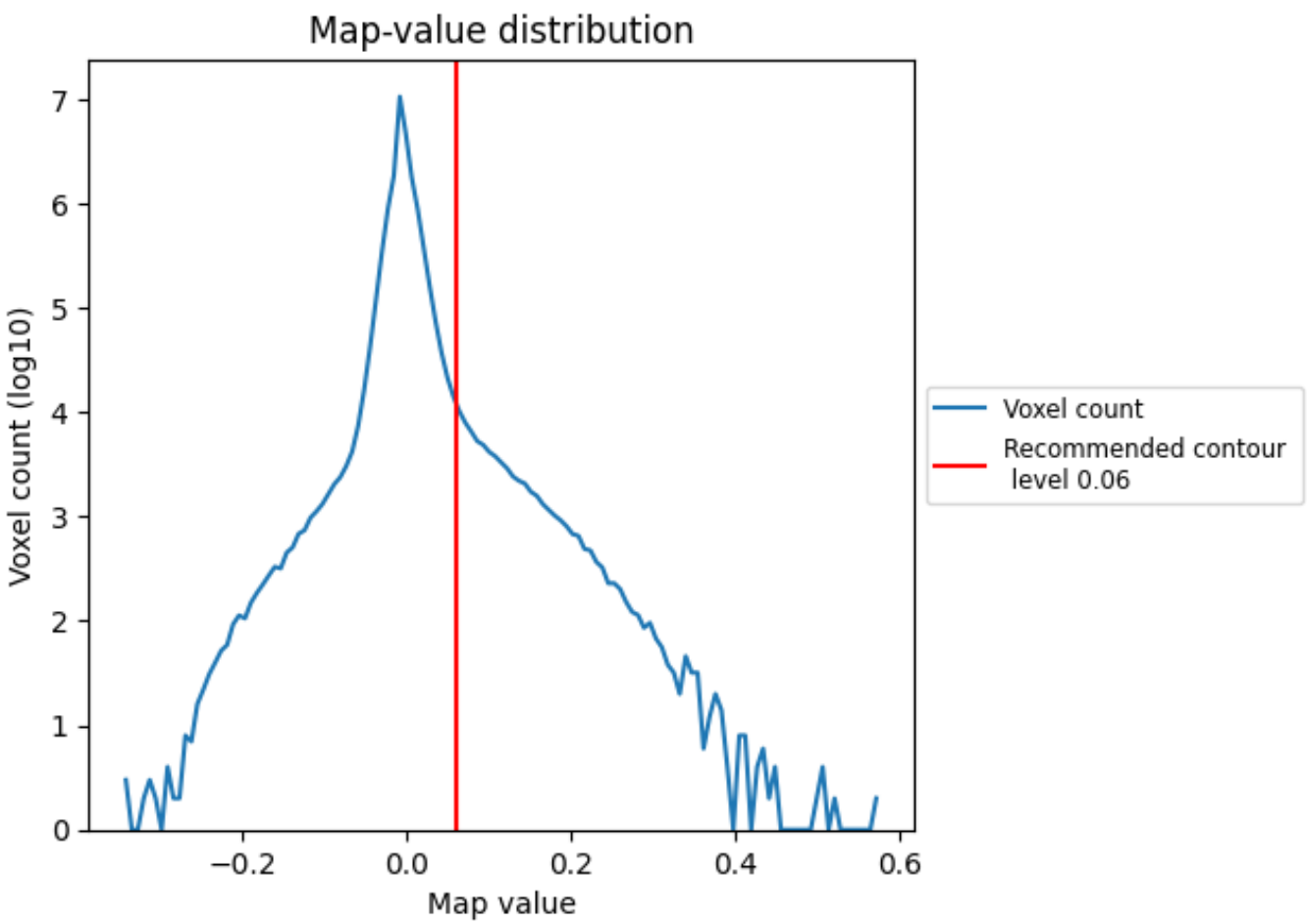
6.5 Mask visualisation (i)

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

7 Map analysis (i)

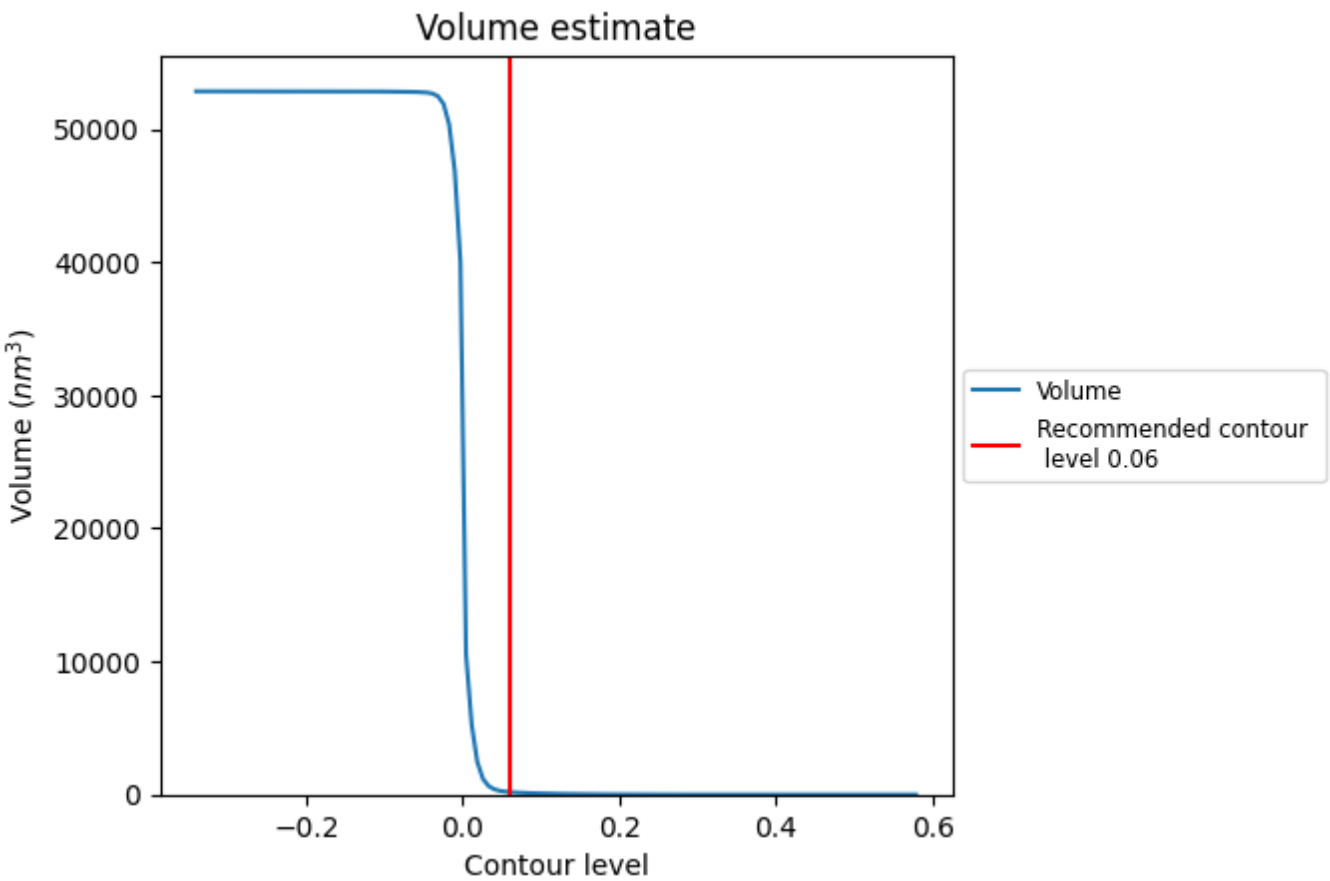
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

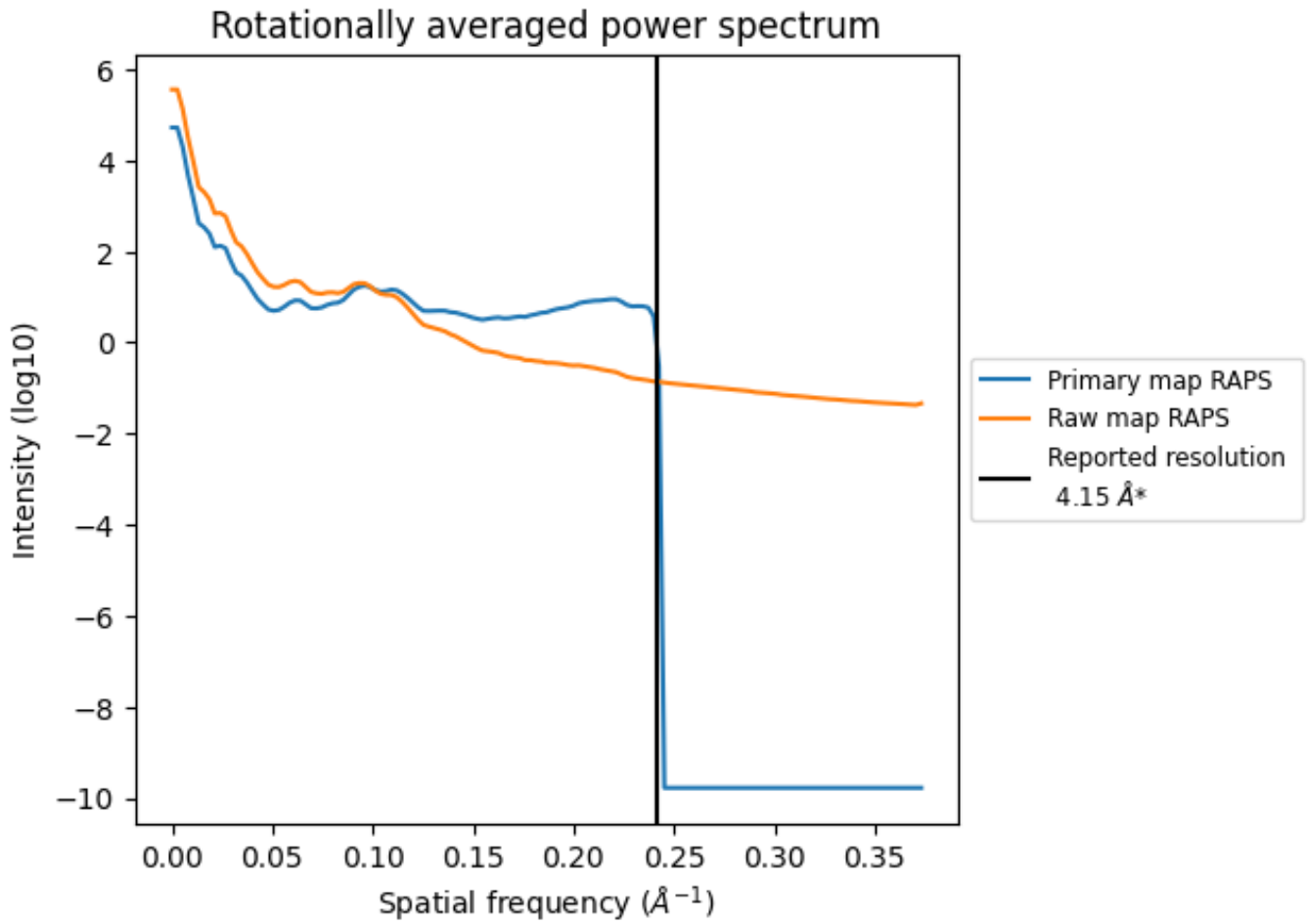
7.2 Volume estimate (i)



The volume at the recommended contour level is 189 nm^3; this corresponds to an approximate mass of 170 kDa.

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

7.3 Rotationally averaged power spectrum (i)

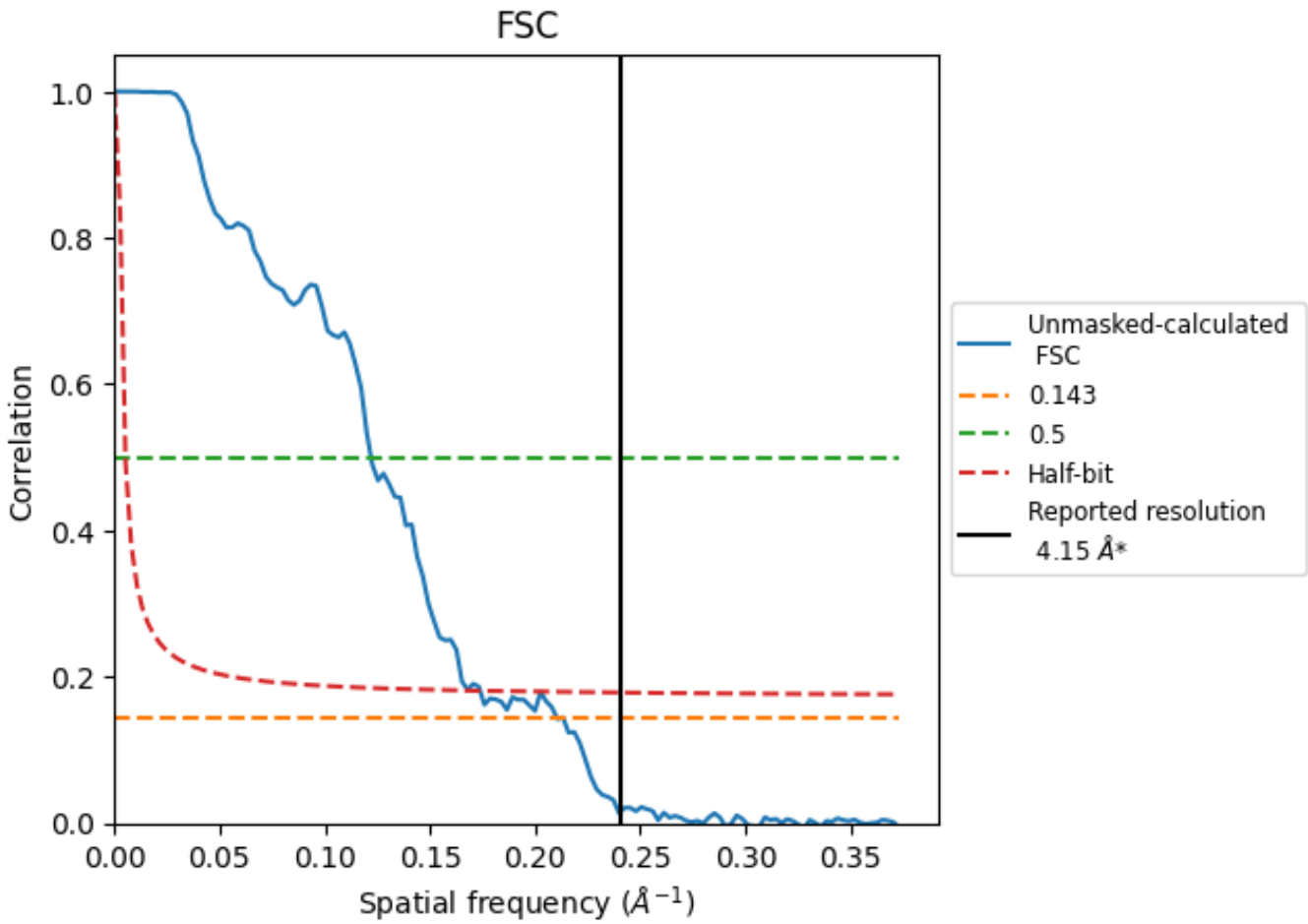


*Reported resolution corresponds to spatial frequency of 0.241 Å^{-1}

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 0.241 Å^{-1}

8.2 Resolution estimates (i)

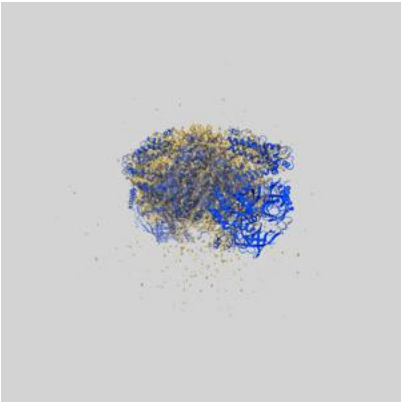
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.15	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.75	8.20	5.75

*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 4.75 differs from the reported value 4.15 by more than 10 %

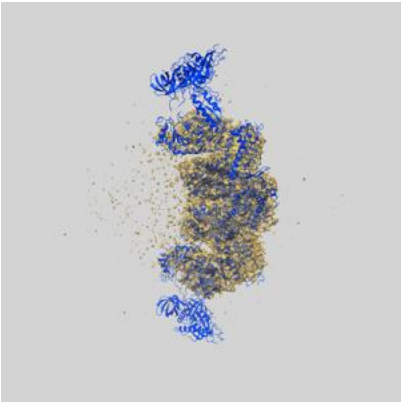
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4543 and PDB model 6QG0. Per-residue inclusion information can be found in section 3 on page 6.

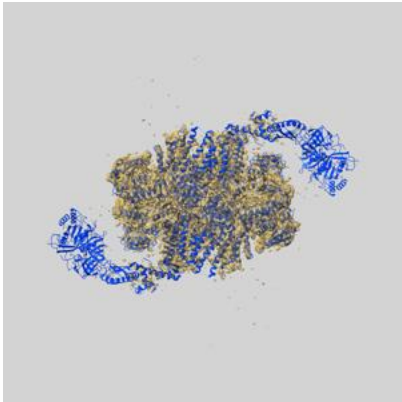
9.1 Map-model overlay (i)



X



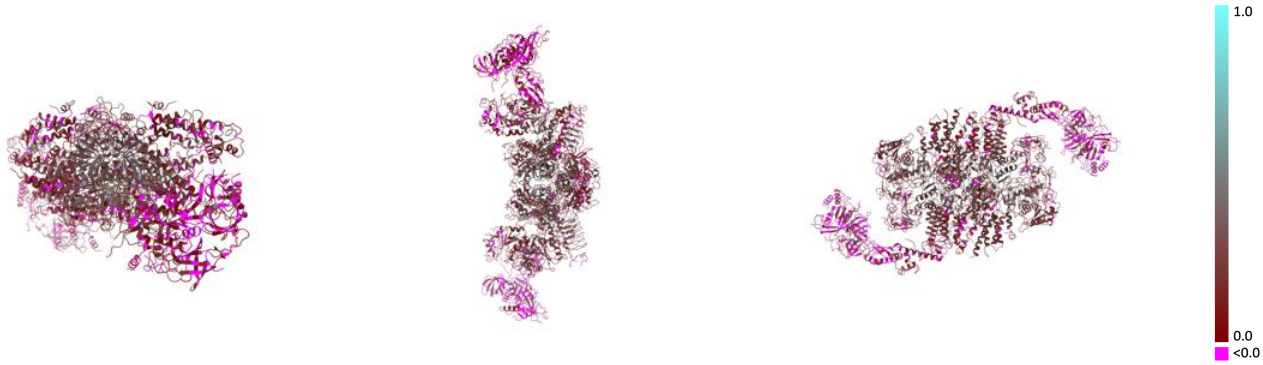
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

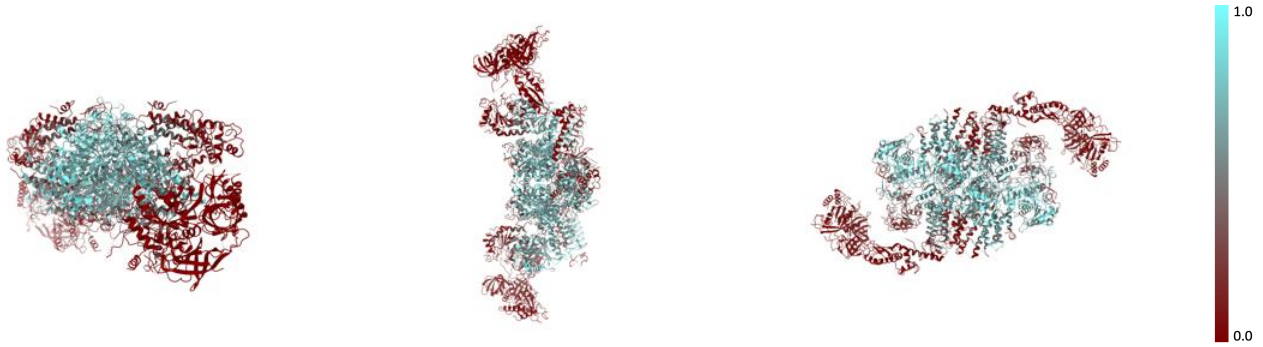
9.2 Q-score mapped to coordinate model (i)



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.

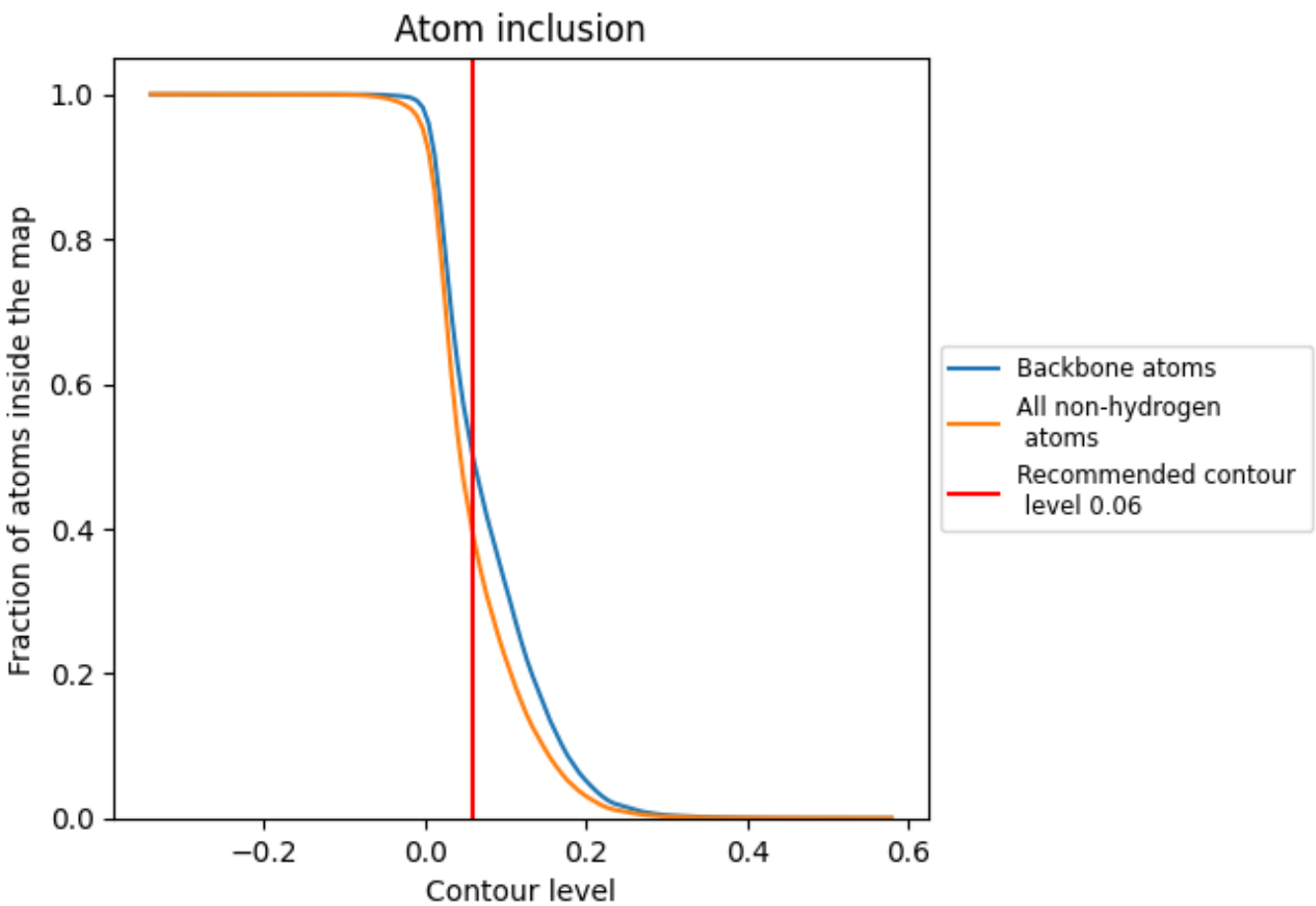
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 50% of all backbone atoms, 39% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3874	0.1950
A	0.4840	0.2220
B	0.4870	0.2170
C	0.6189	0.2960
D	0.6182	0.2930
E	0.2189	0.1470
F	0.2222	0.1510
G	0.5885	0.2820
H	0.5903	0.2900
I	0.6356	0.2680
J	0.6359	0.2700
K	0.0562	0.1120
L	0.0578	0.1090
M	0.0000	0.0240
N	0.0007	0.0230
O	0.0000	0.0020
P	0.0000	-0.0320