wwPDB EM Validation Summary Report (i)

Dec 18, 2023 – 09:14 PM EST

PDB ID	:	1O1E
EMDB ID	:	EMD-1001
Title	:	MOLECULAR MODELS OF AVERAGED RIGOR CROSSBRIDGES FROM TOMOGRAMS OF INSECT FLIGHT MUSCLE
Authors	:	Chen, L.F.; Winkler, H.; Reedy, M.K.; Reedy, M.C.; Taylor, K.A.
Deposited on	:	2002-11-19
Resolution	:	70.00 Å(reported)
Based on initial models	:	2MYS, 1ATN

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

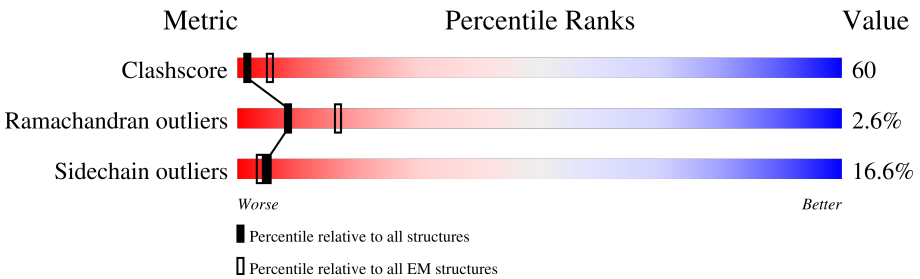
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 70.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
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	840	100% 25% 50% 21% •
1	D	840	100% 26% 51% 19% •
1	G	840	100% 25% 50% 21% •
1	J	840	100% 25% 50% 21% •
1	M	840	100% 25% 51% 20% •
1	P	840	100% 25% 50% 20% 5%
2	B	145	100% 67% 24% 6% •
2	E	145	100% 63% 28% 6% •

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Mol	Chain	Length	Quality of chain
2	H	145	100% 63% 28% 6%
2	K	145	100% 63% 27% 6%
2	N	145	100% 66% 26% 6%
2	Q	145	100% 65% 26% 6%
3	C	147	100% 60% 38%
3	F	147	100% 61% 37%
3	I	147	99% 61% 37%
3	L	147	100% 60% 38%
3	O	147	100% 59% 38%
3	R	147	100% 59% 38%
4	1	375	93% 57% 31% 9%
4	2	375	99% 60% 31% 6%
4	3	375	99% 62% 29% 6%
4	4	375	99% 62% 30% 6%
4	5	375	99% 63% 28% 6%
4	6	375	99% 64% 28% 6%
4	7	375	99% 64% 27% 7%
4	8	375	99% 59% 31% 8%
4	9	375	99% 57% 33% 8%
4	V	375	99% 55% 34% 9%
4	W	375	94% 55% 34% 9%
4	X	375	99% 61% 30% 7%
4	Y	375	98% 61% 30% 7%
4	Z	375	99% 58% 31% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	MLY	A	505	-	-	X	-
1	MLY	A	553	-	-	X	-
1	MLY	A	764	-	-	X	-
1	MLY	A	768	-	-	X	-
1	MLY	A	782	-	-	X	-
1	MLY	A	837	-	-	X	-
1	MLY	D	553	-	-	X	-
1	MLY	D	764	-	-	X	-
1	MLY	D	782	-	-	X	-
1	MLY	G	505	-	-	X	-
1	MLY	G	553	-	-	X	-
1	MLY	G	84	-	-	X	-
1	MLY	J	505	-	-	X	-
1	MLY	J	553	-	-	X	-
1	MLY	J	839	-	-	X	-
1	MLY	J	84	-	-	X	-
1	MLY	M	839	-	-	X	-
1	MLY	M	84	-	-	X	-
1	MLY	P	782	-	-	X	-
1	MLY	P	839	-	-	X	-
1	MLY	P	84	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 94966 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 SKELETAL MUSCLE MYOSIN II.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	840	6797	4382	1135	1243	37	0	0
1	D	840	6797	4382	1135	1243	37	0	0
1	G	840	6797	4382	1135	1243	37	0	0
1	J	840	6797	4382	1135	1243	37	0	0
1	M	840	6797	4382	1135	1243	37	0	0
1	P	840	6797	4382	1135	1243	37	0	0

- Molecule 2 is a protein called SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	145	1127	717	177	227	6	0	0
2	E	145	1127	717	177	227	6	0	0
2	H	145	1127	717	177	227	6	0	0
2	K	145	1127	717	177	227	6	0	0
2	N	145	1127	717	177	227	6	0	0
2	Q	145	1127	717	177	227	6	0	0

- Molecule 3 is a protein called SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	147	1123	698	188	230	7	0	0
3	F	147	1123	698	188	230	7	0	0
3	I	147	1123	698	188	230	7	0	0
3	L	147	1123	698	188	230	7	0	0
3	O	147	1123	698	188	230	7	0	0
3	R	147	1123	698	188	230	7	0	0

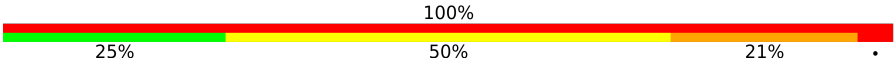
- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

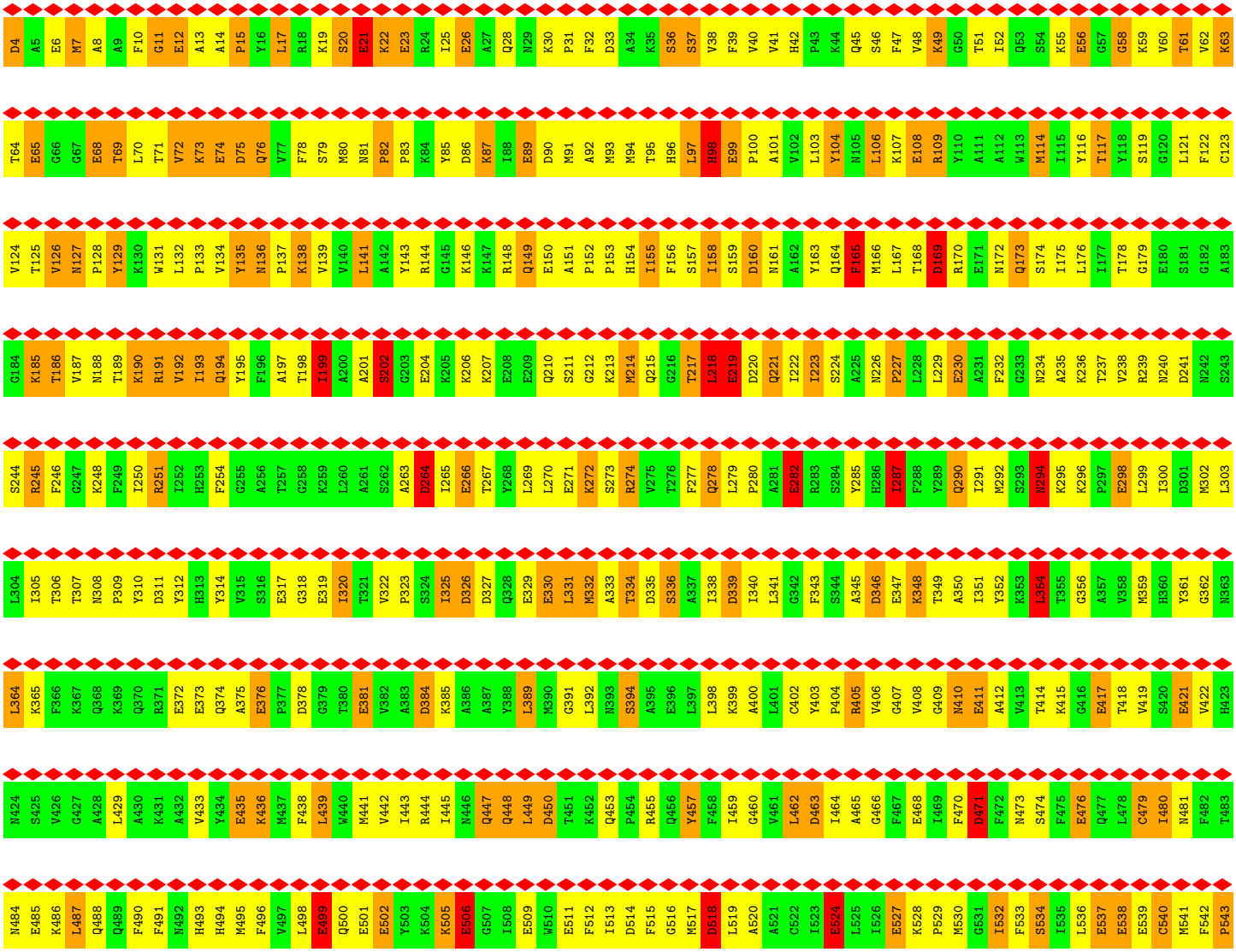
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	1	372	2906	1836	489	561	20	0	0
4	2	372	2906	1836	489	561	20	0	0
4	3	372	2906	1836	489	561	20	0	0
4	4	372	2906	1836	489	561	20	0	0
4	5	372	2906	1836	489	561	20	0	0
4	6	372	2906	1836	489	561	20	0	0
4	7	372	2906	1836	489	561	20	0	0
4	8	372	2906	1836	489	561	20	0	0
4	9	372	2906	1836	489	561	20	0	0
4	V	372	2906	1836	489	561	20	0	0
4	W	372	2906	1836	489	561	20	0	0
4	X	372	2906	1836	489	561	20	0	0
4	Y	372	2906	1836	489	561	20	0	0
4	Z	372	2906	1836	489	561	20	0	0

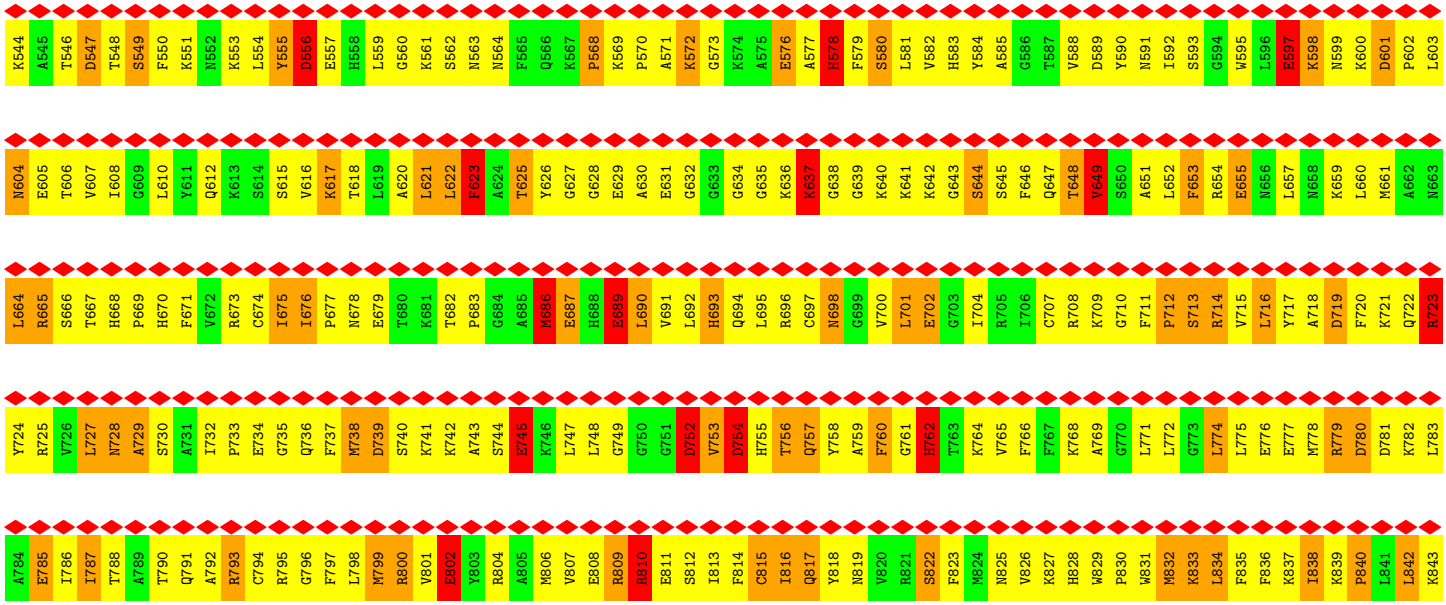
3 Residue-property plots (i)

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: SKELETAL MUSCLE MYOSIN II

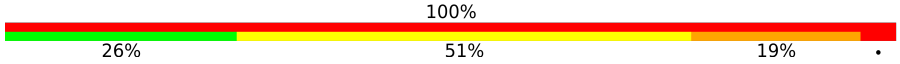
Chain A: 

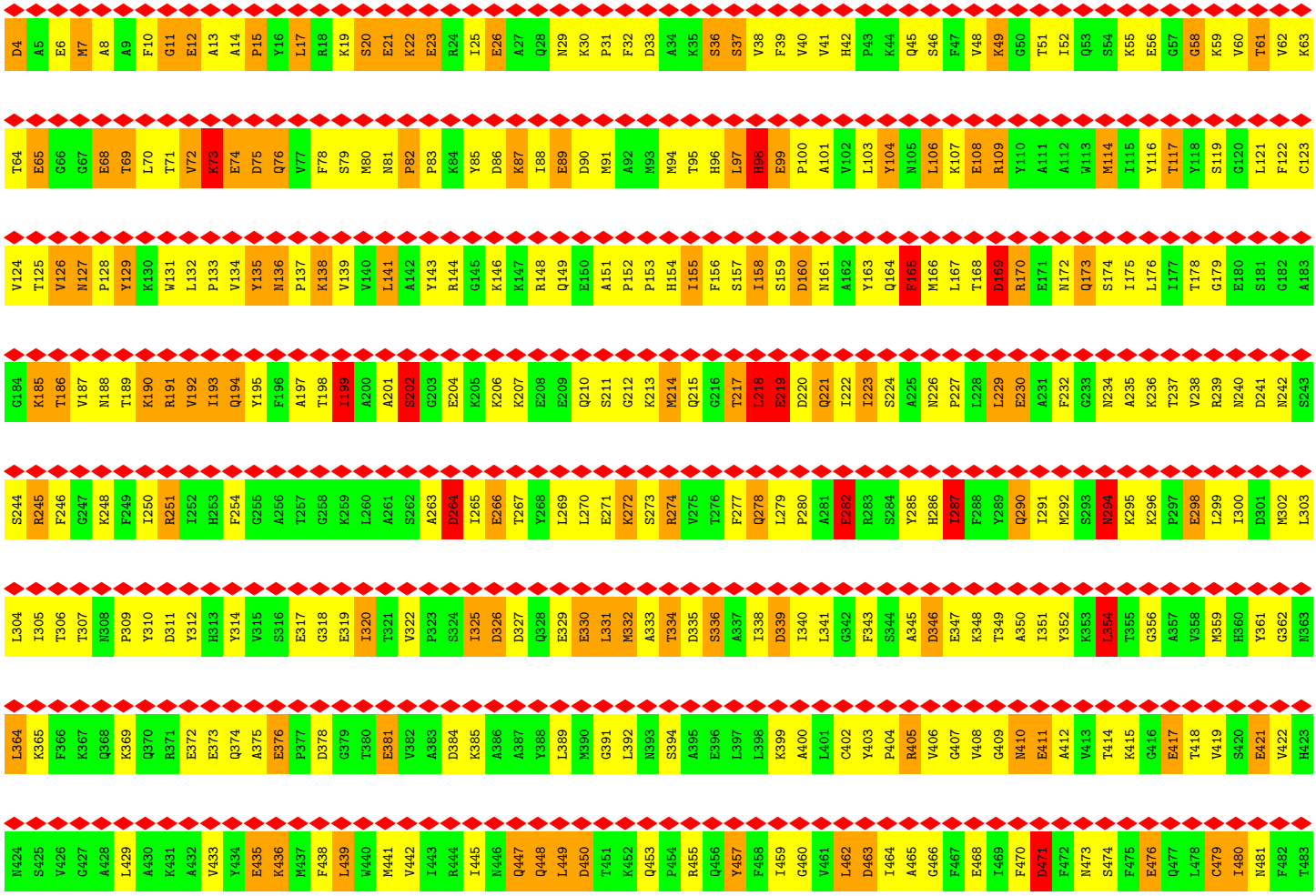




- Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain D:





N484 E485 K486 L487 Q488 Q489 F490 F491 N492 H493 H494 M495 F496 V497 L498 E499 Q500 E501 E502 Y503 K504 K505 E506 G507 I508 E509 W510 E511 F512 I513 D514 F515 G516 M517 D518 L519 A520 A521 C522 I523 E524 L525 I526 E527 K528 P529 M530 G531 I532 F533 S534 I535 L536 E537 E538 E539 C540 M541 F542 P543

K544 A545 T546 D547 T548 S549 F550 K551 N552 K553 L554 Y555 D556 E557 H558 L559 G560 K561 S562 N563 N564 F565 Q566 K567 P568 K569 P570 A571 K572 G573 K574 A575 E576 A577 H578 F579 S580 L581 V582 H583 Y584 A585 G586 T587 V588 D589 Y590 N591 I592 S593 G594 W595 L596 E597 K598 N599 K600 D601 P602 L603

N604 E605 T606 V607 I608 G609 L610 Y611 Q612 K613 S614 S615 V616 K617 T618 L619 A620 L621 L622 F623 A624 T625 Y626 G627 G628 E629 A630 E631 G632 G633 G634 G635 K636 K637 G638 G639 K640 K641 K642 G643 S644 S645 F646 Q647 T648 V649 S650 A651 L652 F653 R654 E655 N656 L657 N658 K659 L660 M661 A662 N663

L664 R665 S666 T667 H668 P669 H670 F671 V672 R673 C674 I675 I676 P677 N678 E679 T680 K681 T682 P683 G684 A685 M686 E687 H688 E689 L690 V691 L692 H693 Q694 L695 R696 C697 N698 G699 V700 L701 E702 G703 I704 R705 I706 C707 R708 K709 G710 F711 P712 S713 R714 V715 L716 Y717 A718 D719 F720 K721 Q722 R723

Y724 R725 V726 L727 N728 A729 S730 A731 I732 P733 E734 G735 Q736 F737 M738 D739 S740 K741 K742 A743 S744 E745 K746 L747 L748 G749 G750 G751 D752 V753 D754 H755 T756 Q757 Y758 A759 F760 G761 H762 T763 K764 V765 F766 F767 K768 A769 G770 L771 L772 G773 L774 L775 E776 E777 M778 R779 D780 D781 K782 L783

A784 E785 I786 I787 T788 A789 T790 Q791 A792 R793 C794 R795 G796 F797 L798 M799 R800 V801 E802 Y803 R804 A805 M806 V807 E808 R809 R810 E811 S812 I813 F814 C815 I816 Q817 Y818 N819 V820 R821 S822 F823 M824 N825 V826 K827 H828 W829 P830 W831 M832 K833 L834 F835 F836 K837 I838 K839 P840 L841 L842 K843

- Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain G: 100% 25% 50% 21%

D4 A5 E6 M7 A8 A9 F10 G11 E12 A13 A14 P15 Y16 L17 R18 K19 S20 E21 K22 E23 R24 I25 E26 A27 Q28 N29 K30 P31 F32 D33 A34 K35 S36 S37 V38 F39 V40 V41 H42 P43 K44 Q45 S46 F47 V48 K49 G50 T51 I52 Q53 S54 K55 E56 G57 G58 K59 V60 T61 V62 K63

T64 E65 G66 G67 E68 T69 L70 T71 V72 K73 E74 D75 Q76 V77 F78 S79 M80 N81 P82 P83 K84 Y85 D86 K87 I88 E89 D90 M91 A92 M93 M94 T95 H96 L97 H98 E99 P100 A101 V102 L103 Y104 N105 L106 K107 E108 R109 Y110 A111 A112 W113 M114 T115 Y116 T117 Y118 S119 G120 L121 F122 C123

V124 T125 V126 N127 P128 Y129 K130 W131 L132 P133 V134 Y135 N136 P137 K138 V139 V140 L141 A142 Y143 R144 G145 K146 K147 R148 Q149 E150 A151 P152 P153 H154 I155 F156 S157 I158 S159 D160 N161 A162 Y163 Q164 F165 M166 L167 T168 D169 R170 E171 N172 Q173 S174 I175 L176 I177 T178 G179 E180 S181 G182 A183

G184 K185 T186 V187 N188 T189 K190 R191 V192 I193 Q194 Y195 F196 A197 T198 I199 A200 A201 S202 G203 E204 K205 K206 K207 E208 E209 Q210 S211 G212 K213 M214 Q215 G216 T217 L218 E219 D220 Q221 I222 I223 S224 A225 N226 P227 L228 L229 E230 A231 F232 G233 N234 A235 K236 T237 V238 R239 N240 D241 N242 S243

S244 R245 F246 G247 K248 F249 I250 R251 I252 H253 F254 G255 A256 T257 G258 K259 L260 A261 S262 A263 D264 I265 E266 T267 Y268 L269 L270 E271 K272 S273 R274 V275 T276 F277 Q278 L279 P280 A281 E282 R283 S284 Y285 H286 I287 F288 Y289 Q290 I291 M292 S293 N294 K295 K296 P297 E298 L299 I300 D301 M302 L303

L304 I305 T306 T307 N308 P309 Y310 D311 Y312 H313 Y314 V315 S316 E317 G318 E319 I320 T321 V322 P323 S324 I325 D326 D327 Q328 E329 E330 L331 M332 A333 T334 D335 S336 A337 I338 D339 I340 L341 G342 F343 S344 A345 D346 E347 K348 T349 A350 I351 Y352 K353 L354 T355 G356 A357 V358 M359 H360 Y361 G362 N363

L364 K365 F366 K367 Q368 K369 Q370 R371 E372 E373 Q374 A375 E376 P377 D378 G379 T380 E381 V382 A383 D384 K385 A386 A387 Y388 L389 M390 G391 L392 N393 S394 A395 E396 L397 L398 K399 A400 L401 C402 Y403 P404 R405 V406 G407 V408 G409 N410 E411 A412 V413 T414 K415 G416 E417 T418 V419 S420 E421 V422 H423

N424 S425 V426 G427 A428 L429 A430 K431 A432 V433 Y434 E435 K436 M437 F438 L439 W440 M441 V442 I443 R444 I445 N446 Q447 Q448 L449 D450 T451 K452 Q453 P454 R455 Q456 Y457 F458 I459 G460 V461 L462 D463 I464 A465 G466 F467 E468 I469 F470 D471 F472 N473 S474 F475 E476 Q477 L478 C479 I480 N481 F482 T483

N484 E485 K486 L487 Q488 Q489 F490 F491 N492 H493 H494 M495 F496 V497 L498 E499 Q500 E501 E502 Y503 K504 K505 E506 G507 I508 E509 W510 E511 F512 I513 D514 F515 G516 M517 D518 L519 A520 A521 C522 I523 E524 L525 I526 E527 K528 P529 M530 G531 I532 F533 S534 I535 L536 E537 E538 E539 C540 M541 F542 P543

K544 A545 T546 D547 T548 S549 F550 K551 N552 K553 L554 Y555 D556 E557 H558 L559 G560 K561 S562 N563 N564 F565 Q566 K567 P568 K569 P570 A571 K572 G573 K574 A575 E576 A577 H578 F579 S580 L581 V582 H583 Y584 A585 G586 T587 V588 D589 Y590 N591 I592 S593 G594 W595 L596 E597 K598 N599 K600 D601 P602 L603

N604 E605 T606 V607 I608 G609 L610 Y611 Q612 K613 S614 S615 V616 K617 T618 L619 A620 L621 L622 F623 A624 T625 Y626 G627 G628 E629 A630 E631 G632 G633 G634 G635 K636 K637 G638 G639 K640 K641 K642 G643 S644 S645 F646 Q647 T648 V649 S650 A651 L652 F653 R654 E655 N656 L657 M658 K659 L660 M661 A662 N663

L664 R665 S666 T667 H668 P669 H670 F671 V672 R673 C674 I675 I676 P677 N678 E679 T680 K681 T682 P683 G684 A685 M686 E687 H688 E689 L690 V691 L692 H693 Q694 L695 R696 C697 N698 G699 V700 L701 E702 G703 I704 R705 I706 C707 R708 K709 G710 F711 P712 S713 R714 V715 L716 Y717 A718 D719 F720 K721 Q722 R723

Y724 R725 V726 L727 N728 A729 S730 A731 I732 P733 E734 G735 Q736 F737 M738 D739 S740 K741 K742 A743 S744 E745 K746 L747 L748 G749 G750 G751 D752 V753 D754 H755 T756 Q757 Y758 A759 F760 G761 H762 T763 K764 V765 F766 F767 K768 A769 G770 L771 L772 G773 L774 L775 E776 E777 M778 R779 D780 D781 K782 L783

A784 E785 I786 I787 T788 A789 T790 Q791 A792 R793 C794 R795 G796 F797 L798 M799 R800 V801 E802 Y803 R804 A805 M806 V807 E808 R809 R810 E811 S812 I813 F814 C815 I816 Q817 Y818 N819 V820 R821 S822 F823 M824 N825 V826 K827 H828 W829 P830 W831 M832 K833 L834 F835 F836 K837 I838 K839 P840 L841 I842 K843

- Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain J: 100% 25% 50% 21% •

D4 A5 E6 M7 A8 A9 F10 G11 E12 A13 A14 P15 Y16 L17 R18 K19 S20 E21 K22 E23 R24 I25 E26 A27 Q28 N29 K30 P31 F32 D33 A34 K35 S36 S37 V38 F39 V40 V41 H42 P43 K44 Q45 S46 F47 V48 K49 G50 T51 I52 Q53 S54 K55 E56 G57 G58 K59 V60 T61 V62 K63

T64 E65 G66 G67 E68 T69 L70 T71 V72 K73 E74 D75 Q76 V77 F78 S79 M80 N81 P82 P83 K84 Y85 D86 K87 I88 E89 D90 M91 A92 M93 M94 T95 H96 L97 H98 E99 P100 A101 V102 L103 Y104 N105 L106 K107 E108 R109 Y110 A111 A112 W113 M114 I115 Y116 T117 Y118 S119 G120 L121 F122 C123

V124 T125 V126 N127 P128 Y129 K130 W131 L132 P133 V134 Y135 N136 P137 K138 V139 V140 L141 A142 Y143 R144 G145 K146 K147 R148 Q149 E150 A151 P152 P153 H154 I155 F156 S157 I158 S159 D160 N161 A162 Y163 Q164 F165 M166 L167 T168 D169 R170 E171 N172 Q173 S174 I175 L176 I177 T178 G179 E180 S181 G182 A183

G184 K185 T186 V187 N188 T189 K190 R191 V192 I193 Q194 Y195 F196 A197 T198 I199 A200 A201 S202 G203 E204 K205 K206 K207 E208 E209 Q210 S211 G212 K213 M214 Q215 G216 T217 L218 E219 D220 Q221 I222 I223 S224 A225 N226 P227 L228 L229 E230 A231 F232 G233 N234 A235 K236 T237 V238 R239 N240 D241 N242 S243

S244 R245 F246 G247 K248 F249 I250 R251 I252 H253 F254 G255 A256 T257 G258 K259 L260 A261 S262 A263 D264 I265 E266 T267 Y268 L269 L270 E271 K272 S273 R274 V275 T276 F277 Q278 L279 P280 A281 E282 R283 S284 Y285 H286 I287 F288 Y289 Q290 I291 M292 S293 N294 K295 K296 P297 E298 I299 I300 D301 M302 L303

L304 I305 T306 T307 N308 P309 Y310 D311 Y312 H313 Y314 V315 S316 E317 G318 E319 I320 T321 V322 P323 S324 I325 D326 D327 Q328 E329 E330 L331 M332 A333 T334 D335 S336 A337 I338 D339 I340 L341 G342 F343 S344 A345 D346 E347 K348 T349 A350 I351 Y352 K353 L354 T355 G356 A357 V358 M359 H360 Y361 G362 N363

L364 K365 F366 K367 Q368 K369 Q370 R371 E372 E373 Q374 A375 E376 P377 D378 G379 T380 E381 V382 A383 D384 K385 A386 A387 Y388 L389 M390 G391 L392 N393 S394 A395 E396 L397 L398 K399 A400 L401 C402 Y403 P404 R405 V406 G407 V408 G409 N410 E411 A412 V413 T414 K415 G416 E417 T418 V419 S420 E421 V422 H423

N424 S425 V426 G427 A428 L429 A430 K431 A432 V433 Y434 E435 K436 M437 F438 L439 W440 M441 V442 I443 R444 I445 N446 Q447 Q448 L449 D450 T451 K452 Q453 P454 R455 Q456 Y457 F458 I459 G460 V461 L462 D463 I464 A465 G466 F467 E468 I469 F470 D471 F472 N473 S474 F475 E476 Q477 L478 C479 I480 N481 F482 T483

N484 E485 K486 L487 Q488 Q489 F490 F491 N492 H493 H494 M495 F496 V497 L498 E499 Q500 E501 E502 Y503 K504 K505 E506 G507 I508 E509 W510 E511 F512 I513 D514 F515 G516 M517 D518 L519 A520 A521 C522 I523 E524 L525 I526 E527 K528 P529 M530 G531 I532 F533 S534 I535 L536 E537 E538 E539 C540 M541 F542 P543

K544 A545 T546 D547 T548 S549 F550 K551 N552 K553 L554 Y555 D556 E557 H558 L559 G560 K561 S562 N563 N564 F565 Q566 K567 P568 K569 P570 A571 K572 G573 K574 A575 E576 A577 H578 F579 S580 L581 V582 H583 Y584 A585 G586 T587 V588 D589 Y590 N591 I592 S593 G594 W595 L596 E597 K598 N599 K600 D601 P602 L603

N604 E605 T606 V607 I608 G609 L610 Y611 Q612 K613 S614 S615 V616 K617 T618 L619 A620 L621 L622 F623 A624 T625 Y626 G627 G628 E629 A630 E631 G632 G633 G634 G635 K636 K637 G638 G639 K640 K641 K642 G643 S644 S645 F646 Q647 T648 V649 S650 A651 L652 F653 R654 E655 N656 L657 N658 K659 L660 M661 A662 N663

L664 R665 S666 T667 H668 P669 H670 F671 V672 R673 C674 I675 I676 P677 N678 E679 T680 K681 T682 P683 G684 A685 M686 E687 H688 E689 L690 V691 L692 H693 Q694 L695 R696 C697 N698 G699 V700 L701 E702 G703 I704 R705 I706 C707 R708 K709 G710 F711 P712 S713 R714 V715 L716 Y717 A718 D719 F720 K721 Q722 R723

Y724 R725 V726 L727 N728 A729 S730 A731 I732 P733 E734 G735 Q736 F737 M738 D739 S740 K741 K742 A743 S744 E745 K746 L747 L748 G749 G750 G751 D752 V753 D754 H755 T756 Q757 Y758 A759 F760 G761 H762 T763 K764 V765 F766 F767 K768 A769 G770 L771 L772 G773 L774 L775 E776 E777 M778 R779 D780 D781 K782 L783

A784 E785 I786 I787 T788 A789 T790 Q791 A792 R793 C794 R795 G796 F797 L798 M799 R800 V801 E802 Y803 R804 A805 M806 V807 E808 R809 R810 E811 S812 I813 F814 C815 I816 Q817 Y818 N819 V820 R821 S822 F823 M824 N825 V826 K827 H828 W829 P830 W831 M832 K833 L834 F835 F836 K837 I838 K839 P840 L841 L842 K843

- Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain M: 100% 25% 51% 20%

D4 A5 E6 M7 A8 A9 F10 G11 E12 A13 A14 P15 Y16 L17 R18 K19 S20 E21 K22 E23 R24 I25 E26 A27 Q28 N29 K30 P31 F32 D33 A34 K35 S36 S37 V38 F39 V40 V41 H42 P43 K44 Q45 S46 F47 V48 K49 G50 T51 I52 Q53 S54 K55 E56 G57 G58 K59 V60 T61 V62 K63

T64 E65 G66 G67 E68 T69 L70 T71 V72 K73 E74 D75 Q76 V77 F78 S79 M80 N81 P82 P83 K84 Y85 D86 K87 I88 E89 D90 M91 A92 M93 M94 T95 H96 L97 H98 E99 P100 A101 V102 L103 Y104 N105 L106 K107 E108 R109 Y110 A111 A112 W113 M114 I115 Y116 T117 Y118 S119 G120 L121 F122 C123

V124 T125 V126 N127 P128 Y129 K130 W131 L132 P133 V134 Y135 N136 P137 K138 V139 V140 L141 A142 Y143 R144 G145 K146 K147 R148 Q149 E150 A151 P152 P153 H154 I155 F156 S157 I158 S159 D160 N161 A162 Y163 Q164 F165 M166 L167 T168 D169 R170 E171 N172 Q173 S174 I175 L176 I177 T178 G179 E180 S181 G182 A183

G184 K185 T186 V187 N188 T189 K190 R191 V192 I193 Q194 Y195 F196 A197 T198 I199 A200 A201 S202 G203 E204 K205 K206 K207 E208 E209 Q210 S211 G212 K213 M214 Q215 G216 T217 L218 E219 D220 Q221 I222 I223 S224 A225 N226 P227 L228 L229 E230 A231 F232 G233 N234 A235 K236 T237 V238 R239 N240 D241 N242 S243

S244 R245 F246 G247 K248 F249 I250 R251 I252 H253 F254 G255 A256 T257 G258 K259 L260 A261 S262 A263 D264 I265 E266 T267 Y268 L269 L270 E271 K272 S273 R274 V275 T276 F277 Q278 L279 P280 A281 E282 R283 S284 Y285 H286 I287 F288 Y289 Q290 I291 M292 S293 N294 K295 K296 P297 E298 L299 I300 D301 M302 L303

L304 I305 T306 T307 N308 P309 Y310 D311 Y312 H313 Y314 V315 S316 E317 G318 E319 I320 T321 V322 P323 S324 I325 D326 D327 Q328 E329 E330 L331 M332 A333 T334 D335 S336 A337 I338 D339 I340 L341 G342 F343 S344 A345 D346 E347 K348 T349 A350 I351 Y352 K353 L354 T355 G356 A357 V358 M359 H360 Y361 G362 N363

L364 K365 F366 K367 Q368 K369 Q370 R371 E372 E373 Q374 A375 E376 P377 D378 G379 T380 E381 V382 A383 D384 K385 A386 A387 Y388 L389 M390 G391 L392 N393 S394 A395 E396 L397 I398 K399 A400 L401 C402 Y403 P404 R405 V406 G407 V408 G409 N410 E411 A412 V413 T414 K415 G416 E417 T418 V419 S420 E421 V422 H423

N424 S425 V426 G427 A428 L429 A430 K431 A432 V433 Y434 E435 K436 M437 F438 L439 W440 M441 V442 I443 R444 I445 N446 Q447 Q448 L449 D450 T451 K452 Q453 P454 R455 Q456 Y457 F458 I459 G460 V461 L462 D463 I464 A465 G466 F467 E468 I469 F470 D471 F472 N473 S474 F475 E476 Q477 L478 C479 I480 N481 F482 T483

N484 E485 K486 L487 Q488 Q489 F490 F491 N492 H493 H494 M495 F496 V497 L498 E499 Q500 E501 E502 Y503 K504 K505 E506 G507 I508 E509 W510 E511 F512 I513 D514 F515 G516 M517 D518 L519 A520 A521 C522 I523 E524 L525 I526 E527 K528 P529 M530 G531 I532 F533 S534 I535 L536 E537 E538 E539 C540 M541 F542 P543

K544 A545 T546 D547 T548 S549 F550 K551 N552 K553 L554 Y555 D556 E557 H558 L559 G560 K561 S562 N563 N564 F565 Q566 K567 P568 K569 P570 A571 K572 G573 K574 A575 E576 A577 H578 F579 S580 L581 V582 H583 Y584 A585 G586 T587 V588 D589 Y590 N591 I592 S593 G594 W595 L596 E597 K598 N599 K600 D601 P602 L603

N604 E605 T606 V607 I608 G609 L610 Y611 Q612 K613 S614 S615 V616 K617 T618 L619 A620 L621 L622 F623 A624 T625 Y626 G627 G628 E629 A630 E631 G632 G633 G634 G635 K636 K637 G638 G639 K640 K641 K642 G643 S644 S645 F646 Q647 T648 V649 S650 A651 L652 F653 R654 E655 N656 L657 N658 K659 L660 M661 A662 N663

L664 R665 S666 T667 H668 P669 H670 F671 V672 R673 C674 I675 I676 P677 N678 E679 T680 K681 T682 P683 G684 A685 M686 E687 H688 E689 L690 V691 L692 H693 Q694 L695 R696 C697 N698 G699 V700 L701 E702 G703 I704 R705 I706 C707 R708 K709 G710 F711 P712 S713 R714 V715 L716 Y717 A718 D719 F720 K721 Q722 R723

Y724 R725 V726 L727 N728 A729 S730 A731 I732 P733 E734 G735 Q736 F737 M738 D739 S740 K741 K742 A743 S744 E745 K746 L747 L748 G749 G750 G751 D752 V753 D754 H755 T756 Q757 Y758 A759 F760 G761 H762 T763 K764 V765 F766 F767 K768 A769 G770 L771 L772 G773 L774 L775 E776 E777 M778 R779 D780 D781 K782 L783

A784 E785 I786 I787 T788 A789 T790 Q791 A792 R793 C794 R795 G796 F797 L798 M799 R800 V801 E802 Y803 R804 A805 M806 V807 E808 R809 R810 E811 S812 I813 F814 C815 I816 Q817 Y818 N819 V820 R821 S822 F823 M824 N825 V826 K827 H828 W829 P830 W831 M832 K833 L834 F835 F836 K837 I838 K839 P840 L841 L842 K843

- Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain P: 100% 25% 50% 20% 5%

D4 A5 E6 M7 A8 A9 F10 G11 E12 A13 A14 P15 Y16 L17 R18 K19 S20 E21 K22 E23 R24 I25 E26 A27 Q28 N29 K30 P31 F32 D33 A34 K35 S36 S37 V38 F39 V40 V41 H42 P43 K44 Q45 S46 F47 V48 K49 G50 T51 I52 Q53 S54 K55 E56 G57 G58 K59 V60 T61 V62 K63

T64 E65 G66 G67 E68 T69 L70 T71 V72 K73 E74 D75 Q76 V77 F78 S79 M80 N81 P82 P83 K84 Y85 D86 K87 I88 E89 D90 M91 A92 M93 M94 T95 H96 L97 H98 E99 P100 A101 V102 L103 Y104 N105 L106 K107 E108 R109 Y110 A111 A112 W113 M114 I115 Y116 T117 Y118 S119 G120 L121 F122 C123

V124 T125 V126 N127 P128 Y129 K130 W131 L132 P133 V134 Y135 N136 P137 K138 V139 V140 L141 A142 Y143 R144 G145 K146 K147 R148 Q149 E150 A151 P152 P153 H154 I155 F156 S157 I158 S159 D160 N161 A162 Y163 Q164 F165 M166 L167 T168 D169 R170 E171 N172 Q173 S174 I175 L176 I177 T178 G179 E180 S181 G182 A183

G184 K185 T186 V187 N188 T189 K190 R191 V192 I193 Q194 Y195 F196 A197 T198 I199 A200 A201 S202 G203 E204 K205 K206 K207 E208 E209 Q210 S211 G212 K213 M214 Q215 G216 T217 L218 E219 D220 Q221 I222 I223 S224 A225 N226 P227 L228 L229 E230 A231 F232 G233 N234 A235 K236 T237 V238 R239 N240 D241 N242 S243

S244 R245 F246 G247 K248 F249 I250 R251 I252 H253 F254 G255 A256 T257 G258 K259 L260 A261 S262 A263 D264 I265 E266 T267 Y268 L269 L270 E271 K272 S273 R274 V275 T276 F277 Q278 L279 P280 A281 E282 R283 S284 Y285 H286 I287 F288 Y289 Q290 I291 M292 S293 N294 K295 K296 P297 E298 L299 I300 D301 M302 L303

L304 I305 T306 T307 N308 P309 Y310 D311 Y312 H313 Y314 V315 S316 E317 G318 E319 I320 T321 V322 P323 S324 I325 D326 D327 Q328 E329 E330 L331 M332 A333 T334 D335 S336 A337 I338 D339 I340 L341 G342 F343 S344 A345 D346 E347 K348 T349 A350 I351 Y352 K353 L354 T355 G356 A357 V358 M359 H360 Y361 G362 N363

L364 K365 F366 K367 Q368 K369 Q370 R371 E372 E373 Q374 A375 E376 P377 D378 G379 T380 E381 V382 A383 D384 K385 A386 A387 Y388 L389 M390 G391 L392 N393 S394 A395 E396 L397 L398 K399 A400 L401 C402 Y403 P404 R405 V406 G407 V408 G409 N410 E411 A412 V413 T414 K415 G416 E417 T418 V419 S420 E421 V422 H423

N424 S425 V426 G427 A428 L429 A430 K431 A432 V433 Y434 E435 K436 M437 F438 L439 W440 M441 V442 I443 R444 I445 N446 Q447 Q448 L449 D450 T451 K452 Q453 P454 R455 Q456 Y457 F458 I459 G460 V461 L462 D463 I464 A465 G466 F467 E468 I469 F470 D471 F472 N473 S474 F475 E476 Q477 L478 C479 I480 N481 F482 T483

N484 E485 K486 L487 Q488 Q489 F490 F491 N492 H493 H494 M495 F496 V497 L498 E499 Q500 E501 E502 Y503 K504 K505 E506 G507 I508 E509 W510 E511 F512 I513 D514 F515 G516 M517 D518 L519 A520 A521 C522 I523 E524 L525 I526 E527 K528 P529 M530 G531 I532 F533 S534 I535 L536 E537 E538 E539 C540 M541 F542 P543

K544 A545 T546 D547 T548 S549 F550 K551 N552 K553 L554 Y555 D556 E557 H558 L559 G560 K561 S562 N563 N564 F565 Q566 K567 P568 K569 P570 A571 K572 G573 K574 A575 E576 A577 H578 F579 S580 L581 V582 H583 Y584 A585 G586 T587 V588 D589 Y590 N591 I592 S593 G594 W595 L596 E597 K598 N599 K600 D601 P602 L603

N604 E605 T606 V607 I608 G609 L610 Y611 Q612 K613 S614 S615 V616 K617 T618 L619 A620 L621 L622 F623 A624 T625 Y626 G627 G628 E629 A630 E631 G632 G633 G634 G635 K636 K637 G638 G639 K640 K641 K642 G643 S644 S645 F646 Q647 T648 V649 S650 A651 L652 F653 R654 E655 N656 L657 N658 K659 L660 M661 A662 N663

L664 R665 S666 T667 H668 P669 H670 F671 V672 R673 C674 I675 I676 P677 N678 E679 T680 K681 T682 P683 G684 A685 M686 E687 H688 E689 L690 V691 L692 H693 Q694 L695 R696 C697 N698 G699 V700 L701 E702 G703 I704 R705 I706 C707 R708 K709 G710 F711 P712 S713 R714 V715 L716 Y717 A718 D719 F720 K721 Q722 R723

Y724 R725 V726 L727 N728 A729 S730 A731 I732 P733 E734 G735 Q736 F737 M738 D739 S740 K741 K742 A743 S744 E745 K746 L747 L748 G749 G750 G751 D752 V753 D754 H755 T756 Q757 Y758 A759 F760 G761 H762 T763 K764 V765 F766 F767 K768 A769 G770 L771 L772 G773 L774 L775 E776 E777 M778 R779 D780 D781 K782 L783

A784 E785 I786 I787 T788 A789 T790 Q791 A792 R793 C794 R795 G796 F797 L798 M799 R800 V801 E802 Y803 R804 A805 M806 V807 E808 R809 R810 E811 S812 I813 F814 C815 I816 Q817 Y818 N819 V820 R821 S822 F823 M824 N825 V826 K827 H828 W829 P830 W831 M832 K833 L834 F835 F836 K837 I838 K839 P840 L841 L842 K843

- Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

Chain B: 100% 67% 24% 6%

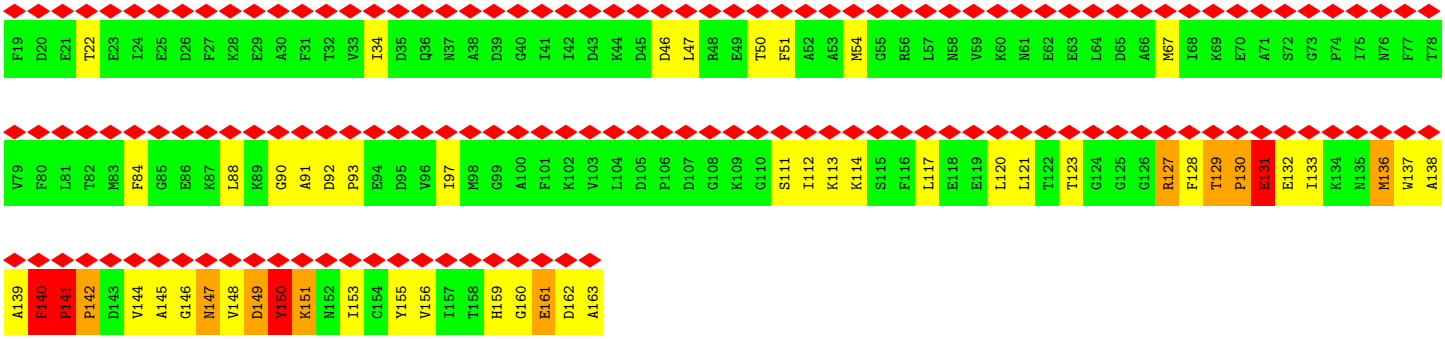
F19 D20 E21 T22 E23 I24 E25 D26 F27 K28 E29 A30 F31 T32 V33 I34 D35 Q36 N37 A38 D39 G40 I41 I42 D43 K44 D45 D46 L47 R48 E49 T50 F51 A52 A53 M54 G55 R56 L57 N58 V59 K60 N61 E62 E63 L64 D65 A66 M67 I68 K69 E70 A71 S72 G73 P74 I75 N76 F77 T78

V79 F80 L81 T82 M83 F84 G85 E86 K87 L88 K89 G90 A91 D92 P93 E94 D95 V96 I97 N98 G99 A100 F101 K102 V103 L104 D105 P106 D107 G108 K109 G110 S111 I112 K113 K114 S115 F116 L117 E118 E119 L120 L121 T122 T123 G124 G125 G126 R127 F128 T129 P130 E131 E132 I133 K134 N135 M136 W137 A138

A139 F140 P141 P142 D143 V144 A145 G146 N147 V148 D149 Y150 K151 N152 I153 C154 Y155 V156 I157 T158 H159 G160 E161 D162 A163

- Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

Chain E:



- Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

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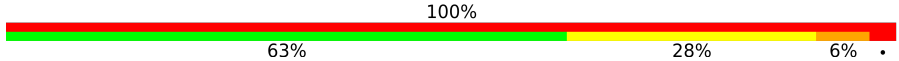
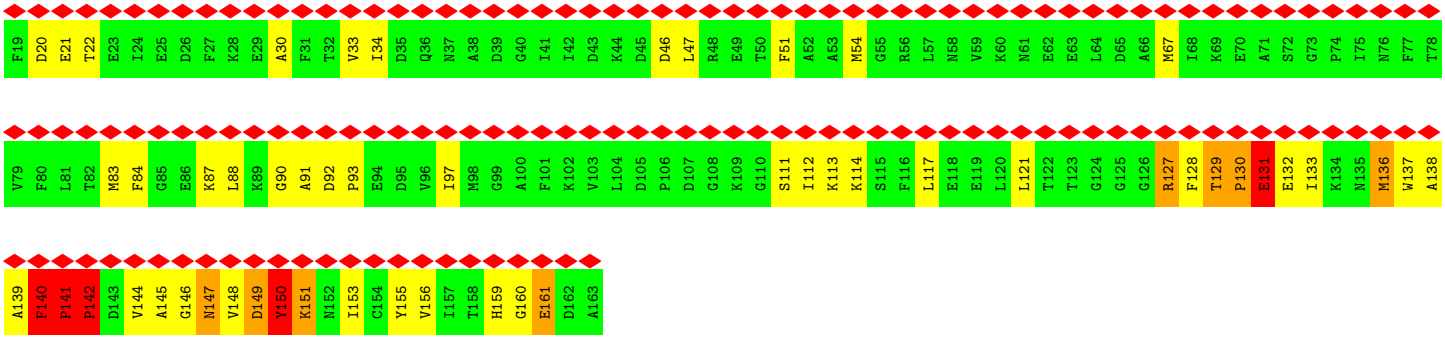
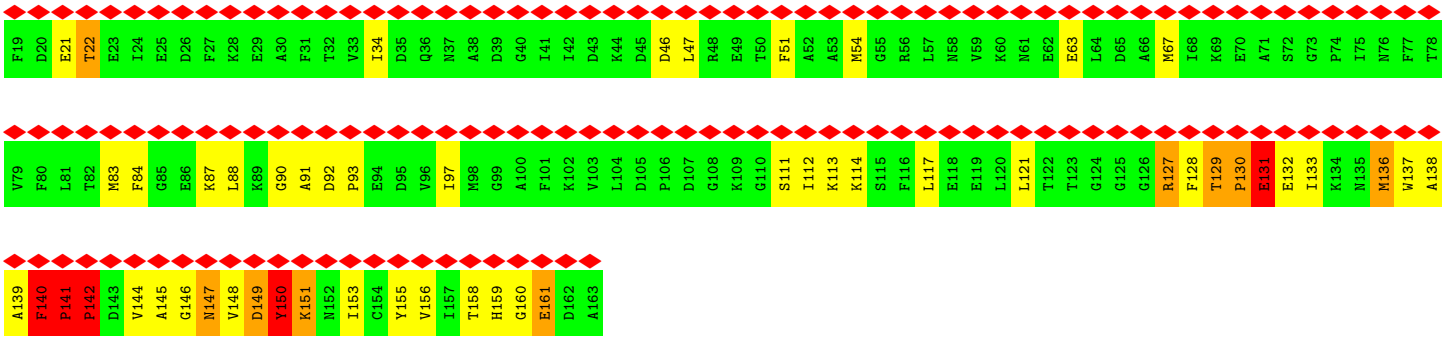




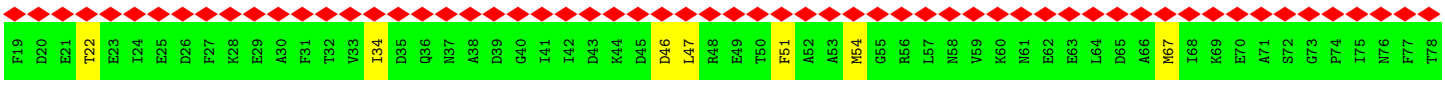
- Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

Chain K:



- Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

Chain N:



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A139 F140 P141 P142 D143 V144 A145 G146 N147 V148 D149 Y150 K151 N152 I153 C154 Y155 V156 I157 T158 H159 G160 E161 D162 A163

- Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

Chain Q:

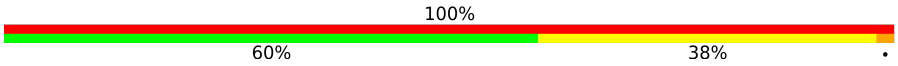
F19 D20 E21 T22 E23 I24 E25 D26 F27 K28 E29 A30 F31 T32 V33 I34 D35 Q36 N37 A38 D39 G40 I41 I42 D43 K44 D45 D46 L47 R48 E49 T50 F51 A52 A53 M54 G55 R56 L57 N58 V59 K60 N61 E62 E63 L64 D65 A66 M67 I68 K69 E70 A71 S72 G73 P74 I75 N76 F77 T78

V79 F80 L81 T82 M83 F84 G85 E86 K87 L88 K89 G90 A91 D92 P93 E94 D95 V96 I97 M98 G99 A100 F101 K102 V103 L104 D105 P106 D107 G108 K109 G110 S111 I112 K113 K114 S115 F116 L117 E118 E119 L120 L121 T122 T123 G124 G125 G126 R127 F128 T129 P130 E131 E132 I133 K134 N135 M136 W137 A138

A139 F140 P141 P142 D143 V144 A145 G146 N147 V148 D149 Y150 K151 N152 I153 C154 Y155 V156 I157 T158 H159 G160 E161 D162 A163

- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain C:



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I63 T64 F65 E66 E67 F68 L69 P70 M71 L72 Q73 A74 A75 A76 N77 N78 K79 D80 Q81 G82 T83 F84 E85 D86 F87 V88 E89 G90 L91 R92 V93 F94 D95 K96 E97 G98 N99 G100 T101 V102 M103 G104 A105 E106 L107 R108 H109 V110 L111 A112 T113 L114 G115 E116 K117 M118 T119 E120 E121 E122

V123 E124 E125 L126 M127 K128 G129 Q130 E131 D132 S133 N134 G135 C136 I137 N138 Y139 E140 A141 F142 V143 K144 H145 I146 M147 S148 V149

- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain F:

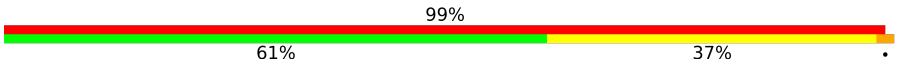
S3 K4 A5 A6 A7 D8 D9 F10 K11 E12 A13 F14 L15 L16 F17 D18 R19 T20 G21 D22 A23 K24 I25 T26 A27 S28 Q29 V30 G31 D32 I33 A34 R35 A36 L37 G38 Q39 N40 P41 T42 N43 A44 E45 I46 N47 K48 I49 L50 G51 N52 P53 S54 K55 E56 E57 M58 N59 A60 A61 A62

I63 T64 F65 E66 E67 F68 L69 P70 M71 L72 Q73 A74 A75 A76 N77 N78 K79 D80 Q81 G82 T83 F84 E85 D86 F87 V88 E89 G90 L91 R92 V93 F94 D95 K96 E97 G98 N99 G100 T101 V102 M103 G104 A105 E106 L107 R108 H109 V110 L111 A112 T113 L114 G115 E116 K117 M118 T119 E120 E121 E122

V123 E124 E125 L126 M127 K128 G129 Q130 E131 D132 S133 N134 G135 C136 I137 N138 Y139 E140 A141 F142 V143 K144 H145 I146 M147 S148 V149

• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain I:



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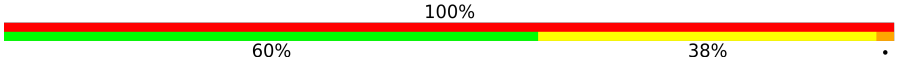
I63 T64 F65 E66 E67 F68 L69 P70 M71 L72 Q73 A74 A75 A76 N77 N78 K79 D80 Q81 G82 T83 F84 E85 D86 F87 V88 E89 G90 L91 R92 V93 F94 D95 K96 E97 G98 N99 G100 T101 V102 M103 G104 A105 E106 L107 R108 H109 V110 L111 A112 T113 L114 G115 E116 K117 M118 T119 E120 E121 E122

V123 E124 E125 L126 M127 K128 G129 Q130 E131 D132 S133 N134 G135 C136 I137 N138 Y139 E140 A141 F142 V143 K144 H145 I146 M147 S148 V149

• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain L:



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I63 T64 F65 E66 E67 F68 L69 P70 M71 L72 Q73 A74 A75 A76 N77 N78 K79 D80 Q81 G82 T83 F84 E85 D86 F87 V88 E89 G90 L91 R92 V93 F94 D95 K96 E97 G98 N99 G100 T101 V102 M103 G104 A105 E106 L107 R108 H109 V110 L111 A112 T113 L114 G115 E116 K117 M118 T119 E120 E121 E122

V123 E124 E125 L126 M127 K128 G129 Q130 E131 D132 S133 N134 G135 C136 I137 N138 Y139 E140 A141 F142 V143 K144 H145 I146 M147 S148 V149

• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain O:

S3 K4 A5 A6 A7 D8 D9 F10 K11 E12 A13 F14 L15 L16 F17 D18 R19 T20 G21 D22 A23 K24 I25 T26 A27 S28 Q29 V30 G31 D32 I33 A34 R35 A36 L37 G38 Q39 N40 P41 T42 N43 A44 E45 I46 M47 K48 I49 L50 G51 N52 P53 S54 K55 E56 E57 M58 N59 A60 A61 A62

I63 T64 F65 E66 E67 F68 L69 P70 M71 L72 Q73 A74 A75 A76 N77 N78 K79 D80 Q81 G82 T83 F84 E85 D86 F87 V88 E89 G90 L91 R92 V93 F94 D95 K96 E97 G98 N99 G100 T101 V102 M103 G104 A105 E106 L107 R108 H109 V110 L111 A112 T113 L114 G115 E116 K117 M118 T119 E120 E121 E122

V123 E124 E125 L126 M127 K128 G129 Q130 E131 D132 S133 N134 G135 C136 I137 N138 Y139 E140 A141 F142 V143 K144 H145 I146 M147 S148 V149

• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain R:

S3 K4 A5 A6 A7 D8 D9 F10 K11 E12 A13 F14 L15 L16 F17 D18 R19 T20 G21 D22 A23 K24 I25 T26 A27 S28 Q29 V30 G31 D32 I33 A34 R35 A36 L37 G38 Q39 N40 P41 T42 N43 A44 E45 I46 M47 K48 I49 L50 G51 N52 P53 S54 K55 E56 E57 M58 N59 A60 A61 A62

I63 T64 F65 E66 E67 F68 L69 P70 M71 L72 Q73 A74 A75 A76 N77 N78 K79 D80 Q81 G82 T83 F84 E85 D86 F87 V88 E89 G90 L91 R92 V93 F94 D95 K96 E97 G98 N99 G100 T101 V102 M103 G104 A105 E106 L107 R108 H109 V110 L111 A112 T113 L114 G115 E116 K117 M118 T119 E120 E121 E122

V123 E124 E125 L126 M127 K128 G129 Q130 E131 D132 S133 N134 G135 C136 I137 N138 Y139 E140 A141 F142 V143 K144 H145 I146 M147 S148 V149

- Molecule 4: SKELETAL MUSCLE ACTIN

Chain 1: 93% 57% 31% 9%

D1 E2 D3 E4 T5 T6 A7 L8 V9 C10 D11 N12 G13 S14 G15 L16 V17 K18 A19 G20 F21 A22 G23 D24 D25 A26 P27 R28 A29 V30 F31 P32 S33 I34 V35 G36 R37 P38 R39 H40 Q41 G42 V43 M44 V45 G46 M47 G48 Q49 K50 D51 S52 Y53 V54 G55 D56 E57 A58 Q59 S60

K61 R62 G63 I64 L65 T66 L67 K68 Y69 P70 I71 E72 H73 G74 I75 I76 T77 N78 W79 D80 D81 M82 E83 K84 I85 W86 H87 H88 T89 F90 Y91 N92 E93 L94 R95 V96 A97 P98 E99 E100 H101 P102 T103 L104 L105 T106 E107 A108 P109 L110 N111 P112 K113 A114 N115 R116 E117 K118 M119 T120

Q121 I122 M123 F124 E125 T126 F127 N128 V129 P130 A131 M132 Y133 V134 A135 I136 Q137 A138 V139 L140 S141 L142 Y143 A144 S145 G146 R147 T148 T149 G150 I151 V152 L153 D154 S155 G156 D157 G158 V159 T160 H161 N162 V163 P164 I165 Y166 E167 G168 Y169 A170 L171 P172 H173 A174 I175 M176 R177 L178 D179 L180

A181 G182 R183 D184 L185 T186 D187 Y188 L189 M190 K191 I192 L193 T194 E195 R196 G197 Y198 S199 F200 V201 T202 T203 A204 E205 R206 E207 I208 V209 R210 D211 I212 K213 E214 K215 L216 C217 Y218 V219 A220 L221 D222 F223 E224 N225 E226 M227 A228 T229 S233 E237 K238 S239 Y240 E241 L242 P243 D244

G245 Q246 V247 T248 T249 I250 G251 N252 E253 R254 F255 R256 C257 P258 E259 T260 L261 F262 Q263 P264 S265 F266 I267 G268 M269 E270 S271 A272 G273 I274 H275 E276 T277 T278 Y279 N280 S281 T282 M283 K284 C285 D286 I287 D288 I289 R290 K291 D292 L293 Y294 A295 N296 N297 V298 M299 S300 G301 G302 T303 T304

M305 Y306 P307 G308 I309 A310 D311 R312 M313 Q314 K315 E316 I317 T318 A319 L320 A321 P322 S323 T324 M325 K326 I327 K328 I329 I330 A331 P332 P333 E334 R335 K336 Y337 S338 V339 W340 I341 G342 G343 S344 I345 L346 A347 S348 L349 S350 T351 F352 Q353 Q354 M355 W356 I357 T358 K359 Q360 E361 Y362 D363 E364

A365 G366 P367 S368 I369 V370 H371 R372 LYS CYS PHE

- Molecule 4: SKELETAL MUSCLE ACTIN

Chain 2: 99% 60% 31% 6%

D1 E2 D3 E4 T5 T6 A7 L8 V9 C10 D11 N12 G13 S14 G15 L16 V17 K18 A19 G20 F21 A22 G23 D24 D25 A26 P27 R28 A29 V30 F31 P32 S33 I34 V35 G36 R37 P38 R39 H40 Q41 G42 V43 M44 V45 G46 M47 G48 Q49 K50 D51 S52 Y53 V54 G55 D56 E57 A58 Q59 S60

K61 R62 G63 I64 L65 T66 L67 K68 Y69 P70 I71 E72 H73 G74 I75 I76 T77 N78 W79 D80 D81 M82 E83 K84 I85 W86 H87 H88 T89 F90 Y91 N92 E93 L94 R95 V96 A97 P98 E99 E100 H101 P102 T103 L104 L105 T106 E107 A108 P109 L110 N111 P112 K113 A114 N115 R116 E117 K118 M119 T120

Q121 I122 M123 F124 E125 T126 F127 N128 V129 P130 A131 M132 Y133 V134 A135 I136 Q137 A138 V139 L140 S141 L142 Y143 A144 S145 G146 R147 T148 T149 G150 I151 V152 L153 D154 S155 G156 D157 G158 V159 T160 H161 N162 V163 P164 I165 Y166 E167 G168 Y169 A170 L171 P172 H173 A174 I175 M176 R177 L178 D179 L180

A181 G182 R183 D184 L185 T186 D187 Y188 L189 M190 K191 I192 L193 T194 E195 R196 G197 Y198 S199 F200 V201 T202 T203 A204 E205 R206 E207 I208 V209 R210 D211 I212 K213 E214 K215 L216 C217 Y218 V219 A220 L221 D222 F223 E224 N225 E226 M227 A228 T229 A230 A231 S232 S233 S234 S235 L236 E237 K238 S239 Y240

E241 L242 P243 D244 G245 Q246 V247 I248 T249 I250 G251 N252 E253 R254 F255 R256 C257 P258 E259 T260 L261 F262 Q263 P264 S265 F266 I267 G268 M269 E270 S271 A272 G273 I274 H275 E276 T277 T278 Y279 N280 S281 I282 M283 K284 C285 D286 I287 D288 I289 R290 K291 D292 L293 Y294 A295 N296 N297 V298 M299 S300

G301 G302 T303 T304 M305 Y306 P307 G308 I309 A310 D311 R312 M313 Q314 K315 E316 I317 T318 A319 L320 A321 P322 S323 T324 M325 K326 I327 K328 I329 I330 A331 P332 P333 E334 R335 K336 Y337 S338 V339 W340 I341 G342 G343 S344 I345 L346 A347 S348 L349 S350 T351 F352 Q353 Q354 M355 W356 I357 T358 K359 Q360

E361 Y362 D363 E364 A365 G366 P367 S368 I369 V370 H371 R372 LYS CYS PHE

- Molecule 4: SKELETAL MUSCLE ACTIN

Chain 3: 99% 62% 29% 6%

D1 E2 D3 E4 T5 T6 A7 L8 V9 C10 D11 N12 G13 S14 G15 L16 V17 K18 A19 G20 F21 A22 G23 D24 D25 A26 P27 R28 A29 V30 F31 P32 S33 I34 V35 G36 R37 P38 R39 H40 Q41 G42 V43 M44 V45 G46 M47 G48 Q49 K50 D51 S52 Y53 V54 G55 D56 E57 A58 Q59 S60

K61 R62 G63 I64 L65 T66 L67 K68 Y69 P70 I71 E72 H73 G74 I75 I76 T77 N78 W79 D80 D81 M82 E83 K84 I85 W86 H87 H88 T89 F90 Y91 N92 E93 L94 R95 V96 A97 P98 E99 E100 H101 P102 T103 L104 L105 T106 E107 A108 P109 L110 N111 P112 K113 A114 N115 R116 E117 K118 M119 T120

Q121 I122 M123 F124 E125 T126 F127 N128 V129 P130 A131 M132 Y133 V134 A135 I136 Q137 A138 V139 L140 S141 L142 Y143 A144 S145 G146 R147 T148 T149 G150 I151 V152 L153 D154 S155 G156 D157 G158 V159 T160 H161 N162 V163 P164 I165 Y166 E167 G168 Y169 A170 L171 P172 H173 A174 I175 M176 R177 L178 D179 L180

A181 G182 R183 D184 L185 T186 D187 Y188 L189 M190 K191 I192 L193 T194 E195 R196 G197 Y198 S199 F200 V201 T202 T203 A204 E205 R206 E207 I208 V209 R210 D211 I212 K213 E214 K215 L216 C217 Y218 V219 A220 L221 D222 F223 E224 N225 E226 M227 A228 T229 A230 A231 S232 S233 S234 S235 L236 E237 K238 S239 Y240

E241 L242 P243 D244 G245 Q246 V247 I248 T249 I250 G251 N252 E253 R254 F255 R256 C257 P258 E259 T260 L261 F262 Q263 P264 S265 F266 I267 G268 M269 E270 S271 A272 G273 I274 H275 E276 T277 T278 Y279 N280 S281 I282 M283 K284 C285 D286 I287 D288 I289 R290 K291 D292 L293 Y294 A295 N296 N297 V298 M299 S300

G301 G302 T303 T304 M305 Y306 P307 G308 I309 A310 D311 R312 M313 Q314 K315 E316 I317 T318 A319 L320 A321 P322 S323 T324 M325 K326 I327 K328 I329 I330 A331 P332 P333 E334 R335 K336 Y337 S338 V339 W340 I341 G342 G343 S344 I345 L346 A347 S348 L349 S350 T351 F352 Q353 Q354 M355 W356 I357 T358 K359 Q360

E361 Y362 D363 E364 A365 G366 P367 S368 I369 V370 H371 R372 LYS CYS PHE

- Molecule 4: SKELETAL MUSCLE ACTIN

Chain 4: 99% 62% 30% 6%

D1 E2 D3 E4 T5 T6 A7 L8 V9 C10 D11 N12 G13 S14 G15 L16 V17 K18 A19 G20 F21 A22 G23 D24 D25 A26 P27 R28 A29 V30 F31 P32 S33 I34 V35 G36 R37 P38 R39 H40 Q41 G42 V43 M44 V45 G46 M47 G48 Q49 K50 D51 S52 Y53 V54 G55 D56 E57 A58 Q59 S60

K61 R62 G63 I64 L65 T66 L67 K68 Y69 P70 I71 E72 H73 G74 I75 I76 T77 N78 W79 D80 D81 M82 E83 K84 I85 W86 H87 H88 T89 F90 Y91 N92 E93 L94 R95 V96 A97 P98 E99 E100 H101 P102 T103 L104 L105 T106 E107 A108 P109 L110 N111 P112 K113 A114 N115 R116 E117 K118 M119 T120

Q121 I122 M123 F124 E125 T126 F127 N128 V129 P130 A131 M132 Y133 V134 A135 I136 Q137 A138 V139 L140 S141 L142 Y143 A144 S145 G146 R147 T148 T149 G150 I151 V152 L153 D154 S155 G156 D157 G158 V159 T160 H161 N162 V163 P164 I165 Y166 E167 G168 Y169 A170 L171 P172 H173 A174 I175 M176 R177 L178 D179 L180

A181 G182 R183 D184 L185 T186 D187 Y188 L189 M190 K191 I192 L193 T194 E195 R196 G197 Y198 S199 F200 V201 T202 T203 A204 E205 R206 E207 I208 V209 R210 D211 I212 K213 E214 K215 L216 C217 Y218 V219 A220 L221 D222 F223 E224 N225 E226 M227 A228 T229 A230 A231 S232 S233 S234 S235 L236 E237 K238 S239 Y240

E241 L242 P243 D244 G245 Q246 V247 I248 T249 I250 G251 N252 E253 R254 F255 R256 C257 P258 E259 T260 L261 F262 Q263 P264 S265 F266 I267 G268 M269 E270 S271 A272 G273 I274 H275 E276 T277 T278 Y279 N280 S281 I282 M283 K284 C285 D286 I287 D288 I289 R290 K291 D292 L293 Y294 A295 N296 N297 V298 M299 S300

G301 G302 T303 T304 M305 Y306 P307 G308 I309 A310 D311 R312 M313 Q314 K315 E316 I317 T318 A319 L320 A321 P322 S323 T324 M325 K326 I327 K328 I329 I330 A331 P332 P333 E334 R335 K336 Y337 S338 V339 W340 I341 G342 G343 S344 I345 L346 A347 S348 L349 S350 T351 F352 Q353 Q354 M355 W356 I357 T358 K359 Q360

E361 Y362 D363 E364 A365 G366 P367 S368 I369 V370 H371 R372 LYS CYS PHE

- Molecule 4: SKELETAL MUSCLE ACTIN

Chain 5: 99% 63% 28% 6%

D1 E2 D3 E4 T5 T6 A7 L8 V9 C10 D11 N12 G13 S14 G15 L16 V17 K18 A19 G20 F21 A22 G23 D24 D25 A26 P27 R28 A29 V30 F31 P32 S33 I34 V35 G36 R37 P38 R39 H40 Q41 G42 V43 M44 V45 G46 M47 G48 Q49 K50 D51 S52 Y53 V54 G55 D56 E57 A58 Q59 S60

K61 R62 G63 I64 L65 T66 L67 K68 Y69 P70 I71 E72 H73 G74 I75 I76 T77 N78 W79 D80 D81 M82 E83 K84 I85 W86 H87 H88 T89 F90 Y91 N92 E93 L94 R95 V96 A97 P98 E99 E100 H101 P102 T103 L104 L105 T106 E107 A108 P109 L110 N111 P112 K113 A114 N115 R116 E117 K118 M119 T120

Q121 I122 M123 F124 E125 T126 F127 N128 V129 P130 A131 M132 Y133 V134 A135 I136 Q137 A138 V139 L140 S141 L142 Y143 A144 S145 G146 R147 T148 T149 G150 I151 V152 L153 D154 S155 G156 D157 G158 V159 T160 H161 N162 V163 P164 I165 Y166 E167 G168 Y169 A170 L171 P172 H173 A174 I175 M176 R177 L178 D179 L180

A181 G182 R183 D184 L185 T186 D187 Y188 L189 M190 K191 I192 L193 T194 E195 R196 G197 Y198 S199 F200 V201 T202 T203 A204 E205 R206 E207 I208 V209 R210 D211 I212 K213 E214 K215 L216 C217 Y218 V219 A220 L221 D222 F223 E224 N225 E226 M227 A228 T229 A230 A231 S232 S233 S234 S235 L236 E237 K238 S239 Y240

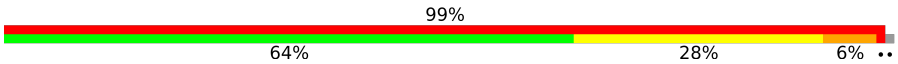
E241 L242 P243 D244 G245 Q246 V247 I248 T249 I250 G251 N252 E253 R254 F255 R256 C257 P258 E259 T260 L261 F262 Q263 P264 S265 F266 I267 G268 M269 E270 S271 A272 G273 I274 H275 E276 T277 T278 Y279 N280 S281 I282 M283 K284 C285 D286 I287 D288 I289 R290 K291 D292 L293 Y294 A295 N296 N297 V298 M299 S300

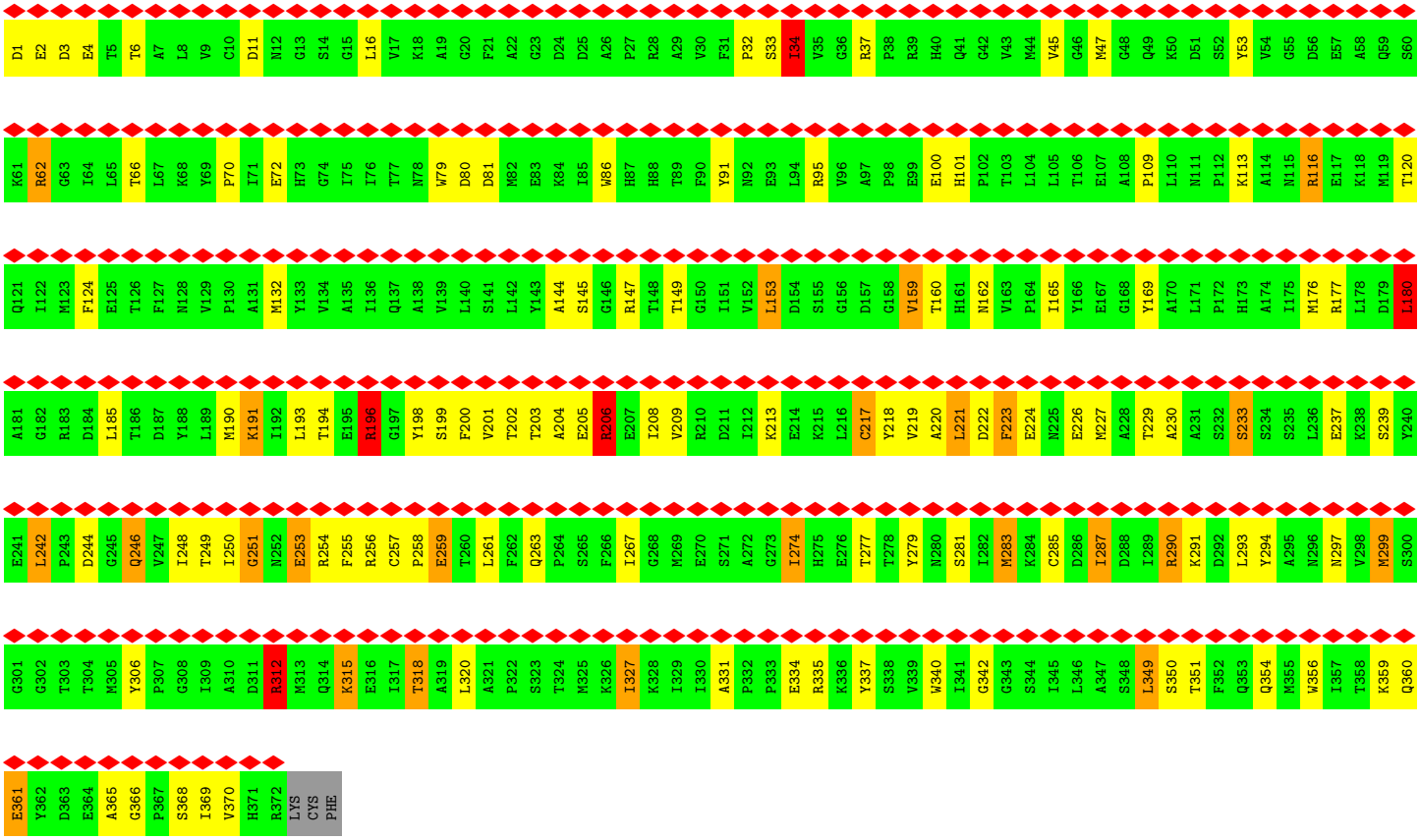
G301 G302 T303 T304 M305 Y306 P307 G308 I309 A310 D311 R312 M313 Q314 K315 E316 I317 T318 A319 L320 A321 P322 S323 T324 M325 K326 I327 K328 I329 I330 A331 P332 P333 E334 R335 K336 Y337 S338 V339 W340 I341 G342 G343 S344 I345 L346 A347 S348 L349 S350 T351 F352 Q353 Q354 M355 W356 I357 T358 K359 Q360

E361 Y362 D363 E364 A365 G366 P367 S368 I369 V370 H371 R372 LYS CYS PHE

- Molecule 4: SKELETAL MUSCLE ACTIN

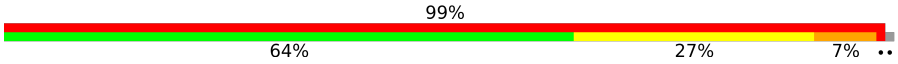
Chain 6:

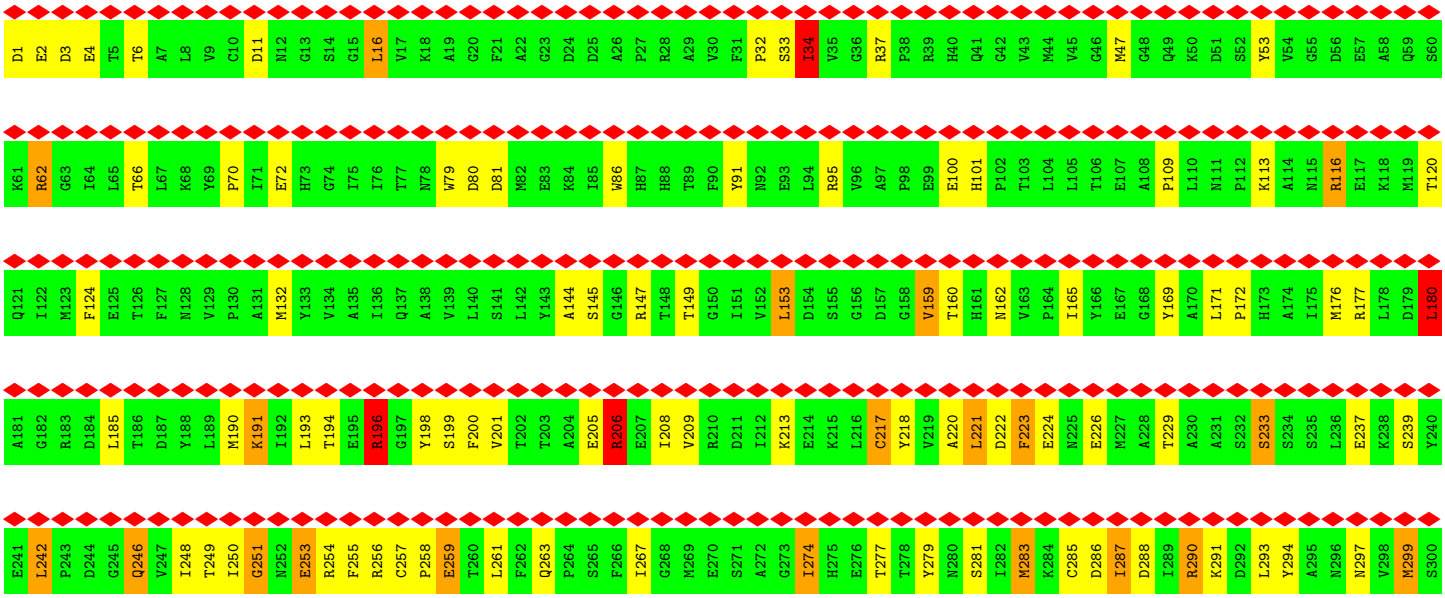




- Molecule 4: SKELETAL MUSCLE ACTIN

Chain 7:





G301 G302 T303 T304 M305 Y306 P307 G308 I309 A310 D311 R312 M313 Q314 K315 E316 I317 T318 A319 L320 A321 P322 S323 T324 M325 K326 I327 K328 I329 I330 A331 P332 P333 E334 R335 K336 Y337 S338 V339 W340 I341 G342 G343 S344 I345 L346 A347 S348 L349 S350 T351 F352 Q353 Q354 M355 W356 I357 T358 K359 Q360

E361 Y362 D363 E364 A365 G366 P367 S368 I369 V370 H371 R372 LYS CYS PHE

- Molecule 4: SKELETAL MUSCLE ACTIN

Chain 8: 99% 59% 31% 8%

D1 E2 D3 E4 T5 T6 A7 L8 V9 C10 D11 N12 G13 S14 G15 L16 V17 K18 A19 G20 F21 A22 G23 D24 D25 A26 P27 R28 A29 V30 F31 P32 S33 I34 V35 G36 R37 P38 R39 H40 Q41 G42 V43 M44 V45 G46 M47 G48 Q49 K50 D51 S52 Y53 V54 G55 D56 E57 A58 Q59 S60

K61 R62 G63 I64 L65 T66 L67 K68 Y69 P70 I71 E72 H73 G74 I75 I76 T77 N78 W79 D80 D81 M82 E83 K84 I85 W86 H87 H88 T89 F90 Y91 N92 E93 L94 R95 V96 A97 P98 E99 E100 H101 P102 T103 L104 L105 T106 E107 A108 P109 L110 N111 P112 K113 A114 N115 R116 E117 K118 M119 T120

Q121 I122 M123 F124 E125 T126 F127 N128 V129 P130 A131 M132 Y133 V134 A135 I136 Q137 A138 V139 L140 S141 L142 Y143 A144 S145 G146 R147 T148 T149 G150 I151 V152 L153 D154 S155 G156 D157 G158 V159 T160 H161 N162 V163 P164 I165 Y166 E167 G168 Y169 A170 L171 P172 H173 A174 I175 M176 R177 L178 D179 L180

A181 G182 R183 D184 L185 T186 D187 Y188 L189 M190 K191 I192 L193 T194 E195 R196 G197 Y198 S199 F200 V201 T202 T203 A204 E205 R206 E207 I208 V209 R210 D211 I212 K213 E214 K215 L216 C217 Y218 V219 A220 L221 D222 F223 E224 N225 E226 M227 A228 T229 A230 A231 S232 S233 S234 S235 L236 E237 K238 S239 Y240

E241 L242 P243 D244 G245 Q246 V247 I248 T249 I250 G251 N252 E253 R254 F255 R256 C257 P258 E259 T260 L261 F262 Q263 P264 S265 F266 I267 G268 M269 E270 S271 A272 G273 I274 H275 E276 T277 T278 Y279 N280 S281 I282 M283 K284 C285 D286 I287 D288 I289 R290 K291 D292 L293 Y294 A295 N296 N297 V298 M299 S300

G301 G302 T303 T304 M305 Y306 P307 G308 I309 A310 D311 R312 M313 Q314 K315 E316 I317 T318 A319 L320 A321 P322 S323 T324 M325 K326 I327 K328 I329 I330 A331 P332 P333 E334 R335 K336 Y337 S338 V339 W340 I341 G342 G343 S344 I345 L346 A347 S348 L349 S350 T351 F352 Q353 Q354 M355 W356 I357 T358 K359 Q360

E361 Y362 D363 E364 A365 G366 P367 S368 I369 V370 H371 R372 LYS CYS PHE

- Molecule 4: SKELETAL MUSCLE ACTIN

Chain 9: 99% 57% 33% 8%

D1 E2 D3 E4 T5 T6 A7 L8 V9 C10 D11 N12 G13 S14 G15 L16 V17 K18 A19 G20 F21 A22 G23 D24 D25 A26 P27 R28 A29 V30 F31 P32 S33 I34 V35 G36 R37 P38 R39 H40 Q41 G42 V43 M44 V45 G46 M47 G48 Q49 K50 D51 S52 Y53 V54 G55 D56 E57 A58 Q59 S60

K61 R62 G63 I64 L65 T66 L67 K68 Y69 P70 I71 E72 H73 G74 I75 I76 T77 N78 W79 D80 D81 M82 E83 K84 I85 W86 H87 H88 T89 F90 Y91 N92 E93 L94 R95 V96 A97 P98 E99 E100 H101 P102 T103 L104 L105 T106 E107 A108 P109 L110 N111 P112 K113 A114 N115 R116 E117 K118 M119 T120

Q121 I122 M123 F124 E125 T126 F127 N128 V129 P130 A131 M132 Y133 V134 A135 I136 Q137 A138 V139 L140 S141 L142 Y143 A144 S145 G146 R147 T148 T149 G150 I151 V152 L153 D154 S155 G156 D157 G158 V159 T160 H161 N162 V163 P164 I165 Y166 E167 G168 Y169 A170 L171 P172 H173 A174 I175 M176 R177 L178 D179 L180

A181 G182 R183 D184 L185 T186 D187 Y188 L189 M190 K191 I192 L193 T194 E195 R196 G197 Y198 S199 F200 V201 T202 T203 A204 E205 R206 E207 I208 V209 R210 D211 I212 K213 E214 K215 L216 C217 Y218 V219 A220 L221 D222 F223 E224 N225 E226 M227 A228 T229 A230 A231 S232 S233 S234 S235 L236 E237 K238 S239 Y240

E241 L242 P243 D244 G245 Q246 V247 I248 T249 I250 G251 N252 E253 R254 F255 R256 C257 P258 E259 T260 L261 F262 Q263 P264 S265 F266 I267 G268 M269 E270 S271 A272 G273 I274 H275 E276 T277 T278 Y279 N280 S281 I282 M283 K284 C285 D286 I287 D288 I289 R290 K291 D292 L293 Y294 A295 N296 N297 V298 M299 S300

G301 G302 T303 T304 M305 Y306 P307 G308 I309 A310 D311 R312 M313 Q314 K315 E316 I317 T318 A319 L320 A321 P322 S323 T324 M325 K326 I327 K328 I329 I330 A331 P332 P333 E334 R335 K336 Y337 S338 V339 W340 I341 G342 G343 S344 I345 L346 A347 S348 L349 S350 T351 F352 Q353 Q354 M355 W356 I357 T358 K359 Q360

E361 Y362 D363 E364 A365 G366 P367 S368 I369 V370 H371 R372 LYS CYS PHE

- Molecule 4: SKELETAL MUSCLE ACTIN

Chain V: 99% 55% 34% 9% ••

D1 E2 D3 E4 T5 T6 A7 L8 V9 C10 D11 N12 G13 S14 G15 L16 V17 K18 A19 G20 F21 A22 G23 D24 D25 A26 P27 R28 A29 V30 F31 P32 S33 I34 V35 G36 R37 P38 R39 H40 Q41 G42 V43 M44 V45 G46 M47 G48 Q49 K50 D51 S52 Y53 V54 G55 D56 E57 A58 Q59 S60

K61 R62 G63 I64 L65 T66 L67 K68 Y69 P70 I71 E72 H73 G74 I75 I76 T77 N78 W79 D80 D81 M82 E83 K84 I85 W86 H87 H88 T89 F90 Y91 N92 E93 L94 R95 V96 A97 P98 E99 E100 H101 P102 T103 L104 L105 T106 E107 A108 P109 L110 N111 P112 K113 A114 N115 R116 E117 K118 M119 T120

Q121 I122 M123 F124 E125 T126 F127 N128 V129 P130 A131 M132 Y133 V134 A135 I136 Q137 A138 V139 L140 S141 L142 Y143 A144 S145 G146 R147 T148 T149 G150 I151 V152 L153 D154 S155 G156 D157 G158 V159 T160 H161 N162 V163 P164 I165 Y166 E167 G168 Y169 A170 L171 P172 H173 A174 I175 M176 R177 L178 D179 L180

A181 G182 R183 D184 L185 T186 D187 Y188 L189 M190 K191 I192 L193 T194 E195 R196 G197 Y198 S199 F200 V201 T202 T203 A204 E205 R206 E207 I208 V209 R210 D211 I212 K213 E214 K215 L216 C217 Y218 V219 A220 L221 D222 F223 E224 N225 E226 M227 A228 T229 A230 A231 S232 S233 S234 S235 L236 E237 K238 S239 Y240

E241 L242 P243 D244 G245 Q246 V247 I248 T249 I250 G251 N252 E253 R254 F255 R256 C257 P258 E259 T260 L261 F262 Q263 P264 S265 F266 I267 G268 M269 E270 S271 A272 G273 I274 H275 E276 T277 T278 Y279 N280 S281 I282 M283 K284 C285 D286 I287 D288 I289 R290 K291 D292 L293 Y294 A295 N296 N297 V298 M299 S300

G301 G302 T303 T304 M305 Y306 P307 G308 I309 A310 D311 R312 M313 Q314 K315 E316 I317 T318 A319 L320 A321 P322 S323 T324 M325 K326 I327 K328 I329 I330 A331 P332 P333 E334 R335 K336 Y337 S338 V339 W340 I341 G342 G343 S344 I345 L346 A347 S348 L349 S350 T351 F352 Q353 Q354 M355 W356 I357 T358 K359 Q360

E361 Y362 D363 E364 A365 G366 P367 S368 I369 V370 H371 R372 LYS CYS PHE

- Molecule 4: SKELETAL MUSCLE ACTIN

Chain W: 94% 55% 34% 9% ••

D1 E2 D3 E4 T5 T6 A7 L8 V9 C10 D11 N12 G13 S14 G15 L16 V17 K18 A19 G20 F21 A22 G23 D24 D25 A26 P27 R28 A29 V30 F31 P32 S33 I34 V35 G36 R37 P38 R39 H40 Q41 G42 V43 M44 V45 G46 M47 G48 Q49 K50 D51 S52 Y53 V54 G55 D56 E57 A58 Q59 S60

K61 R62 G63 I64 L65 T66 L67 K68 Y69 P70 I71 E72 H73 G74 I75 I76 T77 N78 W79 D80 D81 M82 E83 K84 I85 W86 H87 H88 T89 F90 Y91 N92 E93 L94 R95 V96 A97 P98 E99 E100 H101 P102 T103 L104 L105 T106 E107 A108 P109 L110 N111 P112 K113 A114 N115 R116 E117 K118 M119 T120

Q121 I122 M123 F124 E125 T126 F127 N128 V129 P130 A131 M132 Y133 V134 A135 I136 Q137 A138 V139 L140 S141 L142 Y143 A144 S145 G146 R147 T148 T149 V152 L153 D154 S155 G156 D157 G158 V159 T160 H161 N162 V163 P164 I165 Y169 A170 L171 P172 H173 A174 I175 M176 R177 L178 D179 L180 A181 G182 R183

D184 L185 T186 D187 Y188 L189 M190 K191 I192 L193 T194 E195 R196 G197 Y198 S199 F200 V201 T202 T203 A204 E205 R206 E207 I208 V209 R210 D211 I212 K213 E214 K215 L216 C217 Y218 V219 A220 L221 D222 F223 E224 N225 E226 M227 A228 T229 A230 A231 S232 S233 S234 S235 L236 E237 K238 S239 Y240 E241 L242 P243

D244 G245 Q246 V247 I248 T249 I250 G251 N252 E253 R254 F255 R256 C257 P258 E259 T260 L261 F262 Q263 P264 S265 F266 I267 G268 M269 E270 S271 A272 G273 I274 H275 E276 T277 T278 Y279 N280 S281 I282 M283 K284 C285 D286 I287 D288 I289 R290 K291 D292 L293 Y294 N297 V298 M299 S300 G301 G302 T303 T304

M305 Y306 P307 G308 I309 A310 D311 R312 M313 Q314 K315 E316 I317 T318 A319 L320 A321 P322 S323 T324 M325 K326 I327 K328 I329 I330 A331 P332 P333 E334 R335 K336 Y337 S338 V339 W340 I341 G342 G343 S344 I345 L346 A347 S348 L349 S350 T351 F352 Q353 Q354 M355 W356 I357 T358 K359 Q360 E361 Y362 D363 E364

A365 G366 P367 S368 I369 V370 H371 R372 LYS CYS PHE

- Molecule 4: SKELETAL MUSCLE ACTIN

Chain X: 99% 61% 30% 7%

D1 E2 D3 E4 T5 T6 A7 L8 V9 C10 D11 N12 G13 S14 G15 L16 V17 K18 A19 G20 F21 A22 G23 D24 D25 A26 P27 R28 A29 V30 F31 P32 S33 I34 V35 G36 R37 P38 R39 H40 Q41 G42 V43 M44 V45 G46 M47 G48 Q49 K50 D51 S52 Y53 V54 G55 D56 E57 A58 Q59 S60

K61 R62 G63 I64 L65 T66 L67 K68 Y69 P70 I71 E72 H73 G74 I75 I76 T77 N78 W79 D80 D81 M82 E83 K84 I85 W86 H87 H88 T89 F90 Y91 N92 E93 L94 R95 V96 A97 P98 E99 E100 H101 P102 T103 L104 L105 T106 E107 A108 P109 L110 N111 P112 K113 A114 N115 R116 E117 K118 M119 T120

Q121 I122 M123 F124 E125 T126 F127 N128 V129 P130 A131 M132 Y133 V134 A135 I136 Q137 A138 V139 L140 S141 L142 Y143 A144 S145 G146 R147 T148 T149 G150 I151 V152 L153 D154 S155 G156 D157 G158 V159 T160 H161 N162 V163 P164 I165 Y166 E167 G168 Y169 A170 L171 P172 H173 A174 I175 M176 R177 L178 D179 L180

A181 G182 R183 D184 L185 T186 D187 Y188 L189 M190 K191 I192 L193 T194 E195 R196 G197 Y198 S199 F200 V201 T202 T203 A204 E205 R206 E207 I208 V209 R210 D211 I212 K213 E214 K215 L216 C217 Y218 V219 A220 L221 D222 F223 E224 N225 E226 M227 A228 T229 A230 A231 S232 S233 S234 S235 L236 E237 K238 S239 Y240

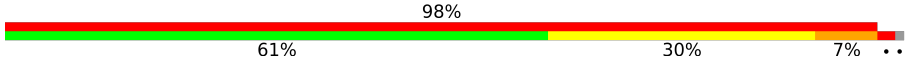
E241 L242 P243 D244 G245 Q246 V247 I248 T249 I250 G251 N252 E253 R254 F255 R256 C257 P258 E259 T260 L261 F262 Q263 P264 S265 F266 I267 G268 M269 E270 S271 A272 G273 I274 H275 E276 T277 T278 Y279 N280 S281 I282 M283 K284 C285 D286 I287 D288 I289 R290 K291 D292 L293 Y294 A295 N296 N297 V298 M299 S300

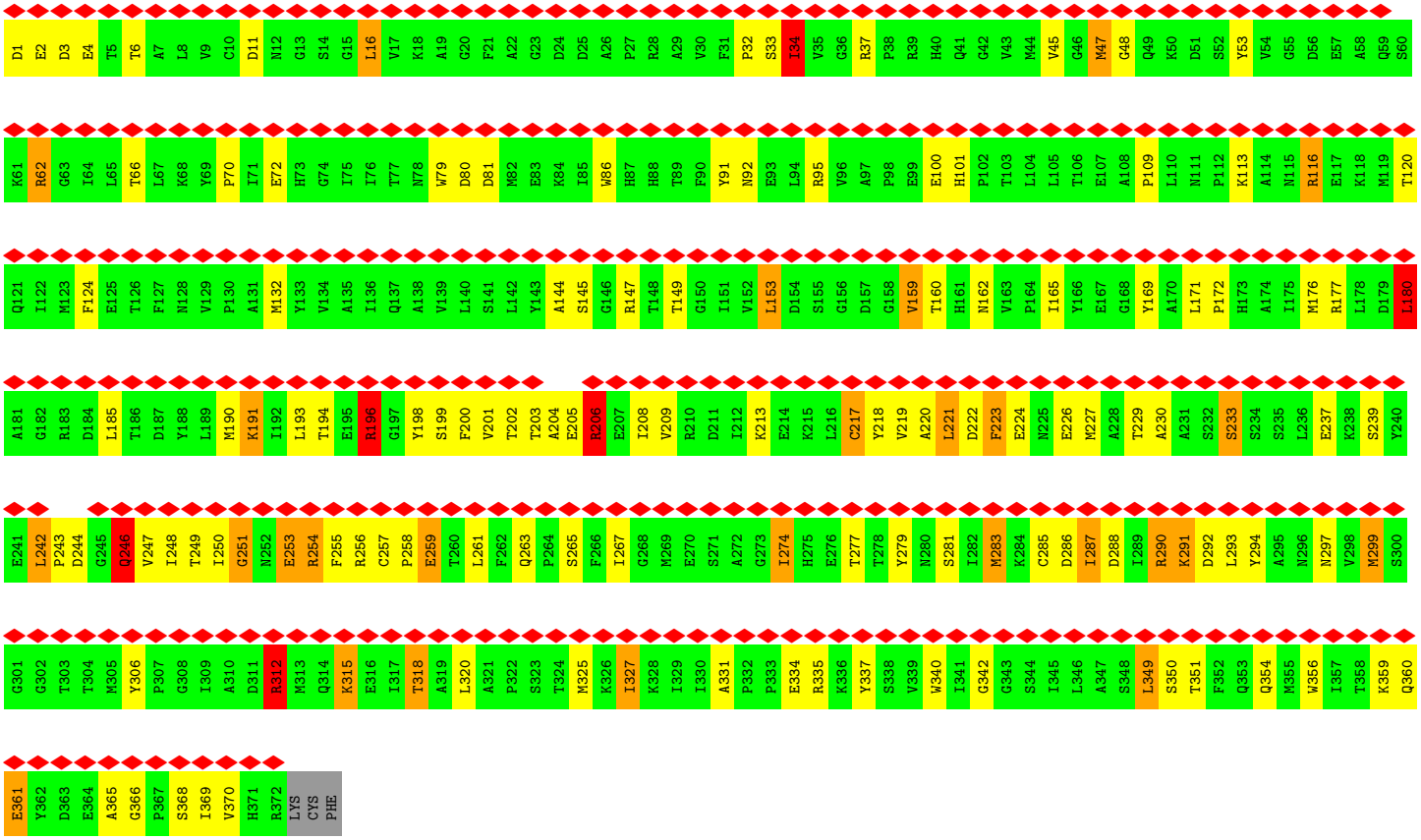
G301 G302 T303 T304 M305 Y306 P307 G308 I309 A310 D311 R312 M313 Q314 K315 E316 I317 T318 A319 L320 A321 P322 S323 T324 M325 K326 I327 K328 I329 I330 A331 P332 P333 E334 R335 K336 Y337 S338 V339 W340 I341 G342 G343 S344 I345 L346 A347 S348 L349 S350 T351 F352 Q353 Q354 M355 W356 I357 T358 K359 Q360

E361 Y362 D363 E364 A365 G366 P367 S368 I369 V370 H371 R372 LYS CYS PHE

- Molecule 4: SKELETAL MUSCLE ACTIN

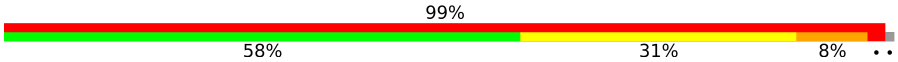
Chain Y:

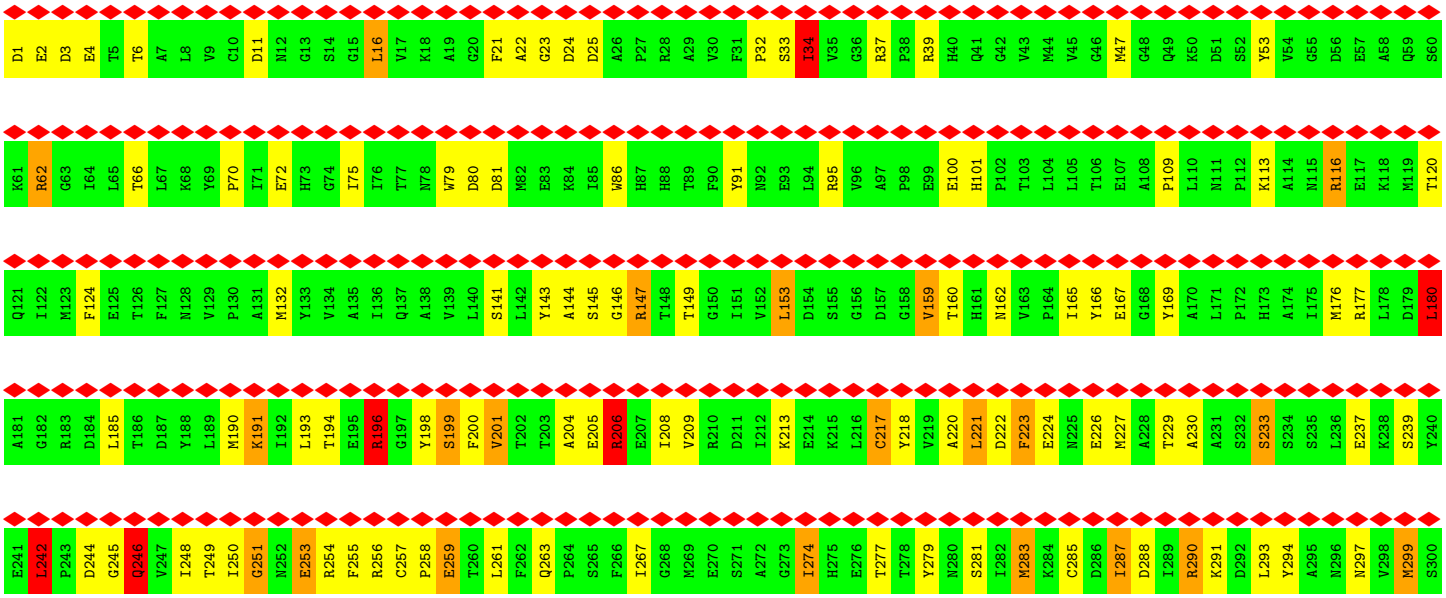


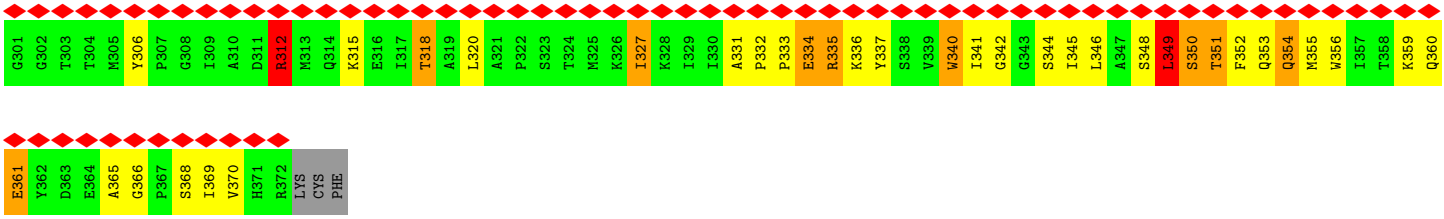


- Molecule 4: SKELETAL MUSCLE ACTIN

Chain Z:






G301
G302
T303
T304
M305
Y306
P307
G308
I309
A310
D311
R312
M313
Q314
K315
E316
I317
T318
A319
L320
A321
P322
S323
T324
M325
K326
I327
K328
I329
I330
A331
P332
P333
E334
R335
K336
Y337
S338
V339
W340
I341
G342
G343
S344
I345
L346
A347
S348
L349
S350
T351
F352
Q353
Q354
M355
W356
I357
T358
K359
Q360

E361
Y362
D363
E364
A365
G366
P367
S368
I369
V370
H371
R372
LYS
CYS
PHE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI/PHILIPS EM400	Depositor
Voltage (kV)	100	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	17000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum voxel value	366.680	Depositor
Minimum voxel value	-417.992	Depositor
Average voxel value	1.860	Depositor
Voxel value standard deviation	47.792	Depositor
Recommended contour level	81.2	Depositor
Tomogram size (Å)	9280, 9280, 464	wwPDB
Tomogram dimensions	600, 600, 30	wwPDB
Tomogram angles (°)	90, 90, 90	wwPDB
Grid spacing (Å)	15.4667, 15.4667, 15.4667	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: MLY

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	1.77	67/6448 (1.0%)	1.82	116/8729 (1.3%)
1	D	1.77	64/6448 (1.0%)	1.82	115/8729 (1.3%)
1	G	1.77	66/6449 (1.0%)	1.82	117/8732 (1.3%)
1	J	1.77	67/6449 (1.0%)	1.87	119/8732 (1.4%)
1	M	1.79	68/6449 (1.1%)	1.91	121/8732 (1.4%)
1	P	1.79	69/6449 (1.1%)	1.90	124/8732 (1.4%)
2	B	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
2	E	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
2	H	1.22	9/1148 (0.8%)	1.62	16/1548 (1.0%)
2	K	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
2	N	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
2	Q	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
3	C	0.80	0/1136	0.95	4/1525 (0.3%)
3	F	0.80	0/1136	0.95	4/1525 (0.3%)
3	I	0.80	0/1136	0.95	4/1525 (0.3%)
3	L	0.79	0/1136	0.94	4/1525 (0.3%)
3	O	0.79	0/1136	0.94	4/1525 (0.3%)
3	R	0.79	0/1136	0.95	4/1525 (0.3%)
4	1	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	2	0.89	1/2968 (0.0%)	1.64	51/4023 (1.3%)
4	3	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	4	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	5	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	6	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	7	0.89	1/2968 (0.0%)	1.64	52/4023 (1.3%)
4	8	0.89	1/2968 (0.0%)	1.64	52/4023 (1.3%)
4	9	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	V	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	W	0.89	1/2968 (0.0%)	1.64	52/4023 (1.3%)
4	X	0.89	1/2968 (0.0%)	1.64	51/4023 (1.3%)
4	Y	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	Z	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	1.34	483/93948 (0.5%)	1.69	1555/127146 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	4
1	D	1	4
1	G	1	5
1	J	1	6
1	M	1	9
1	P	1	8
2	B	0	3
2	E	0	3
2	H	0	3
2	K	0	3
2	N	0	3
2	Q	0	3
3	C	0	2
3	F	0	3
3	I	0	2
3	L	0	2
3	O	0	2
3	R	0	2
4	1	0	1
4	2	0	1
4	3	0	1
4	4	0	1
4	5	0	1
4	6	0	1
4	7	0	1
4	8	0	1
4	9	0	1
4	V	0	1
4	W	0	1
4	X	0	1
4	Y	0	1
4	Z	0	1
All	All	6	81

The worst 5 of 483 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	649	VAL	CB-CG1	53.27	2.64	1.52
1	M	649	VAL	CB-CG1	53.24	2.64	1.52
1	G	649	VAL	CB-CG1	53.23	2.64	1.52
1	J	649	VAL	CB-CG1	53.20	2.64	1.52
1	D	649	VAL	CB-CG1	53.16	2.64	1.52

The worst 5 of 1555 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	637	LYS	O-C-N	-58.52	23.72	123.20
1	P	637	LYS	O-C-N	-58.47	23.80	123.20
1	M	637	LYS	O-C-N	-58.47	23.81	123.20
1	D	637	LYS	O-C-N	-58.46	23.81	123.20
1	J	637	LYS	O-C-N	-58.43	23.87	123.20

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	648	THR	CB
1	D	648	THR	CB
1	G	648	THR	CB
1	J	648	THR	CB
1	M	648	THR	CB

5 of 81 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	623	PHE	Sidechain
1	A	637	LYS	Mainchain
1	A	649	VAL	Mainchain
1	A	98	HIS	Mainchain
2	B	22	THR	Mainchain

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	6797	0	6752	1556	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	6797	0	6754	1441	0
1	G	6797	0	6757	1537	0
1	J	6797	0	6753	1455	0
1	M	6797	0	6770	1482	0
1	P	6797	0	6773	1487	0
2	B	1127	0	1087	260	0
2	E	1127	0	1086	251	0
2	H	1127	0	1088	298	0
2	K	1127	0	1089	272	0
2	N	1127	0	1088	244	0
2	Q	1127	0	1087	245	0
3	C	1123	0	1084	200	0
3	F	1123	0	1083	172	0
3	I	1123	0	1083	187	0
3	L	1123	0	1082	171	0
3	O	1123	0	1082	233	0
3	R	1123	0	1081	225	0
4	1	2906	0	2855	394	0
4	2	2906	0	2863	227	0
4	3	2906	0	2864	137	0
4	4	2906	0	2863	185	0
4	5	2906	0	2865	94	0
4	6	2906	0	2865	102	0
4	7	2906	0	2866	78	0
4	8	2906	0	2857	317	0
4	9	2906	0	2855	346	0
4	V	2906	0	2851	383	0
4	W	2906	0	2851	390	0
4	X	2906	0	2859	215	0
4	Y	2906	0	2863	161	0
4	Z	2906	0	2855	417	0
All	All	94966	0	93611	11358	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 60.

The worst 5 of 11358 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)
1:D:797:PHE:CD1	3:F:146:ILE:HG23	1.25	1.69
1:D:792:ALA:HB2	3:F:42:THR:CG2	1.21	1.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:831:TRP:CZ3	2:B:50:THR:HG21	1.13	1.64
4:2:287:ILE:CG2	4:4:202:THR:HB	1.23	1.63
4:2:287:ILE:HG23	4:4:202:THR:CB	1.26	1.63

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	789/840 (94%)	651 (82%)	112 (14%)	26 (3%)	4	26
1	D	789/840 (94%)	651 (82%)	112 (14%)	26 (3%)	4	26
1	G	791/840 (94%)	651 (82%)	112 (14%)	28 (4%)	3	25
1	J	791/840 (94%)	652 (82%)	112 (14%)	27 (3%)	3	26
1	M	791/840 (94%)	651 (82%)	109 (14%)	31 (4%)	3	23
1	P	791/840 (94%)	649 (82%)	110 (14%)	32 (4%)	3	23
2	B	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
2	E	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
2	H	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
2	K	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
2	N	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
2	Q	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
3	C	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	F	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	I	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	L	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	O	143/147 (97%)	133 (93%)	10 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	R	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
4	1	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	2	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	3	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	4	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	5	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	6	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	7	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	8	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	9	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	V	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	W	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	X	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	Y	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	Z	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
All	All	11638/12042 (97%)	10140 (87%)	1196 (10%)	302 (3%)	8	31

5 of 302 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	LYS
1	A	202	SER
1	A	572	LYS
1	A	712	PRO
1	A	729	ALA

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	672/672 (100%)	512 (76%)	160 (24%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	672/672 (100%)	514 (76%)	158 (24%)	1	4
1	G	672/672 (100%)	513 (76%)	159 (24%)	1	4
1	J	672/672 (100%)	514 (76%)	158 (24%)	1	4
1	M	672/672 (100%)	515 (77%)	157 (23%)	1	4
1	P	672/672 (100%)	514 (76%)	158 (24%)	1	4
2	B	120/120 (100%)	119 (99%)	1 (1%)	81	89
2	E	120/120 (100%)	120 (100%)	0	100	100
2	H	120/120 (100%)	119 (99%)	1 (1%)	81	89
2	K	120/120 (100%)	119 (99%)	1 (1%)	81	89
2	N	120/120 (100%)	119 (99%)	1 (1%)	81	89
2	Q	120/120 (100%)	119 (99%)	1 (1%)	81	89
3	C	117/117 (100%)	112 (96%)	5 (4%)	29	53
3	F	117/117 (100%)	112 (96%)	5 (4%)	29	53
3	I	117/117 (100%)	112 (96%)	5 (4%)	29	53
3	L	117/117 (100%)	112 (96%)	5 (4%)	29	53
3	O	117/117 (100%)	112 (96%)	5 (4%)	29	53
3	R	117/117 (100%)	112 (96%)	5 (4%)	29	53
4	1	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	2	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	3	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	4	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	5	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	6	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	7	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	8	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	9	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	V	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	W	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	X	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	Y	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	Z	315/318 (99%)	268 (85%)	47 (15%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9864/9906 (100%)	8227 (83%)	1637 (17%)	5 12

5 of 1637 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	562	SER
4	4	229	THR
4	Z	116	ARG
1	P	716	LEU
1	P	561	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 240 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	453	GLN
4	W	252	ASN
1	P	453	GLN
4	W	92	ASN
4	Z	92	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)

270 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	$\#\|Z\| > 2$
1	MLY	P	617	1	9,10,11	0.97	1 (11%)	6,11,13	0.33	0
1	MLY	D	296	1	9,10,11	0.65	0	6,11,13	0.38	0
1	MLY	G	107	1	9,10,11	0.46	0	6,11,13	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MLY	G	385	1	9,10,11	1.01	1 (11%)	6,11,13	0.43	0
1	MLY	J	553	1	9,10,11	0.67	0	6,11,13	0.54	0
1	MLY	J	681	1	9,10,11	0.60	0	6,11,13	0.46	0
1	MLY	A	35	1	9,10,11	0.71	0	6,11,13	0.38	0
1	MLY	P	837	1	9,10,11	0.59	0	6,11,13	0.56	0
1	MLY	A	415	1	9,10,11	0.76	0	6,11,13	0.20	0
1	MLY	D	839	1	9,10,11	0.70	0	6,11,13	0.79	0
1	MLY	J	353	1	9,10,11	0.85	0	6,11,13	0.78	0
1	MLY	J	486	1	9,10,11	0.63	0	6,11,13	0.39	0
1	MLY	A	30	1	9,10,11	0.88	0	6,11,13	0.32	0
1	MLY	M	833	1	9,10,11	1.20	1 (11%)	6,11,13	0.30	0
1	MLY	P	84	1	9,10,11	0.50	0	6,11,13	0.80	0
1	MLY	A	138	1	9,10,11	1.33	1 (11%)	6,11,13	0.84	0
1	MLY	M	659	1	9,10,11	0.80	0	6,11,13	0.57	0
1	MLY	A	504	1	9,10,11	0.89	0	6,11,13	0.24	0
1	MLY	G	55	1	9,10,11	0.73	0	6,11,13	0.80	0
1	MLY	P	130	1	9,10,11	0.77	0	6,11,13	0.75	0
1	MLY	G	367	1	9,10,11	0.66	0	6,11,13	0.38	0
1	MLY	D	367	1	9,10,11	0.63	0	6,11,13	0.38	0
1	MLY	A	87	1	9,10,11	1.21	1 (11%)	6,11,13	0.42	0
1	MLY	G	236	1	9,10,11	0.78	1 (11%)	6,11,13	0.47	0
1	MLY	J	436	1	9,10,11	1.07	1 (11%)	6,11,13	0.49	0
1	MLY	A	768	1	9,10,11	0.76	0	6,11,13	0.40	0
1	MLY	A	839	1	9,10,11	0.69	0	6,11,13	0.81	0
1	MLY	M	436	1	9,10,11	1.05	1 (11%)	6,11,13	0.49	0
1	MLY	P	505	1	9,10,11	0.94	1 (11%)	6,11,13	0.33	0
1	MLY	D	59	1	9,10,11	0.86	0	6,11,13	0.50	0
1	MLY	D	505	1	9,10,11	0.87	1 (11%)	6,11,13	0.35	0
1	MLY	P	415	1	9,10,11	0.76	0	6,11,13	0.19	0
1	MLY	P	600	1	9,10,11	0.53	0	6,11,13	0.37	0
1	MLY	A	348	1	9,10,11	0.87	1 (11%)	6,11,13	0.48	0
1	MLY	M	190	1	9,10,11	1.25	1 (11%)	6,11,13	0.52	0
1	MLY	A	369	1	9,10,11	0.71	0	6,11,13	0.44	0
1	MLY	P	598	1	9,10,11	0.86	1 (11%)	6,11,13	0.44	0
1	MLY	M	827	1	9,10,11	0.71	0	6,11,13	0.50	0
1	MLY	M	248	1	9,10,11	0.83	0	6,11,13	0.62	0
1	MLY	M	431	1	9,10,11	0.53	0	6,11,13	0.45	0
1	MLY	M	385	1	9,10,11	1.04	1 (11%)	6,11,13	0.43	0
1	MLY	A	551	1	9,10,11	0.51	0	6,11,13	0.19	0
1	MLY	P	431	1	9,10,11	0.53	0	6,11,13	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MLY	A	130	1	9,10,11	0.81	0	6,11,13	0.75	0
1	MLY	P	839	1	9,10,11	0.69	0	6,11,13	0.76	0
1	MLY	J	504	1	9,10,11	0.83	0	6,11,13	0.23	0
1	MLY	J	598	1	9,10,11	0.89	1 (11%)	6,11,13	0.43	0
1	MLY	G	613	1	9,10,11	0.58	0	6,11,13	0.63	0
1	MLY	J	87	1	9,10,11	1.24	1 (11%)	6,11,13	0.43	0
1	MLY	A	63	1	9,10,11	0.94	1 (11%)	6,11,13	0.44	0
1	MLY	M	598	1	9,10,11	0.91	1 (11%)	6,11,13	0.43	0
1	MLY	M	49	1	9,10,11	1.11	1 (11%)	6,11,13	0.74	0
1	MLY	P	353	1	9,10,11	0.85	0	6,11,13	0.79	0
1	MLY	J	431	1	9,10,11	0.54	0	6,11,13	0.44	0
1	MLY	P	436	1	9,10,11	1.06	1 (11%)	6,11,13	0.50	0
1	MLY	J	659	1	9,10,11	0.81	0	6,11,13	0.58	0
1	MLY	D	837	1	9,10,11	0.61	0	6,11,13	0.57	0
1	MLY	G	617	1	9,10,11	0.96	1 (11%)	6,11,13	0.34	0
1	MLY	D	348	1	9,10,11	0.82	0	6,11,13	0.47	0
1	MLY	M	367	1	9,10,11	0.63	0	6,11,13	0.36	0
1	MLY	M	617	1	9,10,11	0.96	1 (11%)	6,11,13	0.33	0
1	MLY	D	84	1	9,10,11	0.50	0	6,11,13	0.80	0
1	MLY	D	248	1	9,10,11	0.83	0	6,11,13	0.61	0
1	MLY	M	138	1	9,10,11	1.32	1 (11%)	6,11,13	0.83	0
1	MLY	M	353	1	9,10,11	0.86	0	6,11,13	0.78	0
1	MLY	G	35	1	9,10,11	0.72	0	6,11,13	0.39	0
1	MLY	P	385	1	9,10,11	0.99	1 (11%)	6,11,13	0.43	0
1	MLY	P	19	1	9,10,11	1.17	1 (11%)	6,11,13	0.58	0
1	MLY	P	768	1	9,10,11	0.75	0	6,11,13	0.42	0
1	MLY	A	431	1	9,10,11	0.52	0	6,11,13	0.44	0
1	MLY	P	348	1	9,10,11	0.85	0	6,11,13	0.47	0
1	MLY	J	768	1	9,10,11	0.77	0	6,11,13	0.42	0
1	MLY	A	49	1	9,10,11	1.05	1 (11%)	6,11,13	0.74	0
1	MLY	G	431	1	9,10,11	0.53	0	6,11,13	0.47	0
1	MLY	M	768	1	9,10,11	0.76	0	6,11,13	0.42	0
1	MLY	A	436	1	9,10,11	1.05	1 (11%)	6,11,13	0.50	0
1	MLY	P	296	1	9,10,11	0.70	0	6,11,13	0.36	0
1	MLY	A	84	1	9,10,11	0.49	0	6,11,13	0.79	0
1	MLY	P	613	1	9,10,11	0.55	0	6,11,13	0.64	0
1	MLY	D	551	1	9,10,11	0.53	0	6,11,13	0.20	0
1	MLY	P	764	1	9,10,11	0.83	0	6,11,13	0.37	0
1	MLY	A	505	1	9,10,11	0.92	1 (11%)	6,11,13	0.34	0
1	MLY	J	613	1	9,10,11	0.56	0	6,11,13	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MLY	D	436	1	9,10,11	1.11	1 (11%)	6,11,13	0.48	0
1	MLY	J	617	1	9,10,11	0.98	1 (11%)	6,11,13	0.33	0
1	MLY	D	528	1	9,10,11	0.91	0	6,11,13	0.64	0
1	MLY	G	505	1	9,10,11	0.88	1 (11%)	6,11,13	0.36	0
1	MLY	M	505	1	9,10,11	0.93	1 (11%)	6,11,13	0.34	0
1	MLY	J	84	1	9,10,11	0.49	0	6,11,13	0.80	0
1	MLY	A	598	1	9,10,11	0.91	1 (11%)	6,11,13	0.44	0
1	MLY	G	63	1	9,10,11	0.91	0	6,11,13	0.43	0
1	MLY	G	436	1	9,10,11	1.05	1 (11%)	6,11,13	0.48	0
1	MLY	A	833	1	9,10,11	1.16	1 (11%)	6,11,13	0.32	0
1	MLY	P	827	1	9,10,11	0.72	0	6,11,13	0.48	0
1	MLY	D	833	1	9,10,11	1.15	2 (22%)	6,11,13	0.31	0
1	MLY	P	87	1	9,10,11	1.22	1 (11%)	6,11,13	0.42	0
1	MLY	G	30	1	9,10,11	0.87	0	6,11,13	0.30	0
1	MLY	A	659	1	9,10,11	0.84	0	6,11,13	0.60	0
1	MLY	M	30	1	9,10,11	0.88	0	6,11,13	0.31	0
1	MLY	D	138	1	9,10,11	1.38	1 (11%)	6,11,13	0.86	0
1	MLY	D	63	1	9,10,11	0.91	0	6,11,13	0.45	0
1	MLY	D	681	1	9,10,11	0.59	0	6,11,13	0.45	0
1	MLY	J	19	1	9,10,11	1.20	1 (11%)	6,11,13	0.57	0
1	MLY	D	236	1	9,10,11	0.79	1 (11%)	6,11,13	0.46	0
1	MLY	M	296	1	9,10,11	0.69	0	6,11,13	0.35	0
1	MLY	J	600	1	9,10,11	0.53	0	6,11,13	0.37	0
1	MLY	J	415	1	9,10,11	0.79	0	6,11,13	0.18	0
1	MLY	G	415	1	9,10,11	0.76	0	6,11,13	0.19	0
1	MLY	M	782	1	9,10,11	0.78	0	6,11,13	0.36	0
1	MLY	M	415	1	9,10,11	0.77	0	6,11,13	0.18	0
1	MLY	A	486	1	9,10,11	0.65	0	6,11,13	0.38	0
1	MLY	M	528	1	9,10,11	0.87	0	6,11,13	0.66	0
1	MLY	M	837	1	9,10,11	0.59	0	6,11,13	0.54	0
1	MLY	P	833	1	9,10,11	1.20	1 (11%)	6,11,13	0.29	0
1	MLY	G	49	1	9,10,11	1.08	1 (11%)	6,11,13	0.74	0
1	MLY	A	190	1	9,10,11	1.28	1 (11%)	6,11,13	0.51	0
1	MLY	G	486	1	9,10,11	0.65	0	6,11,13	0.38	0
1	MLY	P	138	1	9,10,11	1.32	1 (11%)	6,11,13	0.83	0
1	MLY	A	272	1	9,10,11	0.99	1 (11%)	6,11,13	0.55	0
1	MLY	G	296	1	9,10,11	0.66	0	6,11,13	0.37	0
1	MLY	A	59	1	9,10,11	0.88	0	6,11,13	0.49	0
1	MLY	A	827	1	9,10,11	0.73	0	6,11,13	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MLY	D	35	1	9,10,11	0.72	0	6,11,13	0.38	0
1	MLY	G	190	1	9,10,11	1.26	1 (11%)	6,11,13	0.52	0
1	MLY	J	839	1	9,10,11	0.72	0	6,11,13	0.77	0
1	MLY	M	55	1	9,10,11	0.71	0	6,11,13	0.78	0
1	MLY	P	236	1	9,10,11	0.79	1 (11%)	6,11,13	0.48	0
1	MLY	P	369	1	9,10,11	0.70	0	6,11,13	0.46	0
1	MLY	D	49	1	9,10,11	1.07	1 (11%)	6,11,13	0.74	0
1	MLY	J	295	1	9,10,11	0.79	0	6,11,13	0.34	0
1	MLY	M	272	1	9,10,11	0.98	1 (11%)	6,11,13	0.57	0
1	MLY	M	19	1	9,10,11	1.18	1 (11%)	6,11,13	0.57	0
1	MLY	G	827	1	9,10,11	0.70	0	6,11,13	0.49	0
1	MLY	M	600	1	9,10,11	0.53	0	6,11,13	0.38	0
1	MLY	G	87	1	9,10,11	1.23	1 (11%)	6,11,13	0.43	0
1	MLY	D	19	1	9,10,11	1.21	1 (11%)	6,11,13	0.56	0
1	MLY	D	600	1	9,10,11	0.50	0	6,11,13	0.38	0
1	MLY	M	87	1	9,10,11	1.23	1 (11%)	6,11,13	0.43	0
1	MLY	D	617	1	9,10,11	0.98	1 (11%)	6,11,13	0.34	0
1	MLY	P	190	1	9,10,11	1.29	1 (11%)	6,11,13	0.52	0
1	MLY	A	617	1	9,10,11	0.92	1 (11%)	6,11,13	0.33	0
1	MLY	A	613	1	9,10,11	0.56	0	6,11,13	0.64	0
1	MLY	D	768	1	9,10,11	0.74	0	6,11,13	0.40	0
1	MLY	A	248	1	9,10,11	0.85	0	6,11,13	0.61	0
1	MLY	G	504	1	9,10,11	0.87	0	6,11,13	0.23	0
1	MLY	D	272	1	9,10,11	0.97	1 (11%)	6,11,13	0.57	0
1	MLY	D	353	1	9,10,11	0.86	0	6,11,13	0.80	0
1	MLY	J	385	1	9,10,11	1.02	1 (11%)	6,11,13	0.45	0
1	MLY	J	190	1	9,10,11	1.25	1 (11%)	6,11,13	0.52	0
1	MLY	P	55	1	9,10,11	0.72	0	6,11,13	0.78	0
1	MLY	A	764	1	9,10,11	0.84	0	6,11,13	0.36	0
1	MLY	G	768	1	9,10,11	0.74	0	6,11,13	0.42	0
1	MLY	J	837	1	9,10,11	0.59	0	6,11,13	0.55	0
1	MLY	G	353	1	9,10,11	0.85	0	6,11,13	0.80	0
1	MLY	G	598	1	9,10,11	0.89	1 (11%)	6,11,13	0.43	0
1	MLY	J	348	1	9,10,11	0.83	0	6,11,13	0.48	0
1	MLY	J	55	1	9,10,11	0.72	0	6,11,13	0.78	0
1	MLY	G	348	1	9,10,11	0.86	1 (11%)	6,11,13	0.47	0
1	MLY	M	348	1	9,10,11	0.82	0	6,11,13	0.47	0
1	MLY	M	295	1	9,10,11	0.78	0	6,11,13	0.35	0
1	MLY	P	551	1	9,10,11	0.52	0	6,11,13	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MLY	P	30	1	9,10,11	0.88	0	6,11,13	0.31	0
1	MLY	A	19	1	9,10,11	1.11	1 (11%)	6,11,13	0.58	0
1	MLY	J	296	1	9,10,11	0.68	0	6,11,13	0.37	0
1	MLY	M	764	1	9,10,11	0.87	0	6,11,13	0.38	0
1	MLY	P	528	1	9,10,11	0.89	0	6,11,13	0.64	0
1	MLY	D	55	1	9,10,11	0.71	0	6,11,13	0.79	0
1	MLY	D	369	1	9,10,11	0.69	0	6,11,13	0.44	0
1	MLY	M	59	1	9,10,11	0.88	0	6,11,13	0.49	0
1	MLY	D	30	1	9,10,11	0.92	0	6,11,13	0.32	0
1	MLY	D	295	1	9,10,11	0.79	0	6,11,13	0.35	0
1	MLY	J	764	1	9,10,11	0.84	0	6,11,13	0.37	0
1	MLY	G	764	1	9,10,11	0.83	0	6,11,13	0.36	0
1	MLY	D	130	1	9,10,11	0.81	0	6,11,13	0.74	0
1	MLY	G	369	1	9,10,11	0.71	0	6,11,13	0.45	0
1	MLY	A	55	1	9,10,11	0.71	0	6,11,13	0.78	0
1	MLY	P	272	1	9,10,11	1.03	1 (11%)	6,11,13	0.55	0
1	MLY	A	681	1	9,10,11	0.59	0	6,11,13	0.45	0
1	MLY	G	295	1	9,10,11	0.82	0	6,11,13	0.33	0
1	MLY	P	107	1	9,10,11	0.47	0	6,11,13	0.32	0
1	MLY	G	272	1	9,10,11	0.97	1 (11%)	6,11,13	0.55	0
1	MLY	P	248	1	9,10,11	0.84	0	6,11,13	0.63	0
1	MLY	J	827	1	9,10,11	0.74	0	6,11,13	0.49	0
1	MLY	A	600	1	9,10,11	0.52	0	6,11,13	0.38	0
1	MLY	G	553	4,1	9,10,11	0.68	0	6,11,13	0.55	0
1	MLY	M	553	1	9,10,11	0.66	0	6,11,13	0.53	0
1	MLY	G	782	1	9,10,11	0.78	0	6,11,13	0.35	0
1	MLY	J	248	1	9,10,11	0.83	0	6,11,13	0.61	0
1	MLY	M	551	1	9,10,11	0.51	0	6,11,13	0.19	0
1	MLY	G	84	1	9,10,11	0.49	0	6,11,13	0.80	0
1	MLY	G	248	1	9,10,11	0.81	0	6,11,13	0.63	0
1	MLY	D	486	1	9,10,11	0.65	0	6,11,13	0.39	0
1	MLY	J	528	1	9,10,11	0.88	0	6,11,13	0.65	0
1	MLY	M	84	1	9,10,11	0.49	0	6,11,13	0.80	0
1	MLY	P	63	1	9,10,11	0.93	1 (11%)	6,11,13	0.44	0
1	MLY	J	367	1	9,10,11	0.64	0	6,11,13	0.37	0
1	MLY	P	35	1	9,10,11	0.72	0	6,11,13	0.39	0
1	MLY	M	504	1	9,10,11	0.84	0	6,11,13	0.23	0
1	MLY	J	551	1	9,10,11	0.52	0	6,11,13	0.20	0
1	MLY	D	782	1	9,10,11	0.78	0	6,11,13	0.34	0
1	MLY	A	782	1	9,10,11	0.78	0	6,11,13	0.37	0
1	MLY	G	551	1	9,10,11	0.51	0	6,11,13	0.19	0
1	MLY	J	833	1	9,10,11	1.18	1 (11%)	6,11,13	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MLY	A	837	1	9,10,11	0.60	0	6,11,13	0.53	0
1	MLY	P	59	1	9,10,11	0.87	0	6,11,13	0.49	0
1	MLY	G	19	1	9,10,11	1.16	1 (11%)	6,11,13	0.58	0
1	MLY	G	600	1	9,10,11	0.52	0	6,11,13	0.36	0
1	MLY	J	138	1	9,10,11	1.33	1 (11%)	6,11,13	0.84	0
1	MLY	P	553	1	9,10,11	0.69	0	6,11,13	0.54	0
1	MLY	M	63	1	9,10,11	0.93	1 (11%)	6,11,13	0.43	0
1	MLY	J	369	1	9,10,11	0.68	0	6,11,13	0.47	0
1	MLY	M	681	1	9,10,11	0.59	0	6,11,13	0.46	0
1	MLY	G	837	1	9,10,11	0.60	0	6,11,13	0.53	0
1	MLY	J	505	1	9,10,11	0.93	1 (11%)	6,11,13	0.33	0
1	MLY	P	681	1	9,10,11	0.61	0	6,11,13	0.46	0
1	MLY	A	296	1	9,10,11	0.62	0	6,11,13	0.37	0
1	MLY	J	59	1	9,10,11	0.88	0	6,11,13	0.49	0
1	MLY	M	107	1	9,10,11	0.47	0	6,11,13	0.33	0
1	MLY	M	486	1	9,10,11	0.64	0	6,11,13	0.39	0
1	MLY	P	782	1	9,10,11	0.76	0	6,11,13	0.37	0
1	MLY	G	681	1	9,10,11	0.61	0	6,11,13	0.44	0
1	MLY	G	839	1	9,10,11	0.72	0	6,11,13	0.80	0
1	MLY	P	49	1	9,10,11	1.09	1 (11%)	6,11,13	0.75	0
1	MLY	D	598	1	9,10,11	0.89	1 (11%)	6,11,13	0.43	0
1	MLY	G	528	1	9,10,11	0.91	0	6,11,13	0.66	0
1	MLY	J	782	1	9,10,11	0.80	0	6,11,13	0.36	0
1	MLY	J	236	1	9,10,11	0.79	1 (11%)	6,11,13	0.47	0
1	MLY	M	35	1	9,10,11	0.72	0	6,11,13	0.40	0
1	MLY	J	49	1	9,10,11	1.09	1 (11%)	6,11,13	0.75	0
1	MLY	M	236	1	9,10,11	0.79	1 (11%)	6,11,13	0.48	0
1	MLY	P	295	1	9,10,11	0.82	0	6,11,13	0.34	0
1	MLY	A	553	4,1	9,10,11	0.66	0	6,11,13	0.54	0
1	MLY	A	107	1	9,10,11	0.46	0	6,11,13	0.34	0
1	MLY	A	353	1	9,10,11	0.87	0	6,11,13	0.78	0
1	MLY	A	385	1	9,10,11	0.99	1 (11%)	6,11,13	0.43	0
1	MLY	G	59	1	9,10,11	0.84	0	6,11,13	0.50	0
1	MLY	J	35	1	9,10,11	0.72	0	6,11,13	0.39	0
1	MLY	G	138	1	9,10,11	1.33	1 (11%)	6,11,13	0.84	0
1	MLY	J	30	1	9,10,11	0.89	0	6,11,13	0.32	0
1	MLY	D	764	1	9,10,11	0.87	0	6,11,13	0.35	0
1	MLY	P	504	1	9,10,11	0.84	0	6,11,13	0.24	0
1	MLY	J	272	1	9,10,11	1.02	1 (11%)	6,11,13	0.56	0
1	MLY	A	367	1	9,10,11	0.63	0	6,11,13	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MLY	D	553	4,1	9,10,11	0.69	0	6,11,13	0.56	0
1	MLY	D	659	1	9,10,11	0.82	0	6,11,13	0.60	0
1	MLY	M	613	1	9,10,11	0.56	0	6,11,13	0.65	0
1	MLY	D	431	1	9,10,11	0.54	0	6,11,13	0.46	0
1	MLY	M	839	1	9,10,11	0.70	0	6,11,13	0.77	0
1	MLY	G	833	1	9,10,11	1.18	2 (22%)	6,11,13	0.32	0
1	MLY	P	486	1	9,10,11	0.64	0	6,11,13	0.39	0
1	MLY	G	659	1	9,10,11	0.85	0	6,11,13	0.58	0
1	MLY	J	107	1	9,10,11	0.47	0	6,11,13	0.34	0
1	MLY	A	295	1	9,10,11	0.82	0	6,11,13	0.32	0
1	MLY	P	367	1	9,10,11	0.63	0	6,11,13	0.38	0
1	MLY	M	369	1	9,10,11	0.69	0	6,11,13	0.45	0
1	MLY	D	613	1	9,10,11	0.56	0	6,11,13	0.64	0
1	MLY	D	190	1	9,10,11	1.23	1 (11%)	6,11,13	0.53	0
1	MLY	G	130	1	9,10,11	0.80	0	6,11,13	0.76	0
1	MLY	J	130	1	9,10,11	0.77	0	6,11,13	0.75	0
1	MLY	M	130	1	9,10,11	0.78	0	6,11,13	0.74	0
1	MLY	J	63	1	9,10,11	0.91	0	6,11,13	0.43	0
1	MLY	D	415	1	9,10,11	0.79	0	6,11,13	0.19	0
1	MLY	D	107	1	9,10,11	0.50	0	6,11,13	0.34	0
1	MLY	D	385	1	9,10,11	1.00	1 (11%)	6,11,13	0.45	0
1	MLY	D	87	1	9,10,11	1.19	1 (11%)	6,11,13	0.44	0
1	MLY	D	827	1	9,10,11	0.68	0	6,11,13	0.48	0
1	MLY	A	528	1	9,10,11	0.88	0	6,11,13	0.66	0
1	MLY	A	236	1	9,10,11	0.79	1 (11%)	6,11,13	0.49	0
1	MLY	P	659	1	9,10,11	0.80	0	6,11,13	0.57	0
1	MLY	D	504	1	9,10,11	0.90	0	6,11,13	0.21	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
1	MLY	P	617	1	-	1/8/9/11	-
1	MLY	D	296	1	-	4/8/9/11	-
1	MLY	G	107	1	-	2/8/9/11	-
1	MLY	G	385	1	-	2/8/9/11	-
1	MLY	J	553	1	-	4/8/9/11	-
1	MLY	J	681	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	35	1	-	3/8/9/11	-
1	MLY	P	837	1	-	5/8/9/11	-
1	MLY	A	415	1	-	3/8/9/11	-
1	MLY	D	839	1	-	3/8/9/11	-
1	MLY	J	353	1	-	4/8/9/11	-
1	MLY	J	486	1	-	2/8/9/11	-
1	MLY	A	30	1	-	2/8/9/11	-
1	MLY	M	833	1	-	6/8/9/11	-
1	MLY	P	84	1	-	4/8/9/11	-
1	MLY	A	138	1	-	4/8/9/11	-
1	MLY	M	659	1	-	3/8/9/11	-
1	MLY	A	504	1	-	4/8/9/11	-
1	MLY	G	55	1	-	6/8/9/11	-
1	MLY	P	130	1	-	5/8/9/11	-
1	MLY	G	367	1	-	2/8/9/11	-
1	MLY	D	367	1	-	2/8/9/11	-
1	MLY	A	87	1	-	2/8/9/11	-
1	MLY	G	236	1	-	3/8/9/11	-
1	MLY	J	436	1	-	4/8/9/11	-
1	MLY	A	768	1	-	4/8/9/11	-
1	MLY	A	839	1	-	3/8/9/11	-
1	MLY	M	436	1	-	4/8/9/11	-
1	MLY	P	505	1	-	5/8/9/11	-
1	MLY	D	59	1	-	3/8/9/11	-
1	MLY	D	505	1	-	5/8/9/11	-
1	MLY	P	415	1	-	3/8/9/11	-
1	MLY	P	600	1	-	3/8/9/11	-
1	MLY	A	348	1	-	5/8/9/11	-
1	MLY	M	190	1	-	5/8/9/11	-
1	MLY	A	369	1	-	2/8/9/11	-
1	MLY	P	598	1	-	5/8/9/11	-
1	MLY	M	827	1	-	0/8/9/11	-
1	MLY	M	248	1	-	6/8/9/11	-
1	MLY	M	431	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	M	385	1	-	2/8/9/11	-
1	MLY	A	551	1	-	3/8/9/11	-
1	MLY	P	431	1	-	4/8/9/11	-
1	MLY	A	130	1	-	5/8/9/11	-
1	MLY	P	839	1	-	3/8/9/11	-
1	MLY	J	504	1	-	4/8/9/11	-
1	MLY	J	598	1	-	5/8/9/11	-
1	MLY	G	613	1	-	4/8/9/11	-
1	MLY	J	87	1	-	2/8/9/11	-
1	MLY	A	63	1	-	4/8/9/11	-
1	MLY	M	598	1	-	5/8/9/11	-
1	MLY	M	49	1	-	3/8/9/11	-
1	MLY	P	353	1	-	4/8/9/11	-
1	MLY	J	431	1	-	4/8/9/11	-
1	MLY	P	436	1	-	4/8/9/11	-
1	MLY	J	659	1	-	3/8/9/11	-
1	MLY	D	837	1	-	5/8/9/11	-
1	MLY	G	617	1	-	1/8/9/11	-
1	MLY	D	348	1	-	5/8/9/11	-
1	MLY	M	367	1	-	2/8/9/11	-
1	MLY	M	617	1	-	1/8/9/11	-
1	MLY	D	84	1	-	4/8/9/11	-
1	MLY	D	248	1	-	6/8/9/11	-
1	MLY	M	138	1	-	4/8/9/11	-
1	MLY	M	353	1	-	4/8/9/11	-
1	MLY	G	35	1	-	3/8/9/11	-
1	MLY	P	385	1	-	2/8/9/11	-
1	MLY	P	19	1	-	4/8/9/11	-
1	MLY	P	768	1	-	4/8/9/11	-
1	MLY	A	431	1	-	4/8/9/11	-
1	MLY	P	348	1	-	5/8/9/11	-
1	MLY	J	768	1	-	4/8/9/11	-
1	MLY	A	49	1	-	3/8/9/11	-
1	MLY	G	431	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	M	768	1	-	4/8/9/11	-
1	MLY	A	436	1	-	4/8/9/11	-
1	MLY	P	296	1	-	4/8/9/11	-
1	MLY	A	84	1	-	4/8/9/11	-
1	MLY	P	613	1	-	4/8/9/11	-
1	MLY	D	551	1	-	3/8/9/11	-
1	MLY	P	764	1	-	2/8/9/11	-
1	MLY	A	505	1	-	5/8/9/11	-
1	MLY	J	613	1	-	4/8/9/11	-
1	MLY	D	436	1	-	4/8/9/11	-
1	MLY	J	617	1	-	1/8/9/11	-
1	MLY	D	528	1	-	4/8/9/11	-
1	MLY	G	505	1	-	5/8/9/11	-
1	MLY	M	505	1	-	5/8/9/11	-
1	MLY	J	84	1	-	4/8/9/11	-
1	MLY	A	598	1	-	5/8/9/11	-
1	MLY	G	63	1	-	4/8/9/11	-
1	MLY	G	436	1	-	4/8/9/11	-
1	MLY	A	833	1	-	6/8/9/11	-
1	MLY	P	827	1	-	0/8/9/11	-
1	MLY	D	833	1	-	6/8/9/11	-
1	MLY	P	87	1	-	2/8/9/11	-
1	MLY	G	30	1	-	2/8/9/11	-
1	MLY	A	659	1	-	3/8/9/11	-
1	MLY	M	30	1	-	2/8/9/11	-
1	MLY	D	138	1	-	4/8/9/11	-
1	MLY	D	63	1	-	4/8/9/11	-
1	MLY	D	681	1	-	4/8/9/11	-
1	MLY	J	19	1	-	4/8/9/11	-
1	MLY	D	236	1	-	3/8/9/11	-
1	MLY	M	296	1	-	4/8/9/11	-
1	MLY	J	600	1	-	3/8/9/11	-
1	MLY	J	415	1	-	3/8/9/11	-
1	MLY	G	415	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	M	782	1	-	6/8/9/11	-
1	MLY	M	415	1	-	3/8/9/11	-
1	MLY	A	486	1	-	2/8/9/11	-
1	MLY	M	528	1	-	5/8/9/11	-
1	MLY	M	837	1	-	5/8/9/11	-
1	MLY	P	833	1	-	6/8/9/11	-
1	MLY	G	49	1	-	3/8/9/11	-
1	MLY	A	190	1	-	5/8/9/11	-
1	MLY	G	486	1	-	2/8/9/11	-
1	MLY	P	138	1	-	4/8/9/11	-
1	MLY	A	272	1	-	3/8/9/11	-
1	MLY	G	296	1	-	4/8/9/11	-
1	MLY	A	59	1	-	3/8/9/11	-
1	MLY	A	827	1	-	0/8/9/11	-
1	MLY	D	35	1	-	3/8/9/11	-
1	MLY	G	190	1	-	5/8/9/11	-
1	MLY	J	839	1	-	3/8/9/11	-
1	MLY	M	55	1	-	6/8/9/11	-
1	MLY	P	236	1	-	3/8/9/11	-
1	MLY	P	369	1	-	2/8/9/11	-
1	MLY	D	49	1	-	3/8/9/11	-
1	MLY	J	295	1	-	2/8/9/11	-
1	MLY	M	272	1	-	3/8/9/11	-
1	MLY	M	19	1	-	4/8/9/11	-
1	MLY	G	827	1	-	0/8/9/11	-
1	MLY	M	600	1	-	3/8/9/11	-
1	MLY	G	87	1	-	2/8/9/11	-
1	MLY	D	19	1	-	4/8/9/11	-
1	MLY	D	600	1	-	3/8/9/11	-
1	MLY	M	87	1	-	2/8/9/11	-
1	MLY	D	617	1	-	1/8/9/11	-
1	MLY	P	190	1	-	5/8/9/11	-
1	MLY	A	617	1	-	1/8/9/11	-
1	MLY	A	613	1	-	4/8/9/11	-
1	MLY	D	768	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	248	1	-	6/8/9/11	-
1	MLY	G	504	1	-	4/8/9/11	-
1	MLY	D	272	1	-	3/8/9/11	-
1	MLY	D	353	1	-	4/8/9/11	-
1	MLY	J	385	1	-	2/8/9/11	-
1	MLY	J	190	1	-	5/8/9/11	-
1	MLY	P	55	1	-	6/8/9/11	-
1	MLY	A	764	1	-	2/8/9/11	-
1	MLY	G	768	1	-	4/8/9/11	-
1	MLY	J	837	1	-	5/8/9/11	-
1	MLY	G	353	1	-	4/8/9/11	-
1	MLY	G	598	1	-	5/8/9/11	-
1	MLY	J	348	1	-	5/8/9/11	-
1	MLY	J	55	1	-	6/8/9/11	-
1	MLY	G	348	1	-	5/8/9/11	-
1	MLY	M	348	1	-	5/8/9/11	-
1	MLY	M	295	1	-	2/8/9/11	-
1	MLY	P	551	1	-	3/8/9/11	-
1	MLY	P	30	1	-	2/8/9/11	-
1	MLY	A	19	1	-	4/8/9/11	-
1	MLY	J	296	1	-	4/8/9/11	-
1	MLY	M	764	1	-	2/8/9/11	-
1	MLY	P	528	1	-	5/8/9/11	-
1	MLY	D	55	1	-	6/8/9/11	-
1	MLY	D	369	1	-	2/8/9/11	-
1	MLY	M	59	1	-	3/8/9/11	-
1	MLY	D	30	1	-	2/8/9/11	-
1	MLY	D	295	1	-	2/8/9/11	-
1	MLY	J	764	1	-	2/8/9/11	-
1	MLY	G	764	1	-	2/8/9/11	-
1	MLY	D	130	1	-	5/8/9/11	-
1	MLY	G	369	1	-	2/8/9/11	-
1	MLY	A	55	1	-	6/8/9/11	-
1	MLY	P	272	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	681	1	-	4/8/9/11	-
1	MLY	G	295	1	-	2/8/9/11	-
1	MLY	P	107	1	-	2/8/9/11	-
1	MLY	G	272	1	-	3/8/9/11	-
1	MLY	P	248	1	-	6/8/9/11	-
1	MLY	J	827	1	-	0/8/9/11	-
1	MLY	A	600	1	-	3/8/9/11	-
1	MLY	G	553	4,1	-	4/8/9/11	-
1	MLY	M	553	1	-	4/8/9/11	-
1	MLY	G	782	1	-	6/8/9/11	-
1	MLY	J	248	1	-	6/8/9/11	-
1	MLY	M	551	1	-	3/8/9/11	-
1	MLY	G	84	1	-	4/8/9/11	-
1	MLY	G	248	1	-	6/8/9/11	-
1	MLY	D	486	1	-	2/8/9/11	-
1	MLY	J	528	1	-	4/8/9/11	-
1	MLY	M	84	1	-	4/8/9/11	-
1	MLY	P	63	1	-	4/8/9/11	-
1	MLY	J	367	1	-	2/8/9/11	-
1	MLY	P	35	1	-	3/8/9/11	-
1	MLY	M	504	1	-	4/8/9/11	-
1	MLY	J	551	1	-	3/8/9/11	-
1	MLY	D	782	1	-	6/8/9/11	-
1	MLY	A	782	1	-	6/8/9/11	-
1	MLY	G	551	1	-	3/8/9/11	-
1	MLY	J	833	1	-	6/8/9/11	-
1	MLY	A	837	1	-	5/8/9/11	-
1	MLY	P	59	1	-	3/8/9/11	-
1	MLY	G	19	1	-	4/8/9/11	-
1	MLY	G	600	1	-	3/8/9/11	-
1	MLY	J	138	1	-	4/8/9/11	-
1	MLY	P	553	1	-	4/8/9/11	-
1	MLY	M	63	1	-	4/8/9/11	-
1	MLY	J	369	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	M	681	1	-	4/8/9/11	-
1	MLY	G	837	1	-	5/8/9/11	-
1	MLY	J	505	1	-	5/8/9/11	-
1	MLY	P	681	1	-	4/8/9/11	-
1	MLY	A	296	1	-	4/8/9/11	-
1	MLY	J	59	1	-	3/8/9/11	-
1	MLY	M	107	1	-	2/8/9/11	-
1	MLY	M	486	1	-	2/8/9/11	-
1	MLY	P	782	1	-	6/8/9/11	-
1	MLY	G	681	1	-	4/8/9/11	-
1	MLY	G	839	1	-	3/8/9/11	-
1	MLY	P	49	1	-	3/8/9/11	-
1	MLY	D	598	1	-	5/8/9/11	-
1	MLY	G	528	1	-	4/8/9/11	-
1	MLY	J	782	1	-	6/8/9/11	-
1	MLY	J	236	1	-	3/8/9/11	-
1	MLY	M	35	1	-	3/8/9/11	-
1	MLY	J	49	1	-	3/8/9/11	-
1	MLY	M	236	1	-	3/8/9/11	-
1	MLY	P	295	1	-	2/8/9/11	-
1	MLY	A	553	4,1	-	4/8/9/11	-
1	MLY	A	107	1	-	2/8/9/11	-
1	MLY	A	353	1	-	4/8/9/11	-
1	MLY	A	385	1	-	2/8/9/11	-
1	MLY	G	59	1	-	3/8/9/11	-
1	MLY	J	35	1	-	3/8/9/11	-
1	MLY	G	138	1	-	4/8/9/11	-
1	MLY	J	30	1	-	2/8/9/11	-
1	MLY	D	764	1	-	2/8/9/11	-
1	MLY	P	504	1	-	4/8/9/11	-
1	MLY	J	272	1	-	3/8/9/11	-
1	MLY	A	367	1	-	2/8/9/11	-
1	MLY	D	553	4,1	-	5/8/9/11	-
1	MLY	D	659	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	M	613	1	-	4/8/9/11	-
1	MLY	D	431	1	-	4/8/9/11	-
1	MLY	M	839	1	-	3/8/9/11	-
1	MLY	G	833	1	-	6/8/9/11	-
1	MLY	P	486	1	-	2/8/9/11	-
1	MLY	G	659	1	-	3/8/9/11	-
1	MLY	J	107	1	-	2/8/9/11	-
1	MLY	A	295	1	-	2/8/9/11	-
1	MLY	P	367	1	-	2/8/9/11	-
1	MLY	M	369	1	-	2/8/9/11	-
1	MLY	D	613	1	-	4/8/9/11	-
1	MLY	D	190	1	-	5/8/9/11	-
1	MLY	G	130	1	-	5/8/9/11	-
1	MLY	J	130	1	-	5/8/9/11	-
1	MLY	M	130	1	-	5/8/9/11	-
1	MLY	J	63	1	-	4/8/9/11	-
1	MLY	D	415	1	-	3/8/9/11	-
1	MLY	D	107	1	-	2/8/9/11	-
1	MLY	D	385	1	-	2/8/9/11	-
1	MLY	D	87	1	-	2/8/9/11	-
1	MLY	D	827	1	-	0/8/9/11	-
1	MLY	A	528	1	-	5/8/9/11	-
1	MLY	A	236	1	-	3/8/9/11	-
1	MLY	P	659	1	-	3/8/9/11	-
1	MLY	D	504	1	-	4/8/9/11	-

The worst 5 of 85 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	138	MLY	CB-CA	-3.79	1.48	1.53
1	A	138	MLY	CB-CA	-3.63	1.48	1.53
1	J	138	MLY	CB-CA	-3.63	1.48	1.53
1	G	138	MLY	CB-CA	-3.63	1.48	1.53
1	P	138	MLY	CB-CA	-3.60	1.48	1.53

There are no bond angle outliers.

There are no chirality outliers.

5 of 958 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	19	MLY	C-CA-CB-CG
1	A	49	MLY	N-CA-CB-CG
1	A	49	MLY	C-CA-CB-CG
1	A	55	MLY	N-CA-CB-CG
1	A	55	MLY	C-CA-CB-CG

There are no ring outliers.

182 monomers are involved in 676 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	617	MLY	1	0
1	D	296	MLY	3	0
1	G	107	MLY	3	0
1	J	553	MLY	12	0
1	P	837	MLY	1	0
1	A	415	MLY	1	0
1	D	839	MLY	4	0
1	J	486	MLY	3	0
1	A	30	MLY	1	0
1	P	84	MLY	15	0
1	A	138	MLY	1	0
1	M	659	MLY	1	0
1	G	55	MLY	1	0
1	A	87	MLY	3	0
1	J	436	MLY	3	0
1	A	768	MLY	10	0
1	A	839	MLY	4	0
1	M	436	MLY	2	0
1	D	59	MLY	3	0
1	P	415	MLY	1	0
1	P	600	MLY	1	0
1	A	348	MLY	6	0
1	M	190	MLY	2	0
1	P	598	MLY	1	0
1	M	248	MLY	2	0
1	A	551	MLY	2	0
1	P	839	MLY	7	0
1	J	598	MLY	1	0
1	J	87	MLY	3	0
1	A	63	MLY	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	M	598	MLY	1	0
1	M	49	MLY	2	0
1	P	436	MLY	3	0
1	J	659	MLY	2	0
1	D	837	MLY	1	0
1	G	617	MLY	1	0
1	D	348	MLY	6	0
1	M	617	MLY	1	0
1	D	248	MLY	2	0
1	M	138	MLY	1	0
1	P	348	MLY	5	0
1	J	768	MLY	1	0
1	A	49	MLY	4	0
1	M	768	MLY	3	0
1	A	436	MLY	3	0
1	P	296	MLY	3	0
1	D	551	MLY	2	0
1	P	764	MLY	1	0
1	A	505	MLY	22	0
1	D	436	MLY	3	0
1	J	617	MLY	1	0
1	D	528	MLY	3	0
1	G	505	MLY	9	0
1	M	505	MLY	1	0
1	J	84	MLY	20	0
1	A	598	MLY	1	0
1	G	63	MLY	3	0
1	G	436	MLY	2	0
1	A	833	MLY	1	0
1	P	87	MLY	3	0
1	G	30	MLY	1	0
1	A	659	MLY	1	0
1	M	30	MLY	1	0
1	D	138	MLY	1	0
1	D	63	MLY	4	0
1	M	296	MLY	3	0
1	J	600	MLY	1	0
1	J	415	MLY	1	0
1	G	415	MLY	1	0
1	M	782	MLY	1	0
1	M	415	MLY	1	0
1	A	486	MLY	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	M	528	MLY	3	0
1	M	837	MLY	1	0
1	G	49	MLY	3	0
1	A	190	MLY	2	0
1	G	486	MLY	3	0
1	P	138	MLY	1	0
1	A	272	MLY	1	0
1	G	296	MLY	3	0
1	A	59	MLY	2	0
1	A	827	MLY	2	0
1	G	190	MLY	2	0
1	J	839	MLY	8	0
1	M	55	MLY	1	0
1	P	369	MLY	1	0
1	D	49	MLY	3	0
1	J	295	MLY	6	0
1	M	272	MLY	1	0
1	M	600	MLY	1	0
1	G	87	MLY	3	0
1	D	600	MLY	1	0
1	M	87	MLY	3	0
1	D	617	MLY	1	0
1	P	190	MLY	2	0
1	A	617	MLY	1	0
1	D	768	MLY	2	0
1	A	248	MLY	2	0
1	D	272	MLY	1	0
1	J	190	MLY	2	0
1	P	55	MLY	1	0
1	A	764	MLY	9	0
1	G	768	MLY	3	0
1	J	837	MLY	1	0
1	G	598	MLY	1	0
1	J	348	MLY	6	0
1	J	55	MLY	1	0
1	G	348	MLY	5	0
1	M	348	MLY	5	0
1	M	295	MLY	6	0
1	P	30	MLY	1	0
1	J	296	MLY	3	0
1	M	764	MLY	2	0
1	P	528	MLY	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	55	MLY	1	0
1	D	369	MLY	1	0
1	M	59	MLY	3	0
1	D	30	MLY	1	0
1	D	295	MLY	6	0
1	J	764	MLY	1	0
1	G	764	MLY	4	0
1	A	55	MLY	1	0
1	P	272	MLY	1	0
1	G	295	MLY	6	0
1	P	107	MLY	3	0
1	G	272	MLY	1	0
1	P	248	MLY	2	0
1	A	600	MLY	1	0
1	G	553	MLY	27	0
1	M	553	MLY	2	0
1	G	782	MLY	1	0
1	J	248	MLY	2	0
1	G	84	MLY	15	0
1	G	248	MLY	2	0
1	D	486	MLY	3	0
1	J	528	MLY	3	0
1	M	84	MLY	11	0
1	P	63	MLY	3	0
1	D	782	MLY	71	0
1	A	782	MLY	7	0
1	A	837	MLY	12	0
1	P	59	MLY	2	0
1	G	600	MLY	1	0
1	J	138	MLY	1	0
1	P	553	MLY	2	0
1	M	63	MLY	3	0
1	J	369	MLY	1	0
1	G	837	MLY	1	0
1	J	505	MLY	9	0
1	A	296	MLY	3	0
1	J	59	MLY	3	0
1	M	107	MLY	3	0
1	M	486	MLY	3	0
1	P	782	MLY	15	0
1	G	839	MLY	4	0
1	P	49	MLY	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	598	MLY	1	0
1	G	528	MLY	2	0
1	J	782	MLY	1	0
1	J	49	MLY	3	0
1	P	295	MLY	6	0
1	A	553	MLY	17	0
1	A	107	MLY	3	0
1	G	59	MLY	2	0
1	G	138	MLY	1	0
1	J	30	MLY	1	0
1	D	764	MLY	7	0
1	J	272	MLY	1	0
1	D	553	MLY	17	0
1	D	659	MLY	2	0
1	M	839	MLY	7	0
1	P	486	MLY	3	0
1	G	659	MLY	2	0
1	J	107	MLY	3	0
1	A	295	MLY	6	0
1	D	190	MLY	2	0
1	J	63	MLY	3	0
1	D	415	MLY	1	0
1	D	107	MLY	3	0
1	D	87	MLY	3	0
1	A	528	MLY	3	0
1	P	659	MLY	2	0

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	P	6
1	D	4
1	A	4
1	M	4
1	J	3
1	G	3
3	C	1
3	F	1
3	I	1
3	L	1
3	O	1
3	R	1
2	B	1
2	E	1
2	H	1
2	K	1
2	N	1
2	Q	1

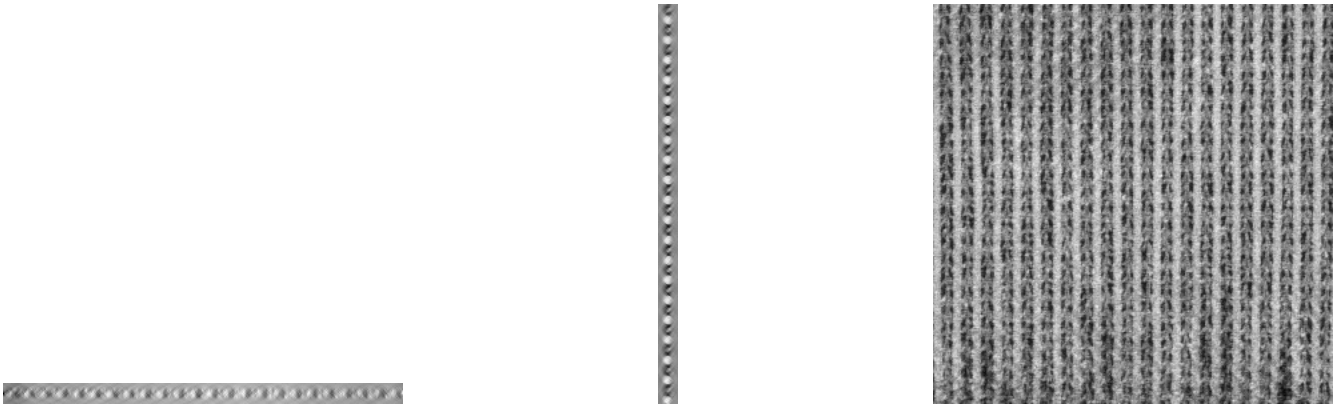
The worst 5 of 36 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	769:ALA	C	770:GLY	N	5.51
1	D	769:ALA	C	770:GLY	N	4.82
1	G	769:ALA	C	770:GLY	N	4.31
1	D	709:LYS	C	710:GLY	N	3.43
1	A	709:LYS	C	710:GLY	N	2.70

6 Tomogram visualisation (i)

This section contains visualisations of the EMDB entry EMD-1001. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

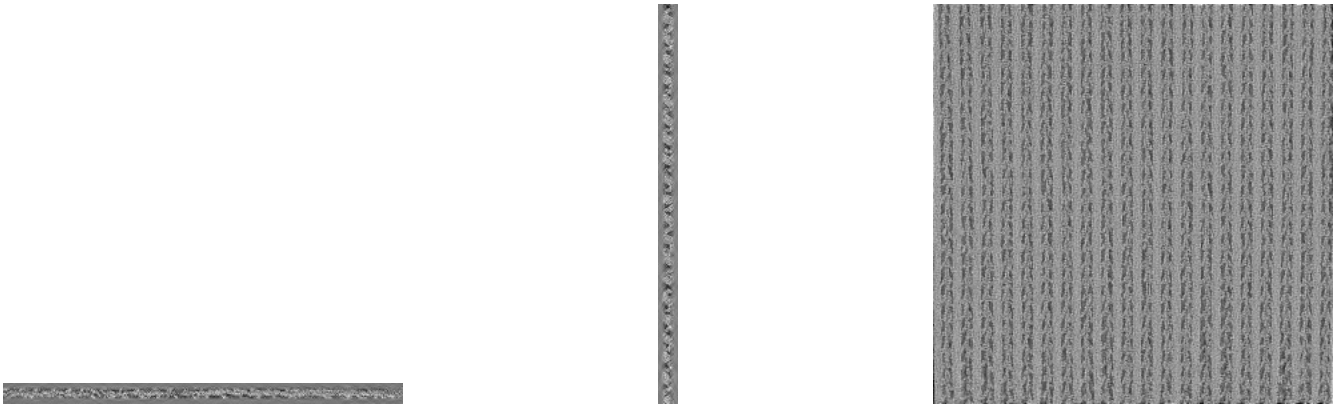
6.1 Orthogonal projections (i)



X Y Z

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

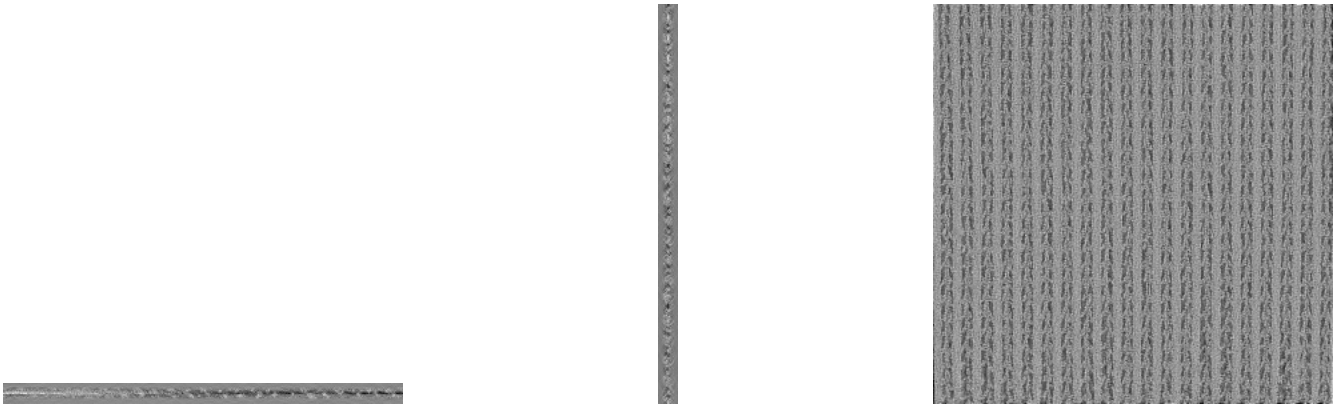
6.2 Central slices (i)



X Index: 300 Y Index: 300 Z Index: 15

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

6.3 Largest variance slices (i)



X Index: 598 Y Index: 598 Z Index: 15

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

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

X Y Z

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

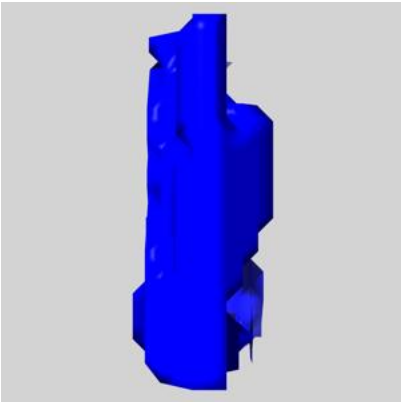
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

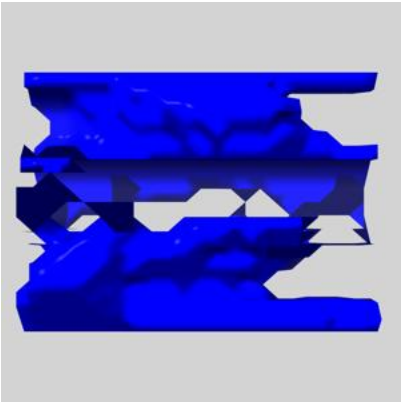
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

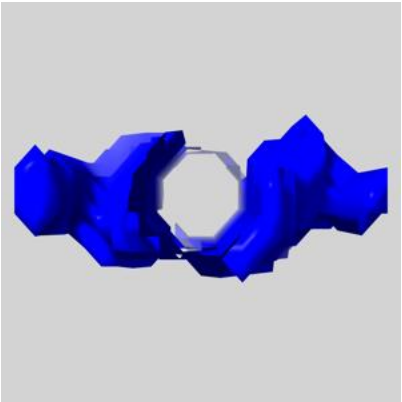
6.5.1 emd_1001_msk_25.map (i)



X

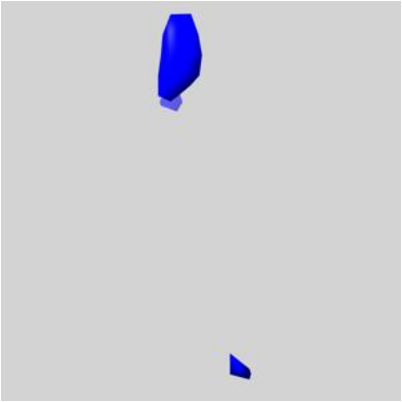


Y

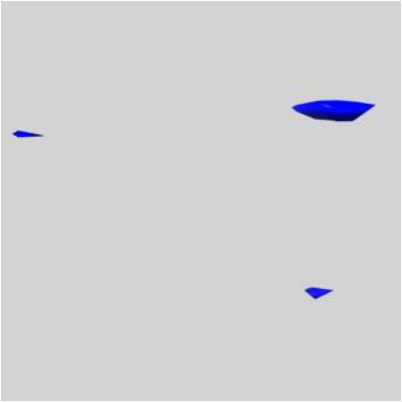


Z

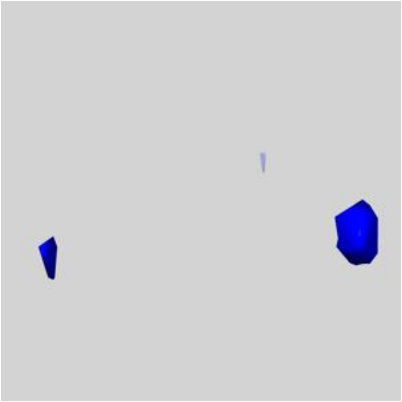
6.5.2 emd_1001_msk_24.map (i)



X

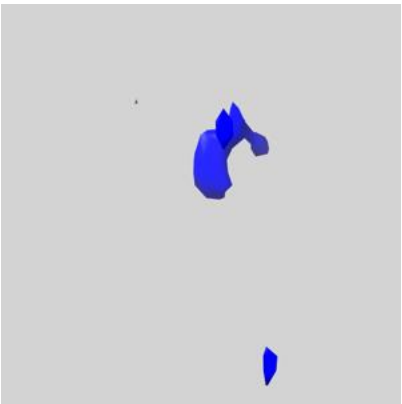


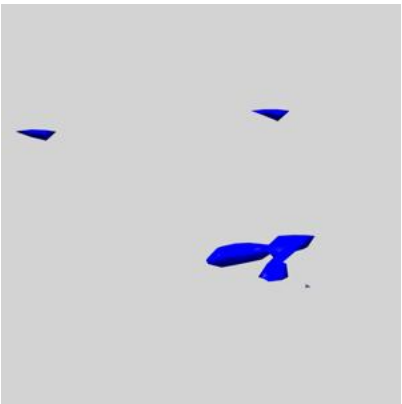
Y

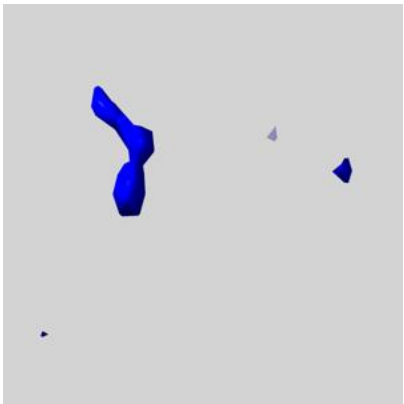


Z

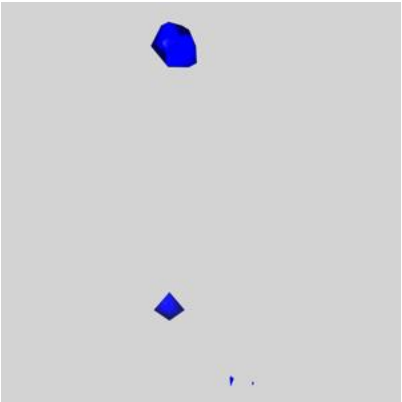
6.5.3 emd_1001_msk_23.map (i)

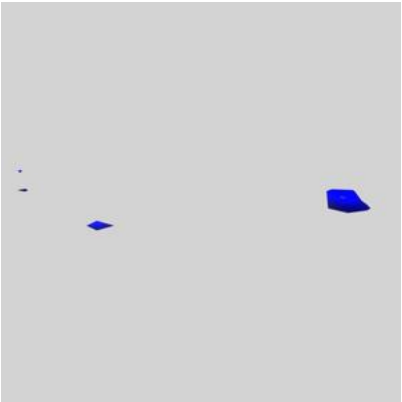

X

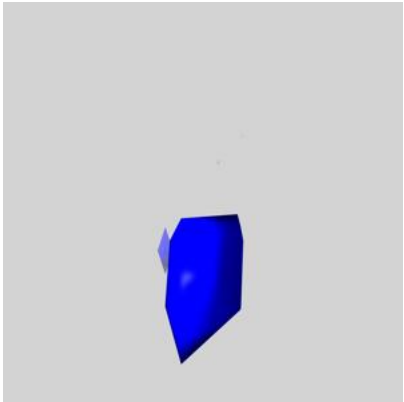

Y


Z

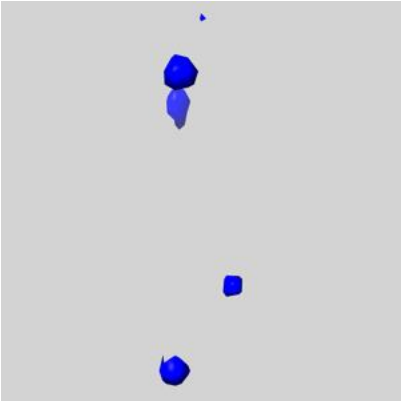
6.5.4 emd_1001_msk_22.map (i)

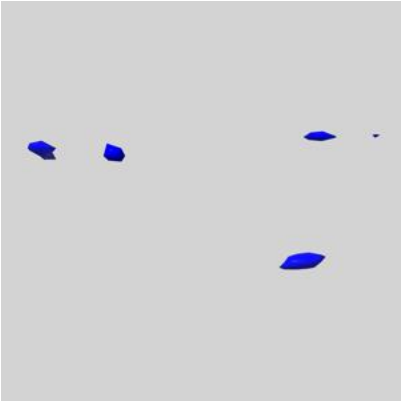

X

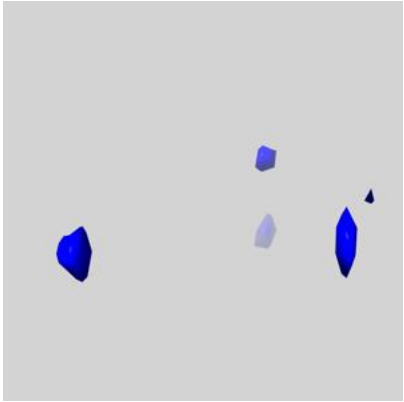

Y


Z

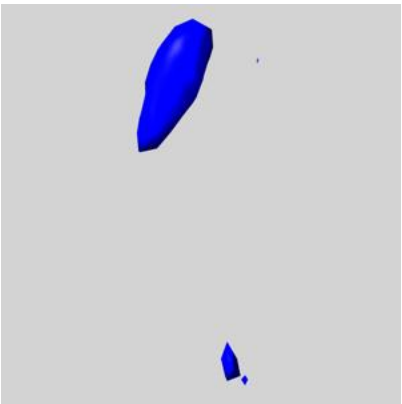
6.5.5 emd_1001_msk_21.map (i)

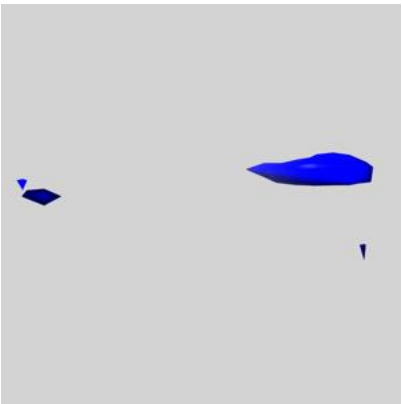

X


Y


Z

6.5.6 emd_1001_msk_20.map (i)


X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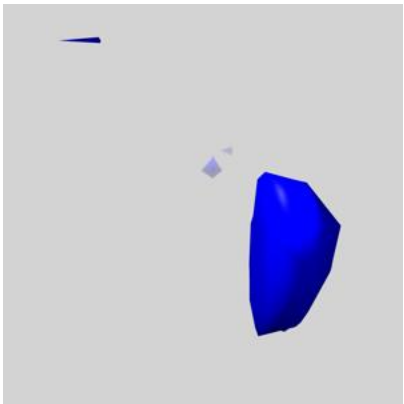
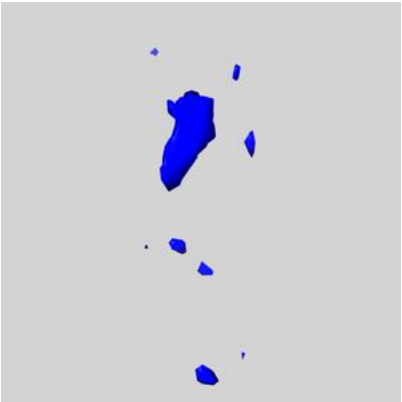

Z

6.5.7 emd_1001_msk_19.map (i)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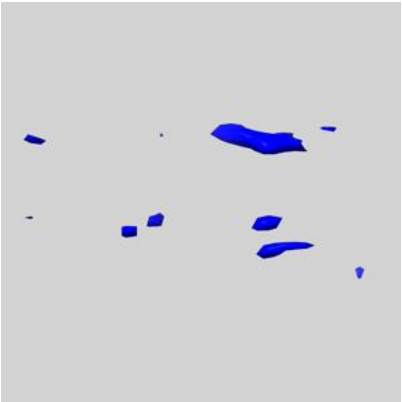
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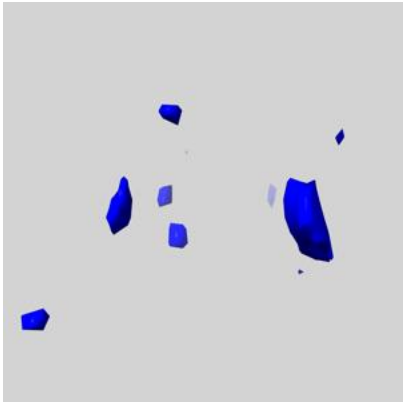
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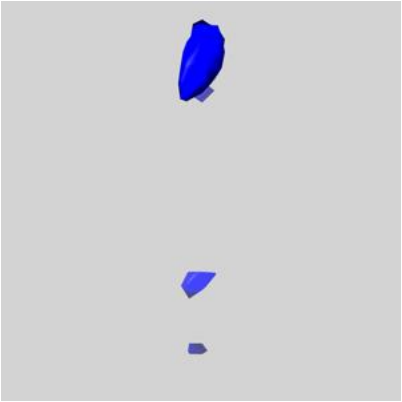
6.5.8 emd_1001_msk_18.map (i)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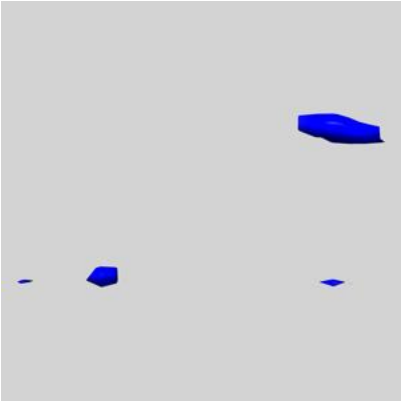
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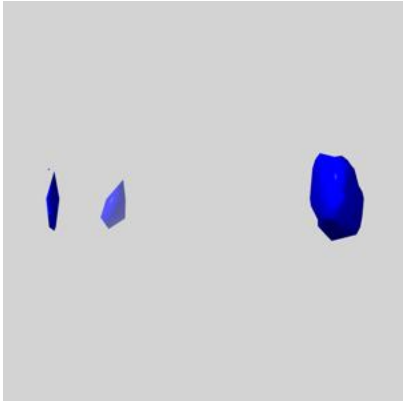
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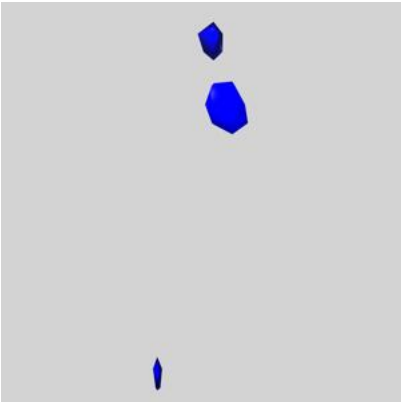
6.5.9 emd_1001_msk_17.map (i)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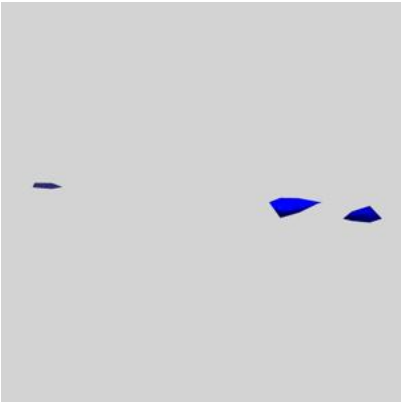
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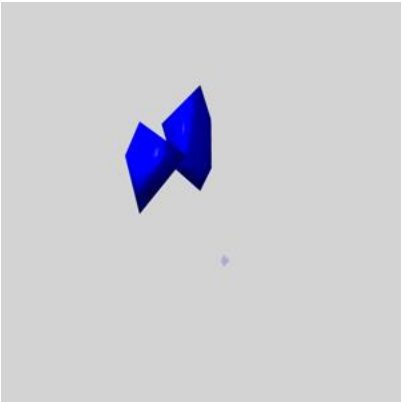
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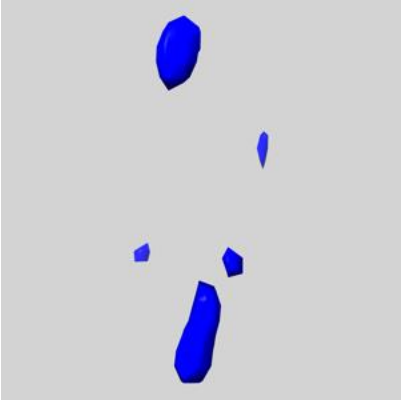
6.5.10 emd_1001_msk_16.map (i)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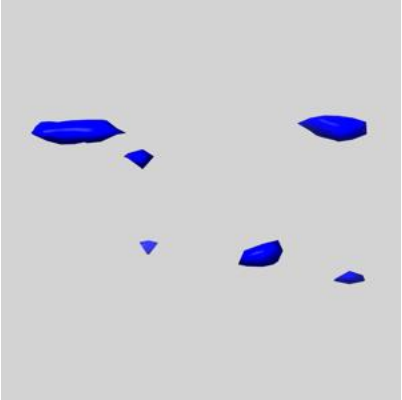
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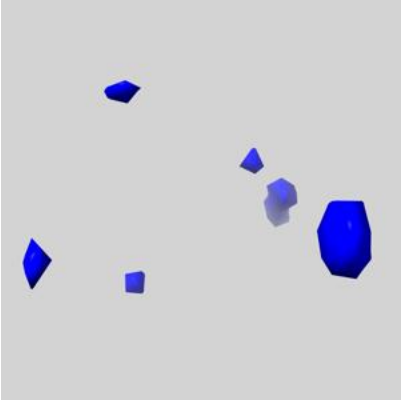
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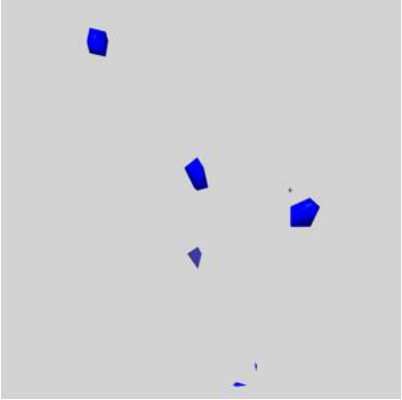
6.5.11 emd_1001_msk_15.map (i)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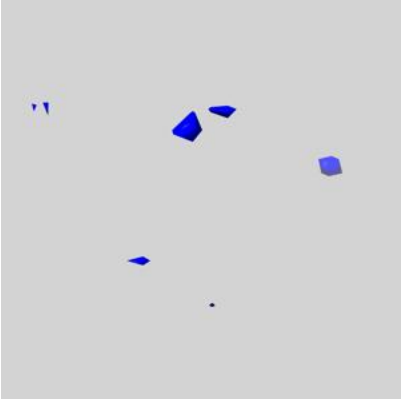
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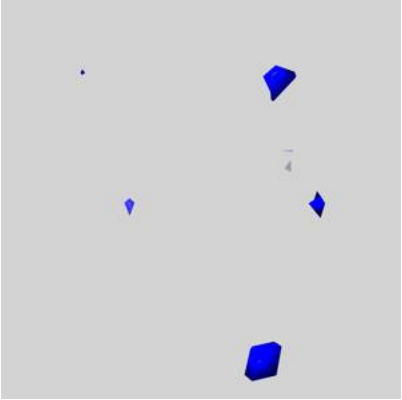
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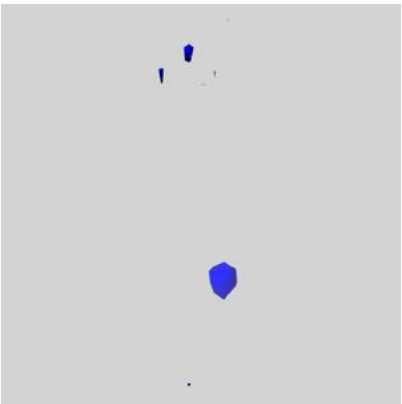
6.5.12 emd_1001_msk_14.map (i)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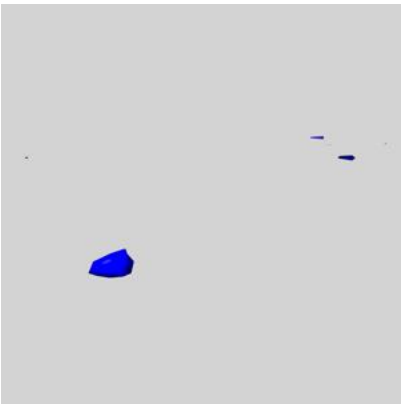
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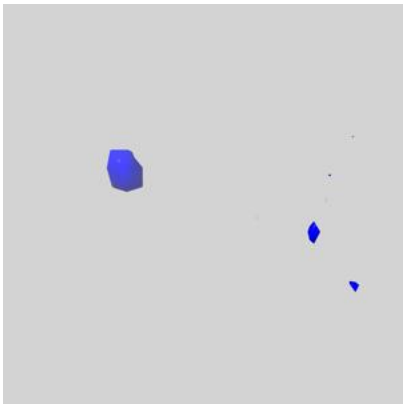
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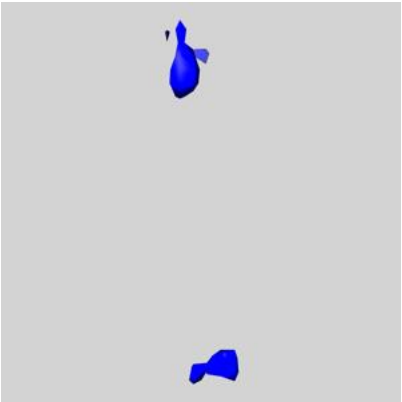
6.5.13 emd_1001_msk_13.map (i)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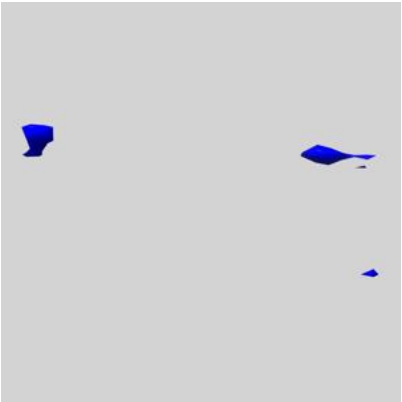
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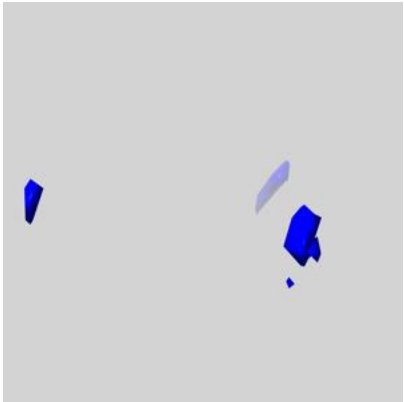
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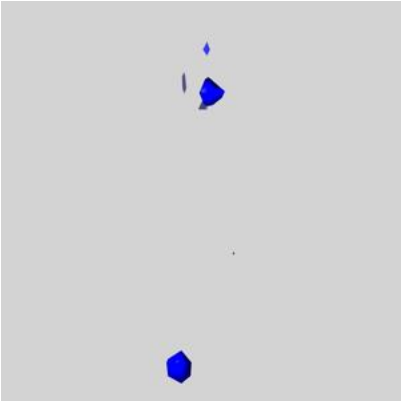
6.5.14 emd_1001_msk_12.map (i)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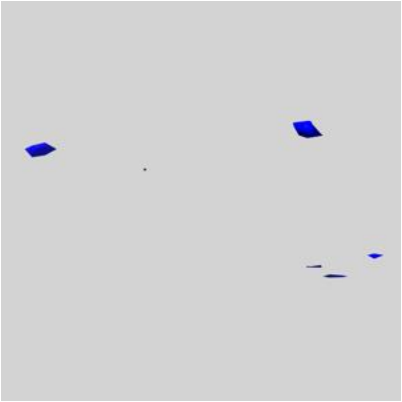
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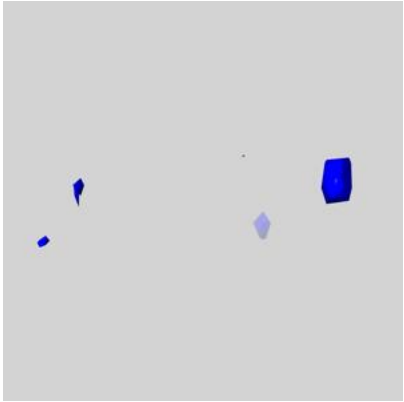
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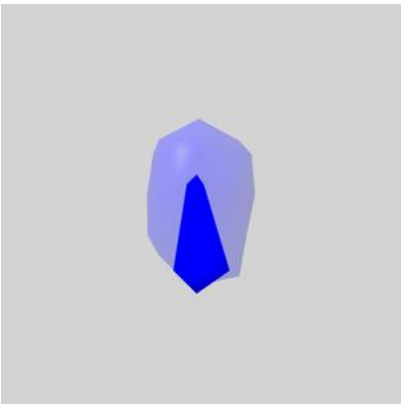
6.5.15 emd_1001_msk_11.map (i)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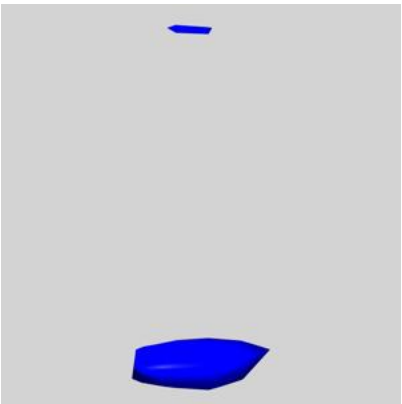
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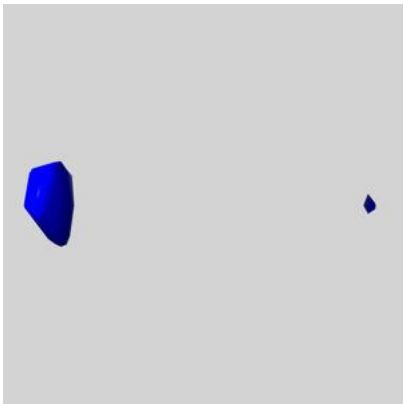
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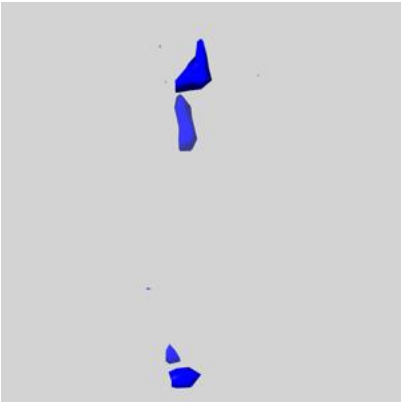
6.5.16 emd_1001_msk_10.map (i)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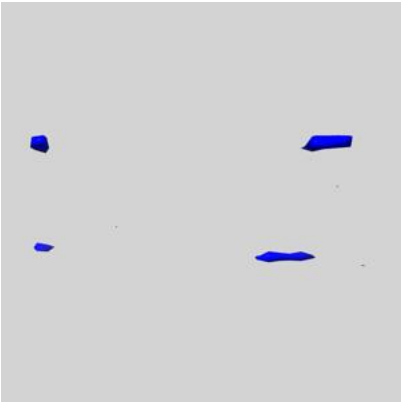
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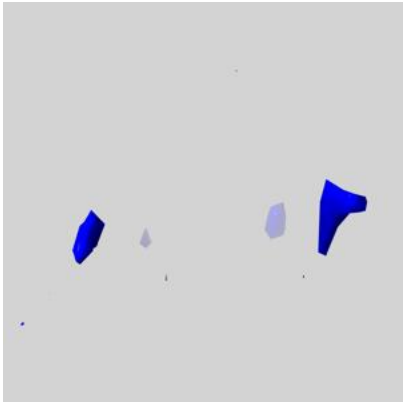
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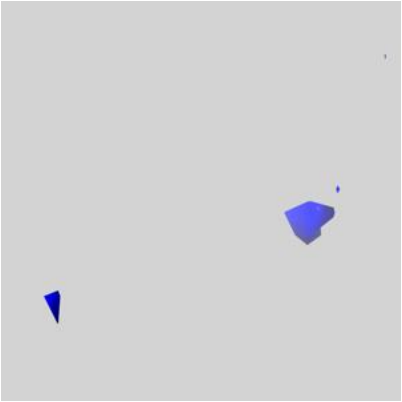
6.5.17 emd_1001_msk_9.map (i)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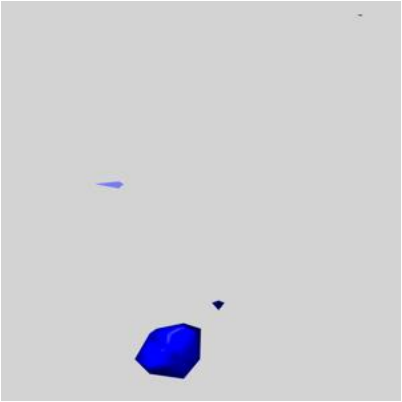
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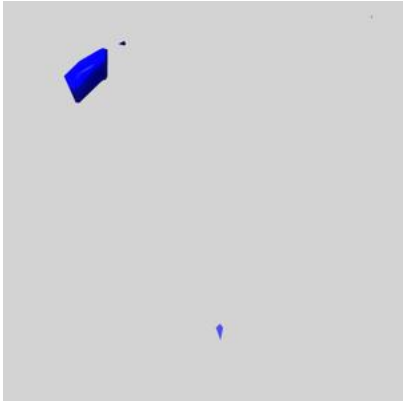
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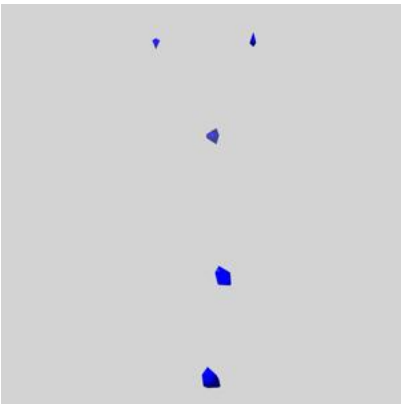
6.5.18 emd_1001_msk_8.map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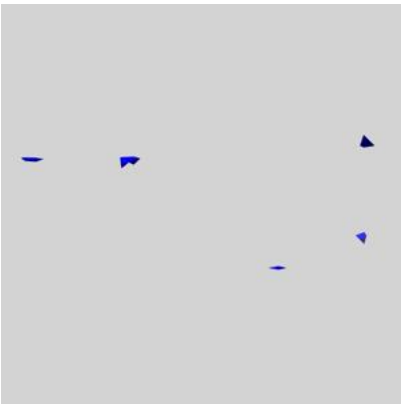
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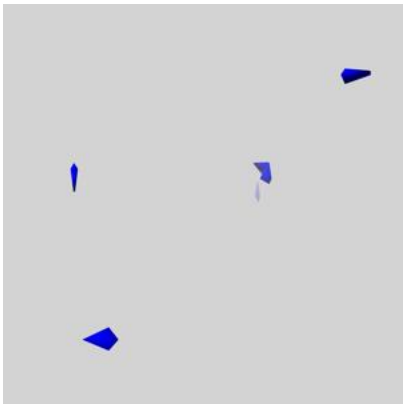
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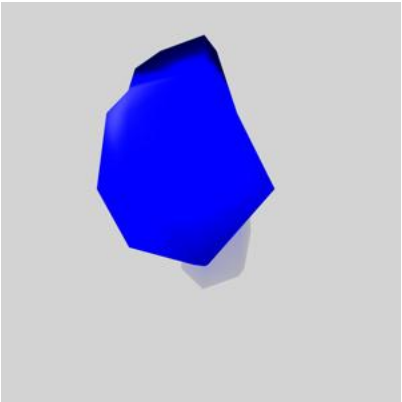
6.5.19 emd_1001_msk_7.map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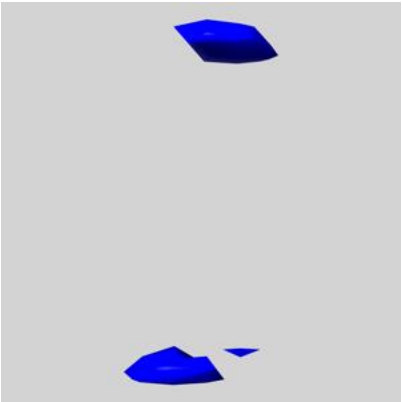
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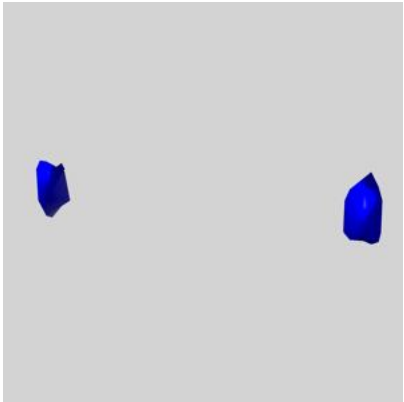
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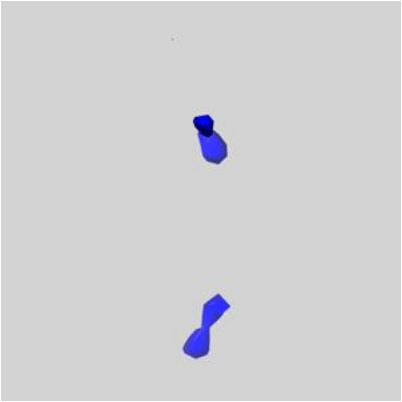
6.5.20 emd_1001_msk_6.map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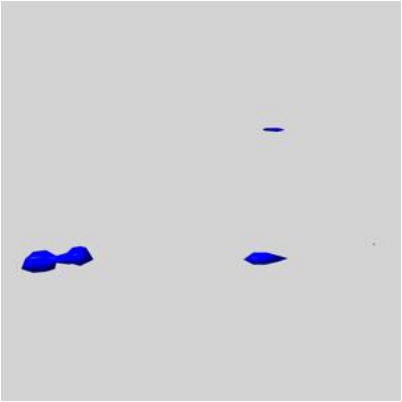
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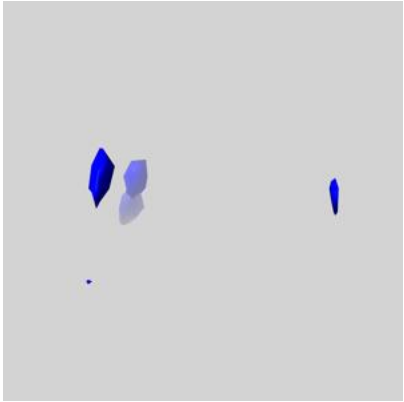
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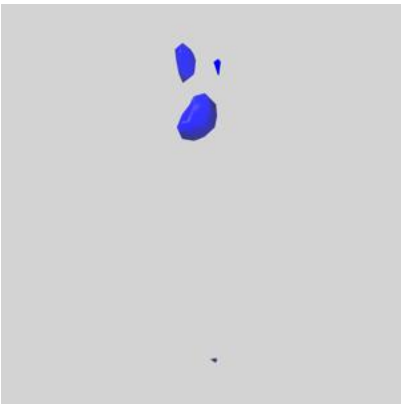
6.5.21 emd_1001_msk_5.map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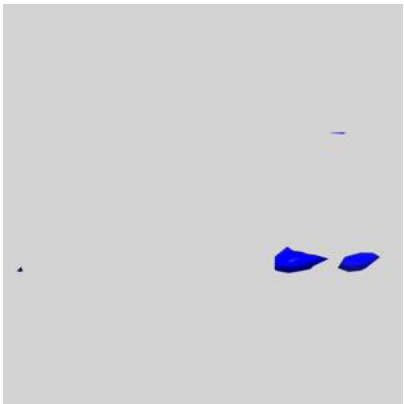
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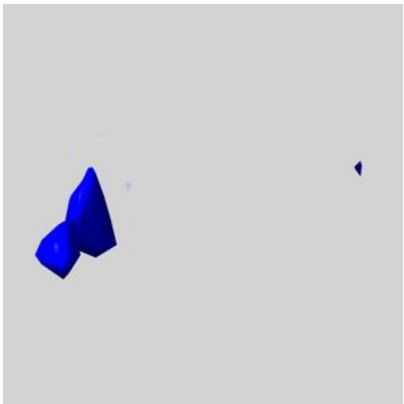
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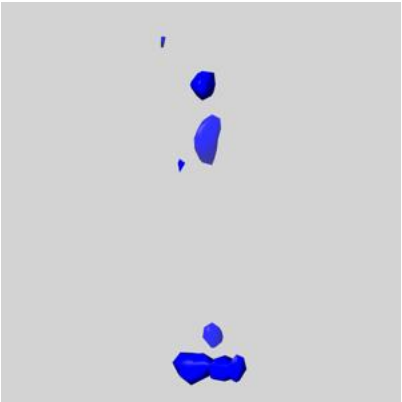
6.5.22 emd_1001_msk_4.map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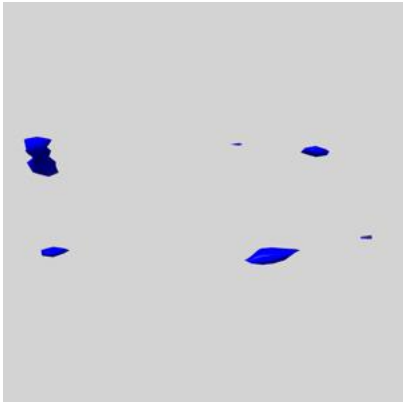
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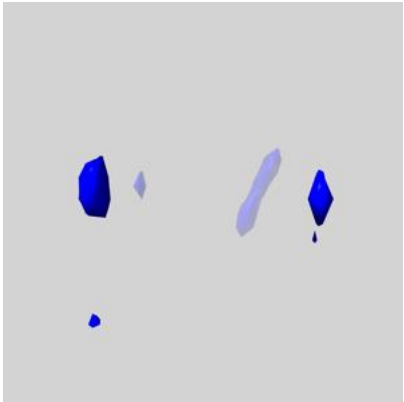
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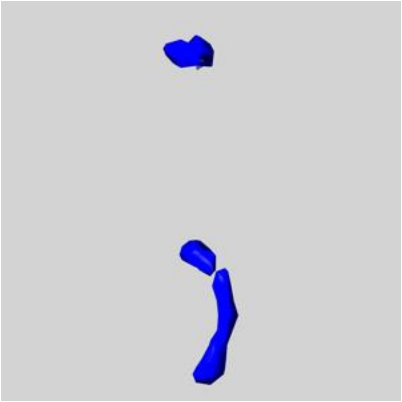
6.5.23 emd_1001_msk_3.map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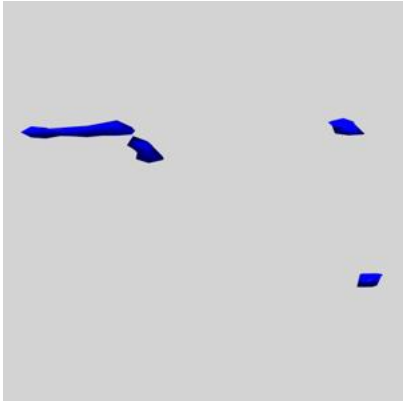
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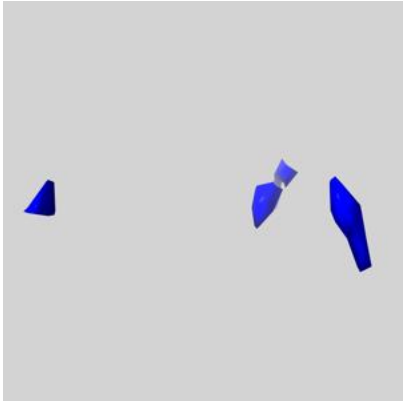
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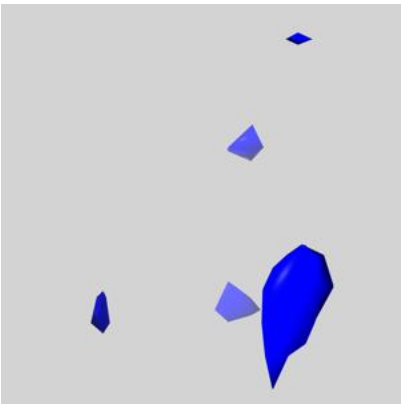
6.5.24 emd_1001_msk_2.map (i)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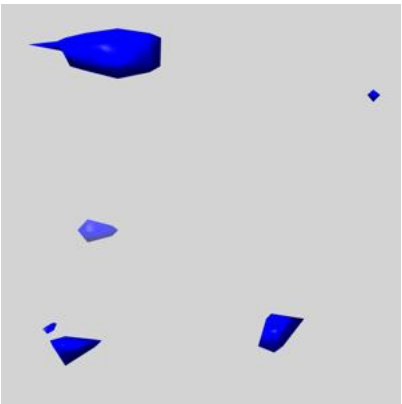
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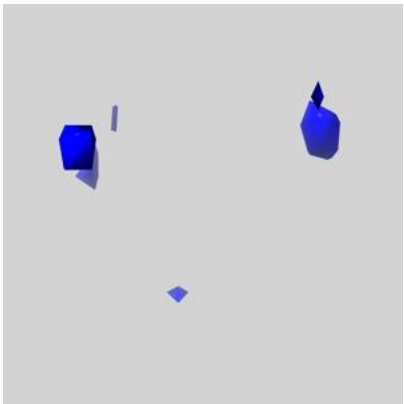
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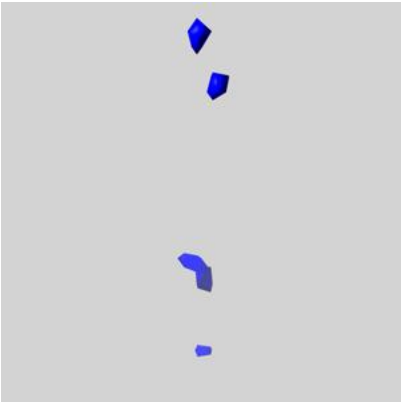
6.5.25 emd_1001_msk_1.map (i)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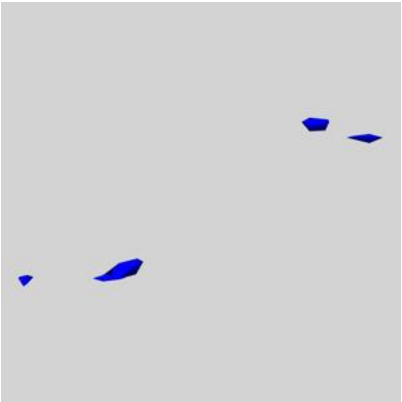
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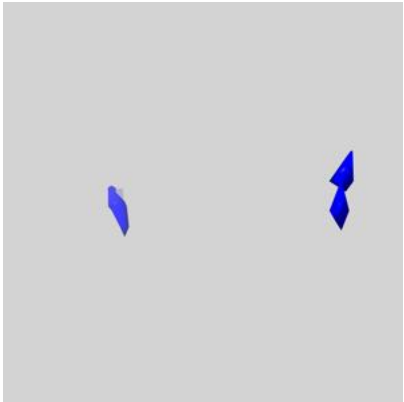
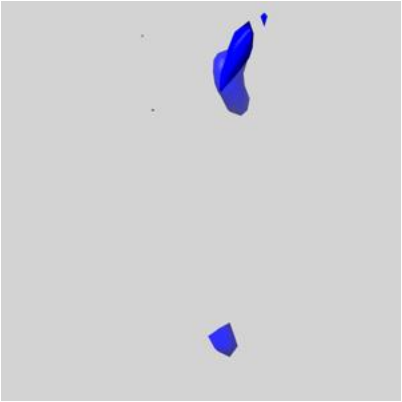
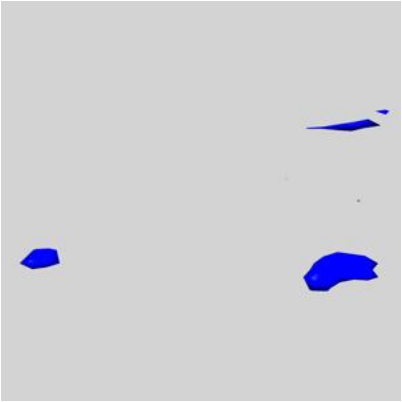
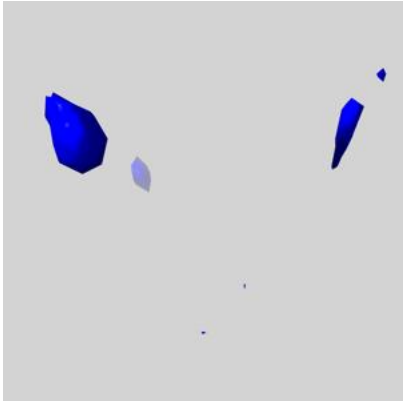

Z

6.5.26 emd_1001_msk_26.map (i)


X

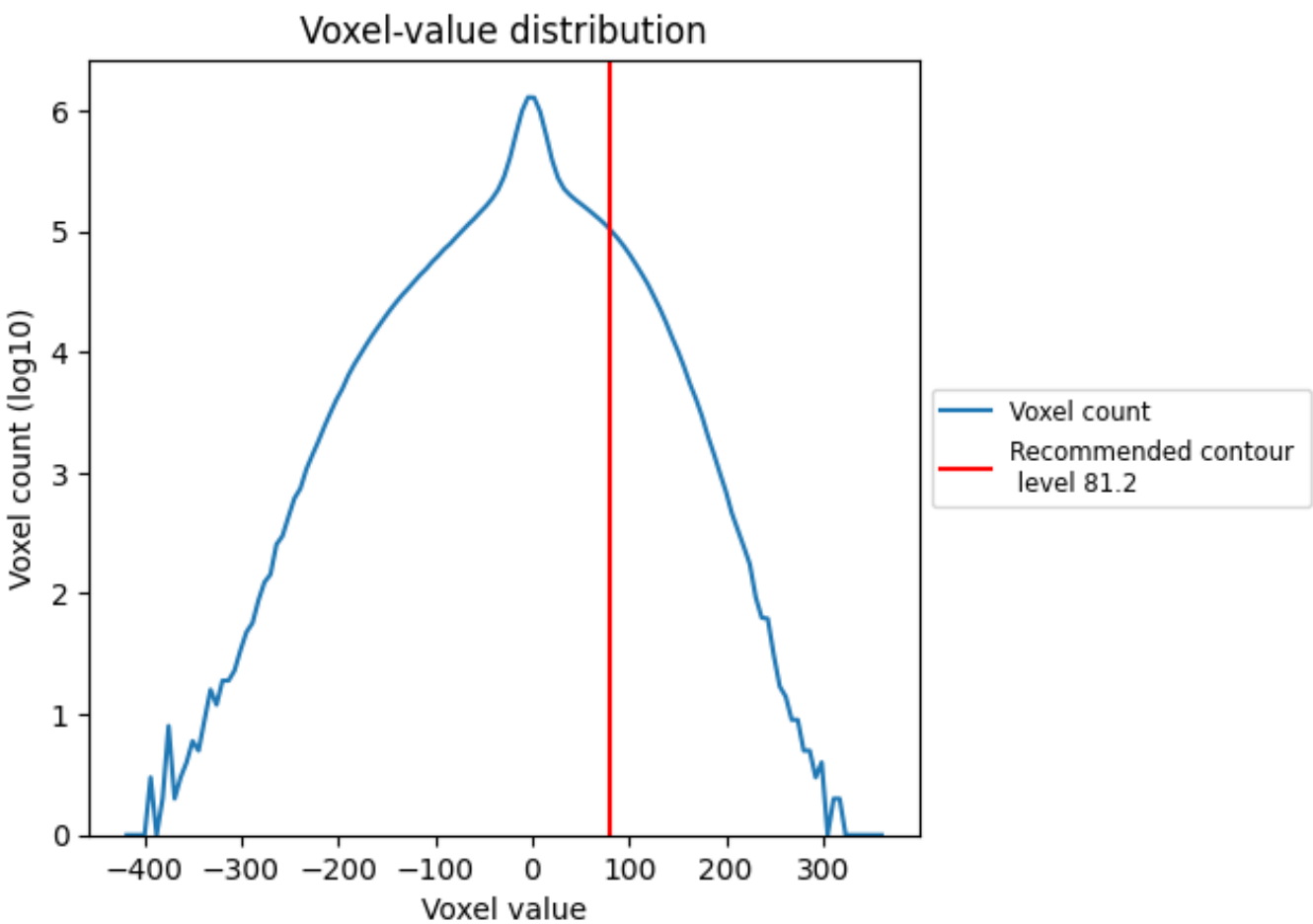

Y


Z

7 Tomogram analysis (i)

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

7.1 Voxel-value distribution (i)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

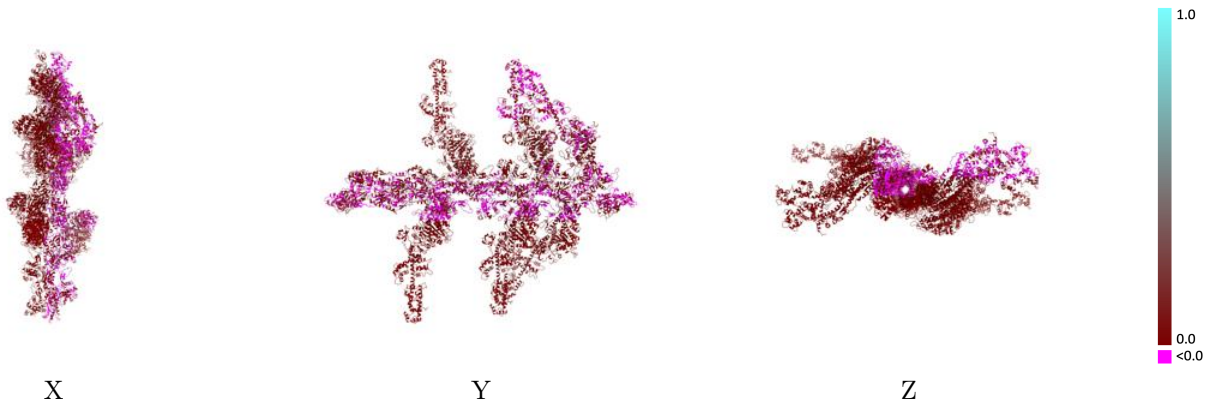
8 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-1001 and PDB model 1O1E. Per-residue inclusion information can be found in section 3 on page 7.

8.1 Map-model overlay (i)

This section was not generated.

8.2 Q-score mapped to coordinate model (i)

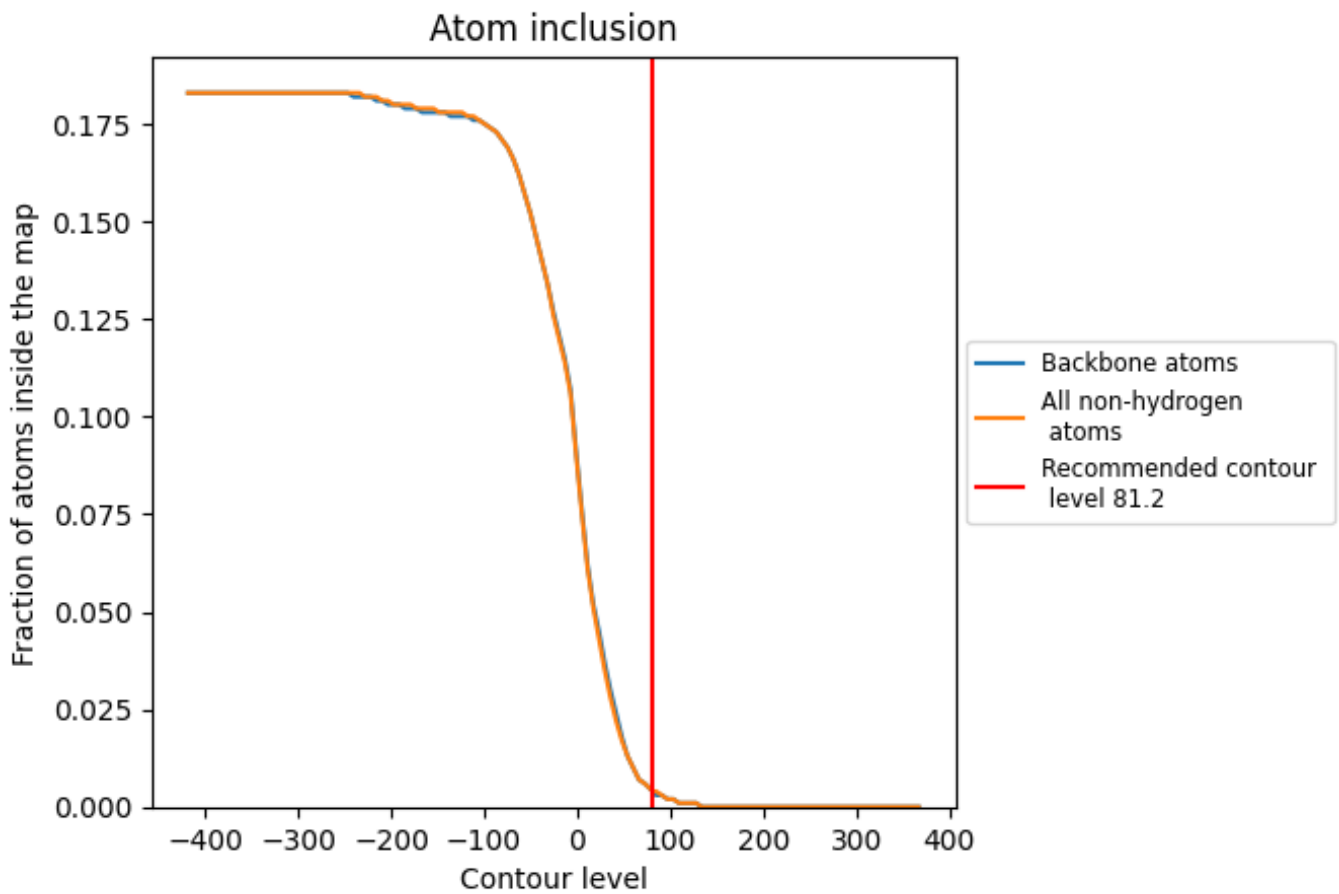


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

8.3 Atom inclusion mapped to coordinate model (i)

This section was not generated.

8.4 Atom inclusion (i)



At the recommended contour level, 0% of all backbone atoms, 0% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (81.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0040	-0.0010
1	0.0680	0.0040
2	0.0000	-0.0080
3	0.0000	0.0220
4	0.0000	-0.0040
5	0.0000	-0.0050
6	0.0000	-0.0010
7	0.0000	-0.0170
8	0.0000	-0.0030
9	0.0000	0.0070
A	0.0000	0.0060
B	0.0000	0.0000
C	0.0000	-0.0190
D	0.0000	-0.0030
E	0.0000	0.0000
F	0.0000	0.0000
G	0.0000	0.0020
H	0.0000	-0.0090
I	0.0050	0.0020
J	0.0000	-0.0010
K	0.0000	0.0000
L	0.0000	0.0000
M	0.0000	0.0000
N	0.0000	0.0000
O	0.0000	0.0000
P	0.0010	-0.0020
Q	0.0000	0.0000
R	0.0000	0.0000
V	0.0000	-0.0020
W	0.0480	-0.0060
X	0.0000	-0.0030
Y	0.0120	-0.0080
Z	0.0000	-0.0000