Full wwPDB EM Validation Report (i)

Aug 6, 2026 – 05:13 pm BST

PDB ID	:	9T67 / pdb_00009t67
EMDB ID	:	EMD-55607
Title	:	Cytoplasmic lattice filament repeat unit with ubiquitin
Authors	:	Singh, K.; Harasimov, K.; Carter, A.
Deposited on	:	2025-11-06
Resolution	:	7.70 Å(reported)

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

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

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

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

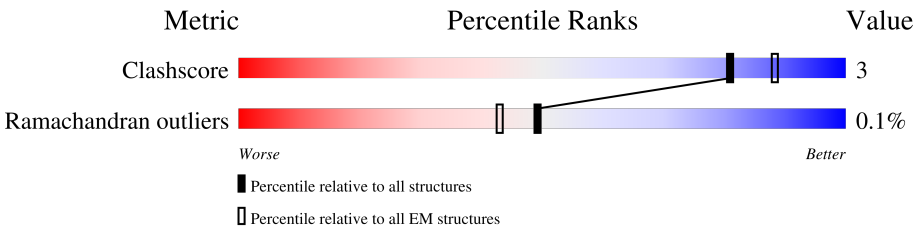
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

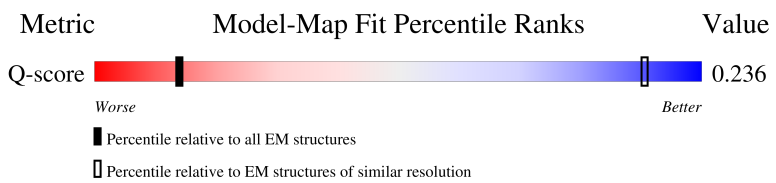
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 7.70 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	384 (7.20 - 8.20)

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	0	440	30% • 69%
1	S	440	29% • 69%
2	1	682	9% 93% 6%
2	2	682	98% 100%
2	3	682	94% 98% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	A	682	92% 8%
2	B	682	6% 94% 6%
2	C	682	7% 97%
2	D	682	7% 93% 7%
2	E	682	11% 97%
2	F	682	12% 96%
2	G	682	5% 91% 9%
2	H	682	97%
2	I	682	8% 96%
2	J	682	94% 6%
2	K	682	94% 99%
2	L	682	87% 99%
2	m	682	94% 6%
2	s	682	6% 94% 6%
2	t	682	5% 96%
2	u	682	5% 94% 6%
2	v	682	10% 96%
2	w	682	10% 98%
2	x	682	5% 93% 7%
2	y	682	95% 5%
2	z	682	14% 98%
3	4	1163	79% 18%
3	7	1163	9% 81% 18%
3	M	1163	78% 18%
3	P	1163	80% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	5	581	61% 37%
4	8	581	8% 62% 37%
4	N	581	60% 37%
4	Q	581	60% 37%
5	6	164	70% 27%
5	9	164	9% 51% 46%
5	O	164	68% 5% 27%
5	R	164	51% 46%
6	AA	228	28% 72%
6	T	228	25% 72%
7	AE	937	22% 98%
7	AF	937	24% 89% 10%
7	X	937	13% 99%
7	Y	937	13% 89% 10%
8	AG	993	9% 96%
8	Z	993	7% 95%
8	n	993	36% 97%
9	AH	782	9% 77% 19%
9	a	782	9% 78% 19%
9	o	782	19% 79% 19%
10	AI	147	96%
10	b	147	95% 5%
10	p	147	5% 99%
11	AJ	449	6% 96%
11	c	449	5% 96%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
11	q	449	33% 97%
12	AK	445	95%
12	d	445	96%
12	r	445	73% 97%
13	AL	466	29% 94% 6%
13	AN	466	96%
13	e	466	15% 94% 6%
13	g	466	92% 8%
14	AM	163	80% 99%
14	AO	163	30% 98%
14	f	163	79% 100%
14	h	163	25% 100%
15	U	76	14% 97%
15	V	76	63% 95%
15	W	76	93% 97%

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 181130 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 KH domain-containing protein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	0	136	673	401	136	136	0	0
1	S	136	673	401	136	136	0	0

- Molecule 2 is a protein called Inactive protein-arginine deiminase type-6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1	682	3373	2009	682	682	0	0
2	2	682	3373	2009	682	682	0	0
2	3	682	3373	2009	682	682	0	0
2	A	682	3373	2009	682	682	0	0
2	B	682	3373	2009	682	682	0	0
2	C	682	3373	2009	682	682	0	0
2	D	682	3373	2009	682	682	0	0
2	E	682	3373	2009	682	682	0	0
2	F	682	3373	2009	682	682	0	0
2	G	682	3373	2009	682	682	0	0
2	H	682	3373	2009	682	682	0	0
2	I	682	3373	2009	682	682	0	0
2	J	682	3373	2009	682	682	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	K	682	3373	2009	682	682	0	0
2	L	682	3373	2009	682	682	0	0
2	m	682	3373	2009	682	682	0	0
2	s	682	3373	2009	682	682	0	0
2	t	682	3373	2009	682	682	0	0
2	u	682	3373	2009	682	682	0	0
2	v	682	3373	2009	682	682	0	0
2	w	682	3373	2009	682	682	0	0
2	x	682	3373	2009	682	682	0	0
2	y	682	3373	2009	682	682	0	0
2	z	682	3373	2009	682	682	0	0

- Molecule 3 is a protein called NACHT, LRR and PYD domains-containing protein 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	4	949	4702	2804	949	949	0	0
3	7	949	4702	2804	949	949	0	0
3	M	949	4702	2804	949	949	0	0
3	P	949	4702	2804	949	949	0	0

- Molecule 4 is a protein called Transducin-like enhancer protein 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	5	367	1812	1078	367	367	0	0
4	8	367	1812	1078	367	367	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	N	367	1812	1078	367	367	0	0
4	Q	367	1812	1078	367	367	0	0

- Molecule 5 is a protein called Oocyte-expressed protein homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	6	119	592	354	119	119	0	0
5	9	89	442	264	89	89	0	0
5	O	119	592	354	119	119	0	0
5	R	89	442	264	89	89	0	0

- Molecule 6 is a protein called Zinc finger BED domain-containing protein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	AA	63	311	185	63	63	0	0
6	T	63	311	185	63	63	0	0

- Molecule 7 is a protein called NLR family, pyrin domain containing 4F.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	AE	935	4643	2773	935	935	0	0
7	AF	845	4196	2506	845	845	0	0
7	X	935	4643	2773	935	935	0	0
7	Y	845	4196	2506	845	845	0	0

- Molecule 8 is a protein called NACHT, LRR and PYD domains-containing protein 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	AG	966	4794	2862	966	966	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	Z	966	4794	2862	966	966	0	0
8	n	966	4794	2862	966	966	0	0

- Molecule 9 is a protein called E3 ubiquitin-protein ligase UHRF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	AH	635	3131	1861	635	635	0	0
9	a	635	3131	1861	635	635	0	0
9	o	635	3131	1861	635	635	0	0

- Molecule 10 is a protein called Ubiquitin-conjugating enzyme E2 D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	AI	147	729	435	147	147	0	0
10	b	147	729	435	147	147	0	0
10	p	147	729	435	147	147	0	0

- Molecule 11 is a protein called Tubulin alpha-1C chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	AJ	440	2167	1287	440	440	0	0
11	c	440	2167	1287	440	440	0	0
11	q	440	2167	1287	440	440	0	0

- Molecule 12 is a protein called Tubulin beta-4B chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	AK	431	2121	1259	431	431	0	0
12	d	431	2121	1259	431	431	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	r	431	2121	1259	431	431	0	0

- Molecule 13 is a protein called F-box/WD repeat-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	AL	466	2312	1380	466	466	0	0
13	AN	466	2312	1380	466	466	0	0
13	e	466	2312	1380	466	466	0	0
13	g	466	2312	1380	466	466	0	0

- Molecule 14 is a protein called S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	AM	163	809	483	163	163	0	0
14	AO	163	809	483	163	163	0	0
14	f	163	809	483	163	163	0	0
14	h	163	809	483	163	163	0	0

- Molecule 15 is a protein called Polyubiquitin-C.

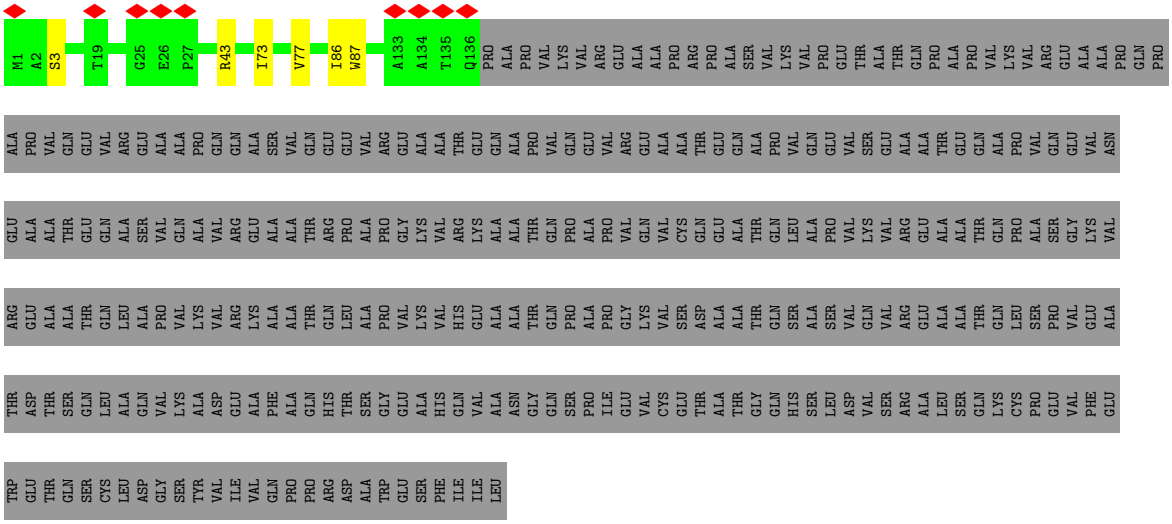
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	U	74	366	218	74	74	0	0
15	V	74	366	218	74	74	0	0
15	W	74	366	218	74	74	0	0

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.

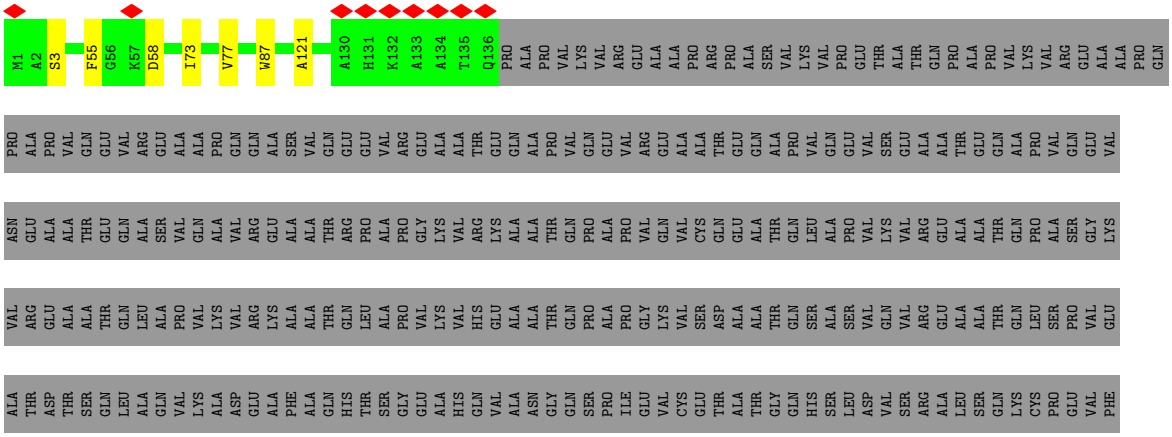
- Molecule 1: KH domain-containing protein 3

Chain 0:



- Molecule 1: KH domain-containing protein 3

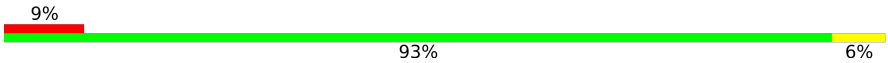
Chain S:



GLU TRP GLU THR GLN SER CYS LEU ASP GLY SER TYR VAL ILE VAL GLN PRO PRO ARG ASP ALA TRP GLU SER PHE ILE ILE LEU

• Molecule 2: Inactive protein-arginine deiminase type-6

Chain 1:



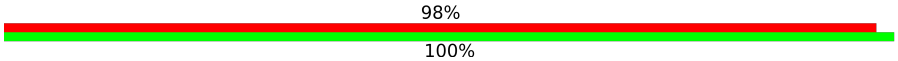
M1 S30 A33 K36 C37 I42 P46 L49 I52 S53 S54 S55 V56 G59 K60 E61 D62 T63 V64 V65 A75 R78 F96 C97 P98 D99 T104 A105 T106 A107 I116 G126 P131 W142 G143 M144 N145 G146 V153 V160 G161 Q162

P163 D164 E165 Q166 S167 F168 Q169 E170 R173 N182 A206 V211 R216 S219 L223 G226 E243 A249 C275 V290 L303 L307 C308 Q312 K333 A356 K359 L373 P384 G385 S386 T393 E394 V398 Q416 S435

Q452 V453 E458 L459 N482 M483 D484 Q485 K486 D487 F488 A493 E517 A539 K562 L565 G566 L567 P576 Q577 L578 F579 P600 G612 K613 D650 Y655 L656 A657 M658 I659 G660 D661 V662 R670 W678 P682

• Molecule 2: Inactive protein-arginine deiminase type-6

Chain 2:



M1 S2 F3 Q4 N5 S6 L7 S8 L9 S10 L11 V12 N13 P14 T15 H16 A17 L18 C19 M20 V21 G22 M23 E24 I25 T26 L27 D28 I29 S30 K31 C32 A33 P34 D35 K36 C37 K38 S39 F40 T41 I42 R43 G44 S45 P46 R47 I48 L49 I50 H51 I52 S53 S54 S55 V56 I57 A58 G59 K60

E61 D62 T63 V64 V65 W66 R67 S68 M69 N70 H71 P72 T73 V74 A75 L76 V77 R78 M79 V80 A81 P82 S83 P84 T85 V86 D87 E88 D89 K90 V91 L92 V93 S94 Y95 F96 C97 P98 D99 Q100 E101 V102 P103 T104 A105 T106 A107 V108 L109 F110 L111 T112 G113 I114 E115 I116 S117 L118 E119 A120

D121 I122 Y123 R124 D125 G126 Q127 L128 D129 M130 P131 S132 D133 K134 Q135 A136 K137 K138 K139 W140 M141 W142 G143 M144 N145 G146 W147 G148 A149 I150 L151 L152 V153 N154 C155 S156 P157 N158 A159 V160 G161 Q162 P163 D164 E165 Q166 S167 F168 Q169 E170 G171 P172 R173 E174 I175 Q176 N177 L178 S179 Q180

M181 T184 V185 E186 G187 P188 T189 S190 I191 L192 Q193 N194 Y195 Q196 L197 I198 L199 H200 T201 S202 E203 E204 E205 A206 K207 K208 T209 R210 V211 Y212 W213 S214 Q215 R216 G217 S218 S219 A220 Y221 E222 L223 V224 V225 G226 P227 N228 K229 P230 V231 Y232 L233 L234 P235 T236 F237 E238 N239 R240 R241

K242 E243 A244 F245 Y246 V247 E248 A249 T250 E251 F252 P253 S254 P255 S256 F257 S258 G259 L260 I261 S262 L263 S264 L265 S266 L267 V268 E269 K270 A271 H272 D273 E274 C275 I276 P277 E278 I279 P280 L281 Y282 K283 D284 T285 V286 M287 F288 R289 V290 A291 P292 Y293 I294 F295 M296 P297 S298 T299 Q300 M301

P302 L303 E304 V305 Y306 L307 C308 R309 E310 L311 Q312 L313 Q314 G315 F316 V317 D318 S319 V320 T321 K322 L323 S324 E325 K326 S327 K328 V329 Q330 V331 V332 K333 V334 Y335 E336 D337 P338 N339 R340 Q341 S342 K343 W344 L345 Q346 D347 E348 M349 A350 F351 C352 Y353 T354 Q355 A356 P357 H358 K359 T360 V361

S362 L363 I364 L365 D366 T367 P368 R369 V370 S371 K372 L373 E374 D375 F376 P377 M378 K379 Y380 T381 L382 T383 P384 G385 S386 G387 Y388 L389 I390 R391 Q392 T393 E394 D395 H396 R397 V398 A399 S400 Q401 D402 S403 I404 G405 N406 L407 M408 F409 S410 P411 P412 V413 K414 A415 Q416 G417 K418 D419 Y420 P421

L422 G423 R424 V425 L426 I427 G428 G429 S430 F431 Y432 P433 S434 S435 E436 G437 R438 D439 M440 N441 K442 G443 L444 R445 E446 F447 V448 Y449 A450 Q451 Q452 V453 Q454 A455 P456 V457 E458 L459 F460 S461 D462 W463 L464 M465 T466 G467 H468 M469 D470 Q471 F472 M473 C474 F475 V476 P477 T478 N479 D480 K481

N482 N483 D484 Q485 K486 D487 F488 R489 L490 L491 L492 A493 S494 P495 S496 A497 C498 F499 E500 L501 F502 E503 Q504 K505 Q506 K507 E508 G509 Y510 G511 N512 V513 T514 L515 F516 E517 D518 I519 G520 A521 E522 Q523 L524 L525 S526 N527 G528 R529 E530 S531 K532 T533 I534 S535 Q536 I537 L538 A539 D540 K541

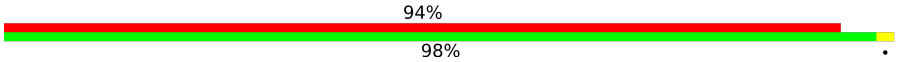
S542 F543 R544 E545 Q546 N547 T548 Y549 V550 E551 K552 C553 I554 S555 L556 N557 R558 T559 L560 L561 K562 T563 E564 L565 G566 L567 E568 D569 K570 D571 I572 I573 L574 I575 P576 Q577 L578 F579 C580 L581 E582 Q583 L584 T585 N586 V587 P588 S589 N590 Q591 Q592 S593 T594 K595 L596 F597 A598 R599 P600 Y601

F602 P603 D604 M605 L606 Q607 I608 I609 V610 L611 G612 K613 N614 L615 G616 I617 P618 K619 P620 F621 G622 P623 K624 I625 N626 G627 T628 C629 C630 L631 E632 E633 K634 V635 C636 G637 L638 L639 E640 P641 L642 G643 L644 K645 C646 T647 F648 I649 D650 D651 F652 D653 C654 Y655 L656 A657 N658 I659 G660 D661

V662 C663 A664 S665 A666 I667 I668 N669 R670 V671 P672 F673 A674 F675 K676 W677 W678 K679 M680 T681 P682

- Molecule 2: Inactive protein-arginine deiminase type-6

Chain 3:



M1 S2 F3 Q4 N5 S6 L7 S8 L9 S10 L11 V12 N13 P14 T15 H16 A17 L18 C19 M20 V21 G22 M23 E24 I25 T26 L27 D28 I29 S30 K31 C32 A33 P34 D35 K36 C37 K38 S39 I42 R43 G44 S45 P46 R47 I50 H51 I52 S53 S54 S55 V56 I57 A58 G59 K60 E61 D62

T63 V64 V65 W66 R67 S68 M69 N70 H71 P72 T73 V74 A75 L76 V77 R78 M79 V80 A81 P82 S83 P84 T85 V86 D87 E88 D89 K90 V91 L92 V93 S94 Y95 F96 C97 P98 D99 Q100 E101 V102 P103 T104 A105 T106 A107 V108 L109 F110 L111 T112 G113 I114 E115 I116 S117 L118 E119 A120 D121 I122

Y123 R124 D125 G126 Q127 L128 D129 M130 P131 S132 D133 K134 Q135 K138 K139 W140 M141 W142 G143 M144 N145 A149 I150 L151 L152 V153 N154 C155 S156 P157 N158 A159 V160 G161 Q162 P163 D164 E165 Q166 S167 F168 Q169 E170 G171 P172 R173 E174 I175 Q176 N177 L178 S179 Q180 M181 N182 V183 T184 V185

E186 G187 P188 T189 S190 I191 L192 Q193 Q196 L199 H200 T201 S202 E203 E204 E205 A206 K207 K208 T209 R210 R216 G217 S218 S219 A220 Y221 E222 L223 V224 V225 G226 P227 N228 K229 P230 V231 Y232 L233 L234 P235 T236 F237 E238 N239 R240 R241 K242 E243 A244 F245 Y246 V247 E248 A249 T250 E251

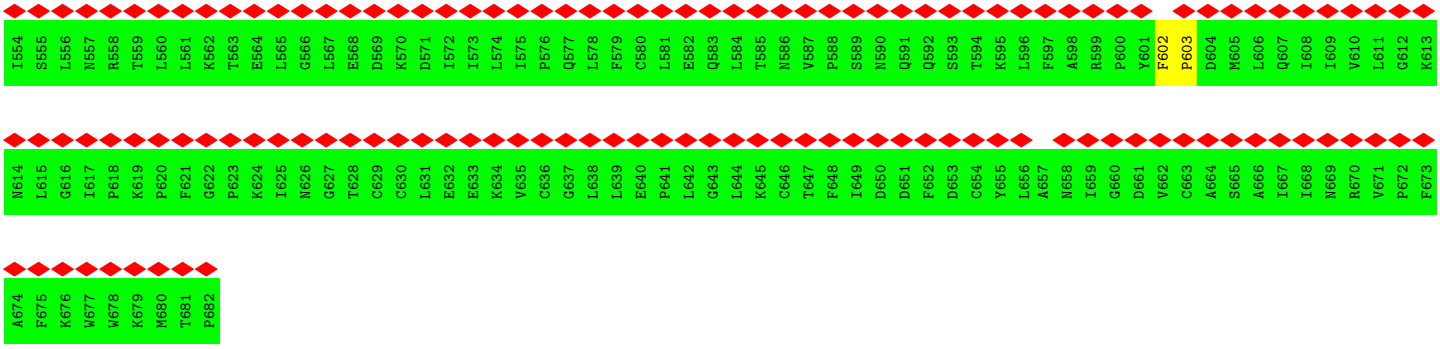
F252 P253 S254 P255 S256 F257 S258 G259 L260 I261 S262 L263 S264 L265 S266 L267 K270 A271 H272 D273 E274 C275 I276 P277 E278 I279 P280 L281 Y282 K283 D284 T285 V286 M287 F288 R289 V290 A291 P292 Y293 I294 F295 M296 P297 S298 T299 Q300 M301 P302 L303 E304 V305 Y306 L307 C308 R309 E310 L311 Q312

L313 Q314 G315 F316 V317 D318 S319 V320 T321 K322 L323 S324 E325 K326 S327 K328 V329 Q330 V331 V332 K333 V334 Y335 E336 D337 P338 N339 S342 K343 W344 L345 Q346 D347 E348 M349 A350 F351 C352 Y353 T354 Q355 A356 P357 H358 K359 T360 V361 S362 L363 I364 L365 D366 T367 P368 R369 V370 S371 K372 L373

E374 D375 F376 P377 M378 K379 Y380 T381 L382 T383 P384 G385 S386 G387 Y388 L389 I390 R391 Q392 T393 E394 D395 H396 R397 V398 A399 S400 L401 D402 S403 I404 G405 N406 L407 M408 V409 S410 P411 P412 V413 K414 A415 Q416 G417 K418 D419 Y420 P421 L422 G423 R424 V425 L426 I427 G428 G429 S430 F431 Y432 P433

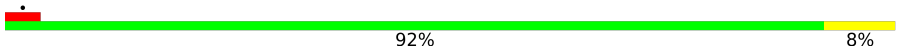
S434 S435 E436 G437 R438 D439 M440 M441 K442 G443 L444 R445 E446 F447 V448 Y449 A450 Q451 Q452 V453 Q454 A455 P456 V457 E458 L459 F460 S461 D462 W463 L464 M465 T466 G467 H468 M469 D470 Q471 F472 M473 C474 F475 V476 P477 T478 M479 D480 K481 M482 N483 D484 Q485 K486 D487 F488 R489 L490 L491 L492 A493

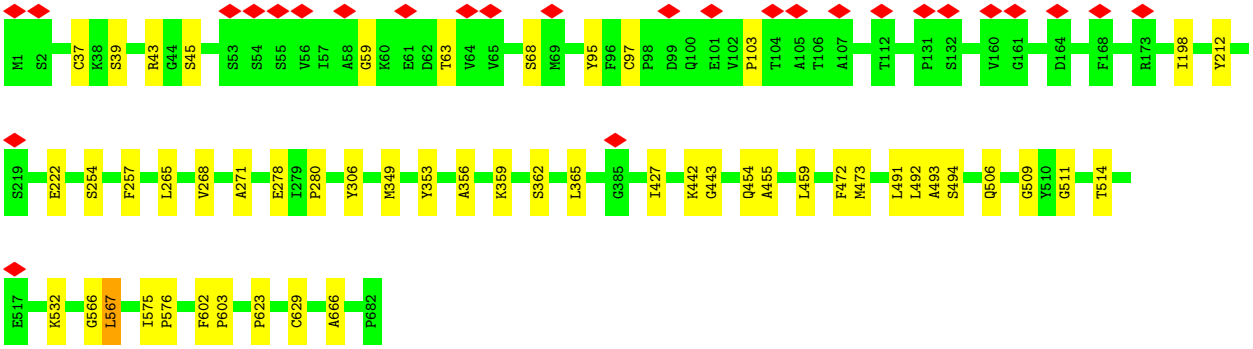
S494 P495 S496 A497 C498 F499 E500 L501 F502 E503 Q504 K505 Q506 K507 E508 G509 Y510 G511 N512 V513 T514 L515 F516 E517 D518 I519 G520 A521 E522 Q523 L524 L525 S526 M527 G528 R529 E530 S531 K532 T533 I534 S535 Q536 I537 L538 A539 D540 K541 S542 F543 R544 E545 Q546 N547 T548 Y549 V550 E551 K552 C553



• Molecule 2: Inactive protein-arginine deiminase type-6

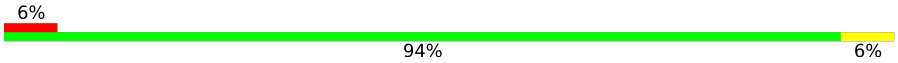
Chain A:

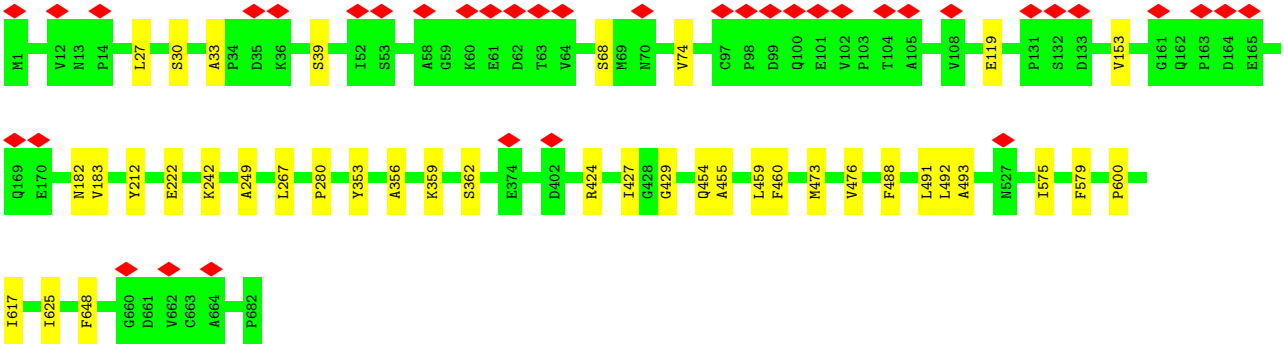




• Molecule 2: Inactive protein-arginine deiminase type-6

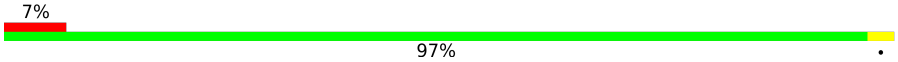
Chain B:

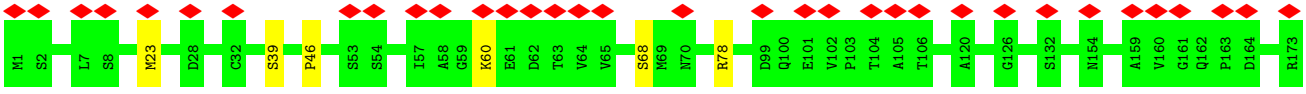


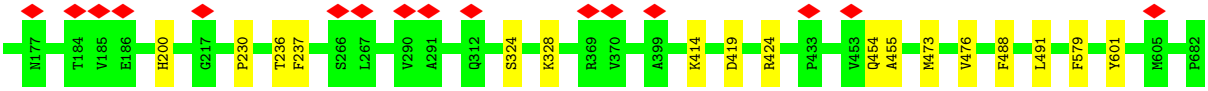


• Molecule 2: Inactive protein-arginine deiminase type-6

Chain C:

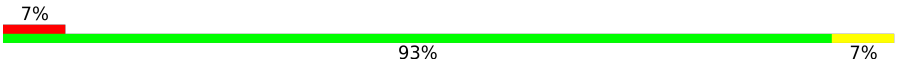


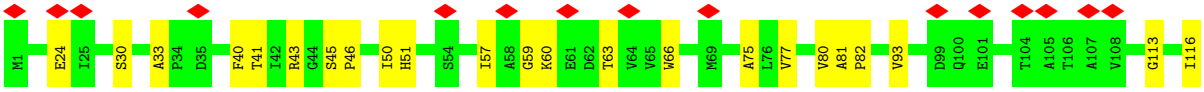


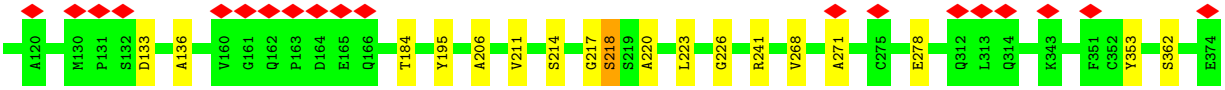


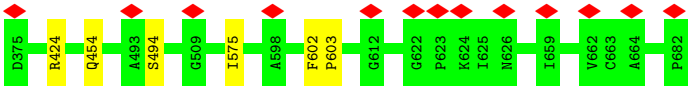
• Molecule 2: Inactive protein-arginine deiminase type-6

Chain D:



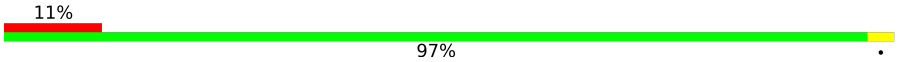


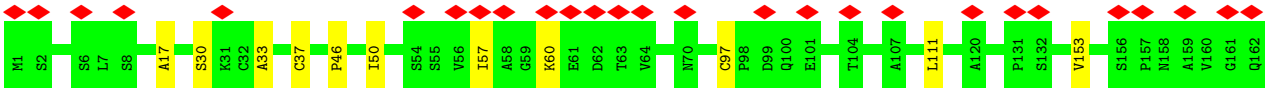


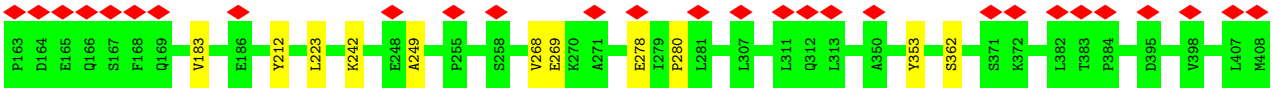


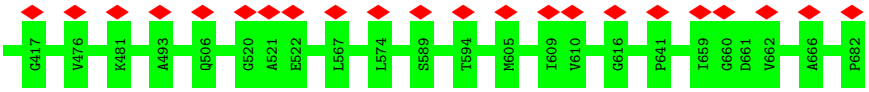
• Molecule 2: Inactive protein-arginine deiminase type-6

Chain E:



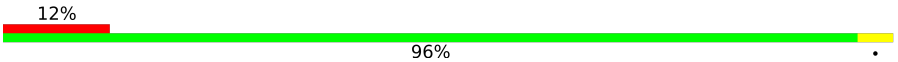


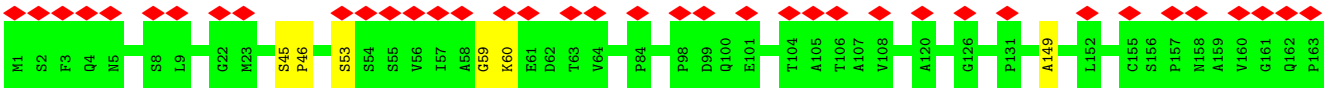


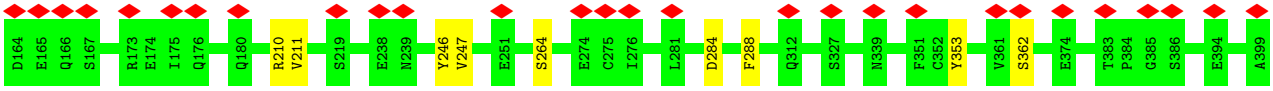


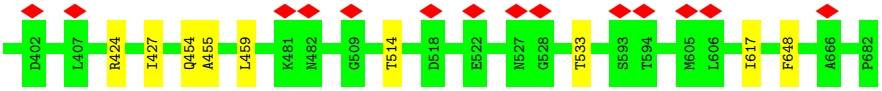
• Molecule 2: Inactive protein-arginine deiminase type-6

Chain F:



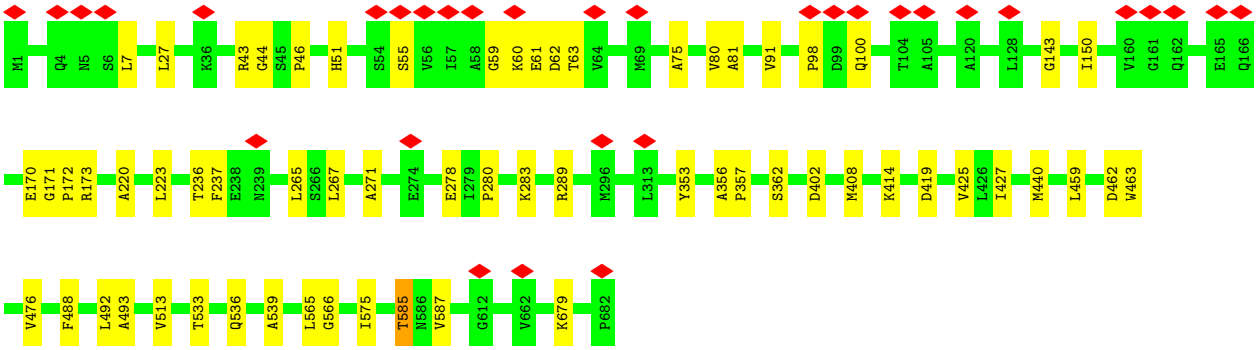






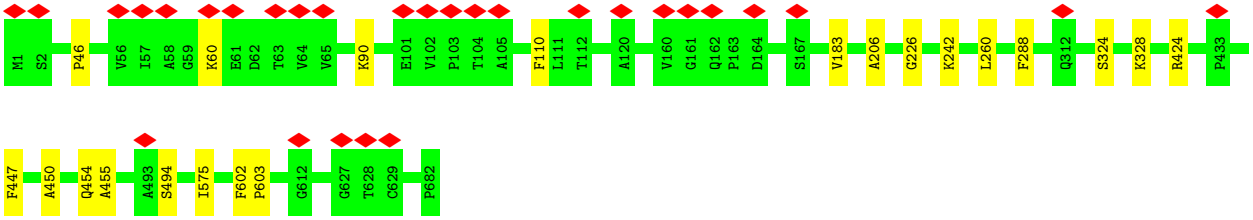
• Molecule 2: Inactive protein-arginine deiminase type-6

Chain G: 5% 91% 9%



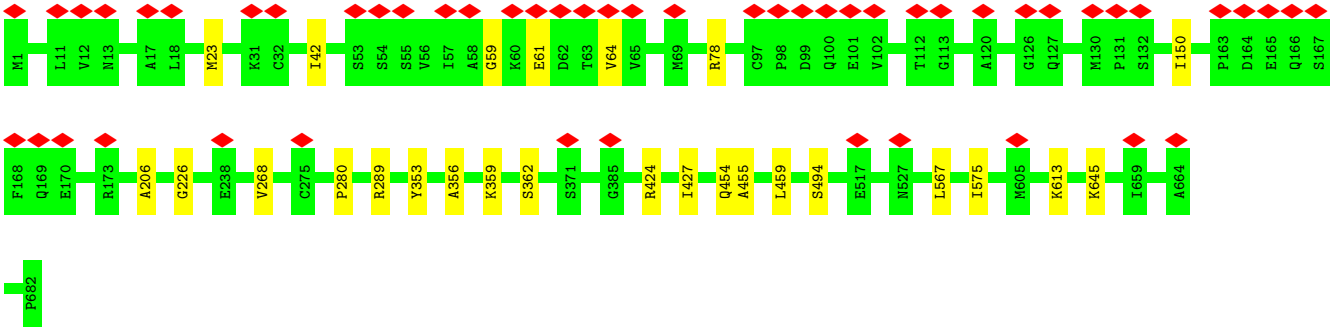
• Molecule 2: Inactive protein-arginine deiminase type-6

Chain H: 97%



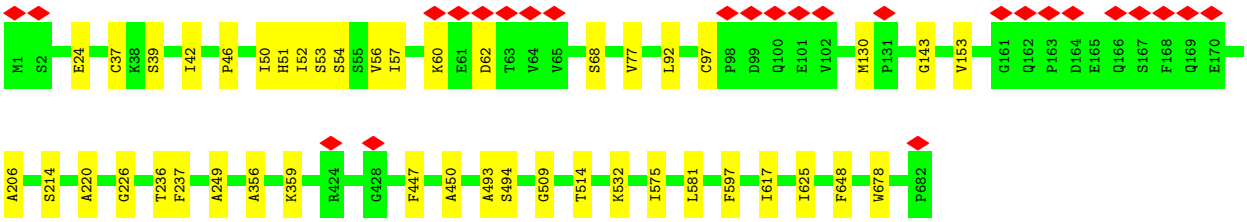
• Molecule 2: Inactive protein-arginine deiminase type-6

Chain I: 8% 96%



• Molecule 2: Inactive protein-arginine deiminase type-6

Chain J: 94% 6%



• Molecule 2: Inactive protein-arginine deiminase type-6

Chain K: 94% 99%

M1 S2 F3 Q4 N5 S6 L7 S8 L9 S10 L11 V12 N13 P14 T15 H16 A17 L18 C19 M20 V21 G22 M23 E24 I25 T26 L27 D28 I29 S30 K31 C32 A33 P34 D35 K36 C37 K38 S39 F40 T41 I42 R43 G44 S45 P46 R47 I48 L49 I50 H51 I52 S53 S54 S55 V56 I57 A58 G59 K60

E61 D62 T63 V64 V65 W66 R67 S68 M69 N70 H71 P72 T73 V74 A75 L76 V77 R78 M79 V80 A81 P82 S83 P84 T85 V86 D87 E88 D89 K90 V91 L92 V93 S94 Y95 F96 C97 P98 D99 Q100 E101 V102 P103 T104 A105 T106 A107 V108 L109 F110 L111 T112 G113 I114 E115 I116 S117 L118 E119 A120

D121 I122 Y123 R124 D125 G126 Q127 L128 D129 M130 P131 S132 D133 K134 Q135 A136 K137 K138 K139 W140 M141 W142 G143 M144 N145 G146 W147 G148 A149 I150 L151 L152 V153 N154 C155 S156 P157 N158 A159 V160 G161 Q162 P163 D164 E165 Q166 S167 F168 Q169 E170 G171 P172 R173 E174 I175 Q176 N177 L178 S179 Q180

M181 N182 V183 T184 V185 E186 G187 P188 T189 S190 I191 L192 Q193 N194 Y195 Q196 L197 I198 L199 H200 T201 S202 E203 E204 E205 A206 K207 K208 T209 R210 V211 V212 W213 S214 Q215 R216 G217 S218 S219 A220 Y221 E222 L223 V224 V225 G226 P227 N228 K229 P230 V231 Y232 L233 L234 P235 T236 F237 E238 N239 R240

R241 K242 E243 A244 F245 Y246 V247 E248 A249 T250 E251 F252 P253 S254 P255 S256 F257 S258 G259 L260 I261 S262 L263 S264 L265 S266 L267 V268 E269 K270 A271 H272 D273 E274 C275 I276 P277 E278 I279 P280 L281 Y282 K283 D284 T285 V286 M287 F288 R289 V290 A291 P292 Y293 I294 F295 M296 P297 S298 T299 Q300

M301 P302 L303 E304 V305 Y306 L307 C308 R309 E310 L311 Q312 L313 Q314 G315 F316 V317 D318 S319 V320 T321 K322 L323 S324 E325 K326 S327 K328 V329 Q330 V331 V332 K333 V334 Y335 E336 D337 P338 N339 R340 Q341 S342 K343 W344 L345 Q346 D347 E348 M349 A350 F351 C352 Y353 T354 Q355 A356 P357 H358 K359 T360

V361 S362 L363 I364 L365 D366 T367 P368 R369 V370 S371 K372 L373 E374 D375 F376 P377 M378 K379 Y380 T381 L382 T383 P384 G385 S386 G387 Y388 L389 I390 R391 Q392 T393 E394 D395 H396 R397 V398 A399 S400 L401 D402 S403 I404 G405 N406 L407 M408 V409 S410 P411 P412 V413 K414 A415 Q416 G417 K418 D419 Y420

P421 L422 G423 R424 V425 L426 I427 G428 G429 S430 F431 Y432 P433 S434 S435 E436 G437 R438 D439 M440 N441 K442 G443 L444 R445 E446 F447 V448 Y449 A450 Q451 Q452 V453 Q454 A455 P456 V457 E458 L459 F460 S461 D462 W463 L464 M465 T466 G467 H468 M469 D470 Q471 F472 M473 C474 F475 V476 P477 T478 N479 D480

K481 N482 N483 D484 Q485 K486 D487 F488 R489 L490 L491 L492 A493 S494 P495 S496 A497 C498 F499 E500 L501 F502 E503 Q504 K505 Q506 K507 E508 G509 Y510 G511 N512 V513 T514 L515 F516 E517 D518 I519 G520 A521 E522 Q523 L524 L525 S526 N527 G528 R529 E530 S531 K532 T533 I534 S535 Q536 I537 L538 A539 D540

R544 E545 Q546 N547 T548 Y549 S555 L556 N557 L560 L561 E564 L565 G566 L567 E568 D569 K570 D571 I572 I573 L574 I575 P576 Q577 L578 F579 C580 L581 E582 Q583 L584 T585 N586 V587 P588 S589 N590 Q591 Q592 S593 T594 K595 L596 F597 A598 R599 P600 Y601 F602 P603 D604 M605 L606 Q607 I608

I609 V610 L611 G612 K613 N614 L615 G616 I617 P620 F621 G622 P623 K624 I625 N626 G627 T628 C629 C630 L631 E632 E633 K634 V635 C636 G637 L638 L639 E640 P641 L642 G643 L644 K645 C646 T647 F648 I649 D650 D651 F652 D653 C654 Y655 L656 A657 N658 I659 G660 D661 V662 C663 A664 S665 A666 I667 I668 N669

R670 V671 P672 F673 A674 F675 K676 W677 W678 K679 M680 T681 P682

• Molecule 2: Inactive protein-arginine deiminase type-6

Chain L: 87% 99%

M1 S2 F3 Q4 N5 S6 L7 S8 L9 S10 L11 V12 N13 P14 T15 H16 A17 L18 C19 M20 V21 G22 M23 E24 I25 T26 L27 D28 I29 S30 K31 C32 A33 P34 D35 K36 C37 K38 S39 S45 P46 R47 I48 L49 I50 H51 I52 S53 S54 S55 V56 I57 A58 G59 K60 E61 D62 T63 V64

V65 S68 M69 N70 H71 P72 T73 V74 A75 L76 V77 V80 A81 P84 T85 V86 D87 E88 D89 K90 V91 L92 V93 C97 P98 D99 Q100 E101 V102 P103 T104 A105 T106 A107 V108 L109 T112 E115 I116 S117 L118 E119 A120 D121 I122 Y123 R124 D125 G126 Q127 L128 D129 M130 P131

S132 D133 K134 Q135 A136 K137 K138 M141 W142 G143 M144 G148 A149 I150 L151 L152 V153 N154 C155 S156 P157 N158 A159 V160 G161 Q162 P163 D164 E165 Q166 S167 F168 Q169 E170 G171 P172 R173 E174 I175 Q176 N177 L178 S179 Q180 M181 T184 V185 E186 G187 S190 I191 L192 Q193 N194 L199

H200 T201 S202 K208 T209 W213 S214 Q215 R216 G217 S218 S219 A220 Y221 P227 N228 K229 P230 V231 P235 T236 F237 E238 N239 R240 E243 A244 F245 Y246 V247 E248 A249 T250 E251 F252 P253 S254 P255 S256 F257 S258 G259 L260 I261 S262 L263 S264 L265 S266 L267 V268 E269 K270 A271 H272

D273 E274 C275 I276 P277 E278 I279 P280 L281 Y282 K283 D284 T285 V286 M287 V290 A291 P292 Y293 I294 F295 M296 P297 S298 T299 Q300 M301 P302 L303 E304 V305 Y306 L307 C308 R309 E310 L311 Q312 L313 Q314 G315 F316 V317 D318 S319 V320 T321 K322 L323 S324 E325 K326 S327 K328 V329 Q330 V331 V332 K333

V334 Y335 E336 D337 P338 N339 R340 Q341 S342 K343 W344 L345 Q346 D347 E348 M349 A350 F351 C352 Y353 T354 Q355 A356 P357 H358 K359 T360 V361 S362 L363 D366 T367 P368 R369 V370 S371 K372 L373 E374 D375 F376 P377 M378 K379 Y380 T381 L382 T383 P384 G385 S386 G387 Y388 L389 I390 R391 Q392 T393 E394

D395 H396 R397 V398 A399 S400 L401 D402 S403 I404 G405 N406 L407 M408 V409 S410 P411 P412 V413 K414 A415 Q416 G417 K418 D419 Y420 P421 L422 G423 R424 V425 L426 I427 G428 G429 S430 F431 Y432 P433 S434 S435 E436 G437 R438 D439 M440 N441 K442 G443 L444 R445 E446 F447 V448 Y449 A450 Q451 Q452 V453 Q454

A455 P456 V457 E458 L459 F460 S461 D462 W463 L464 M465 T466 G467 H468 M469 D470 Q471 F472 M473 C474 F475 V476 P477 T478 N479 D480 K481 N482 N483 D484 Q485 K486 D487 F488 R489 L490 L491 L492 A493 S494 P495 S496 A497 C498 F499 E500 L501 F502 E503 Q504 K505 Q506 K507 E508 G509 Y510 G511 N512 V513 T514

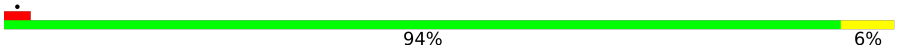
L515 F516 E517 D518 I519 G520 A521 E522 Q523 L524 L525 S526 N527 G528 R529 E530 S531 K532 T533 I534 S535 Q536 I537 L538 A539 D540 K541 S542 F543 R544 E545 Q546 N547 T548 Y549 V550 E551 K552 C553 I554 S555 L556 N557 R558 T559 L560 L561 K562 T563 E564 L565 G566 L567 E568 D569 K570 D571 I572 I573 L574

I575 P576 Q577 L578 F579 C580 L581 E582 Q583 L584 T585 N586 V587 P588 S589 N590 Q591 Q592 S593 T594 K595 L596 F597 A598 Y601 F602 P603 D604 M605 L606 Q607 I608 I609 V610 L611 G612 K613 N614 L615 G616 I617 P618 K619 P620 F621 G622 P623 K624 I625 N626 G627 T628 C629 C630 L631 E632 E633 K634 V635

C636 G637 L638 L639 E640 P641 L642 G643 L644 K645 C646 T647 F648 I649 D650 D651 F652 D653 C654 Y655 L656 A657 N658 I659 G660 D661 V662 C663 A664 S665 A666 I667 I668 N669 R670 V671 P672 F673 A674 F675 K676 W677 M680 T681 P682

- Molecule 2: Inactive protein-arginine deiminase type-6

Chain m:

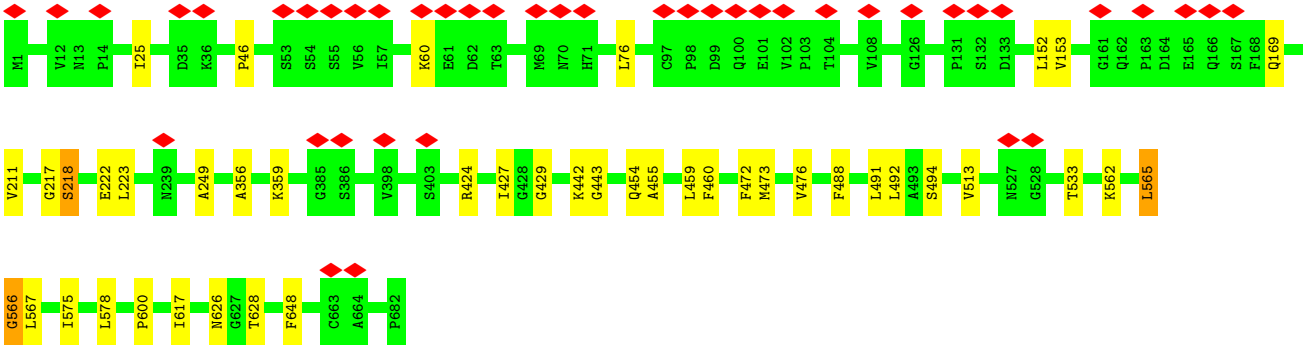


M1 M23 E24 I25 S39 S45 P46 I50 S53 S54 S55 V56 I57 A58 G59 K60 E61 D62 T63 V64 S68 L76 V77 R78 E101 T104 A105 E115 A120 M130 V160 G161 Q166 Q169 V185 Y212 Q215 R216 G217 S218 E222

L223 I261 V268 P280 F288 C308 Q312 L313 V334 Y353 S362 G385 S386 D402 G428 G429 F460 F472 L492 A493 S494 I575 L581 L584 F597 K624 I625 A664 P682

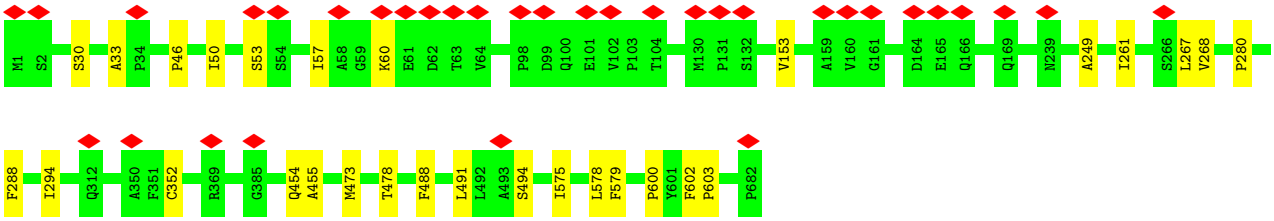
• Molecule 2: Inactive protein-arginine deiminase type-6

Chain s: 6% 94% 6%



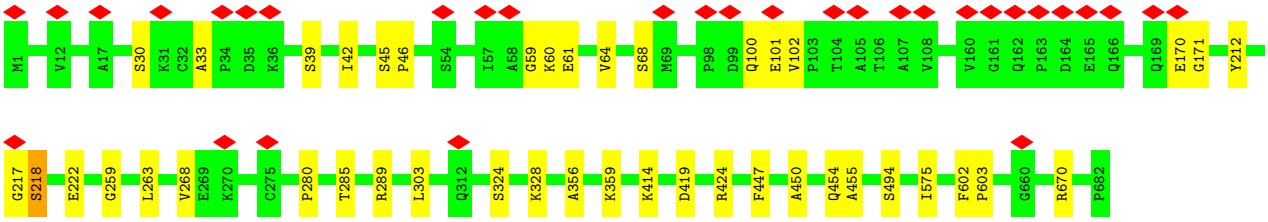
• Molecule 2: Inactive protein-arginine deiminase type-6

Chain t: 5% 96%



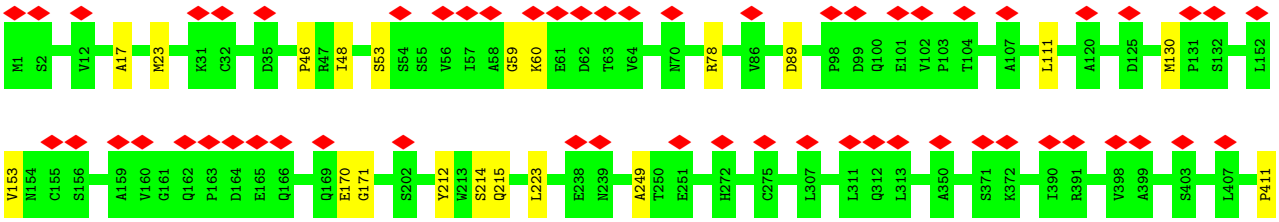
• Molecule 2: Inactive protein-arginine deiminase type-6

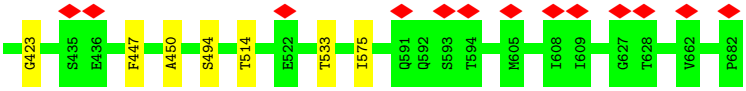
Chain u: 5% 94% 6%



• Molecule 2: Inactive protein-arginine deiminase type-6

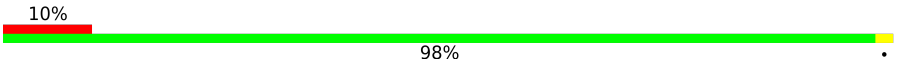
Chain v: 10% 96%

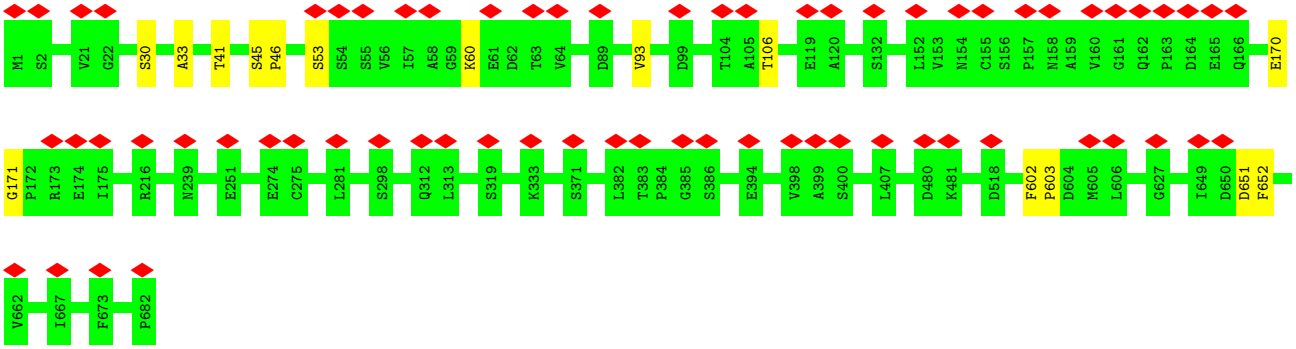




• Molecule 2: Inactive protein-arginine deiminase type-6

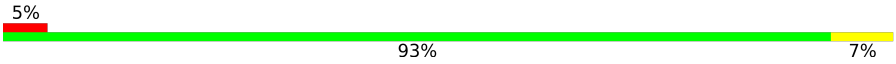
Chain w:

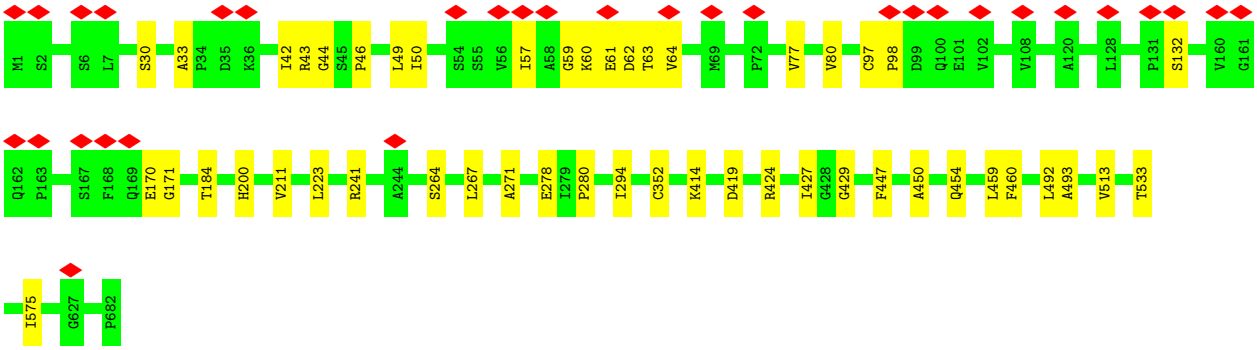




• Molecule 2: Inactive protein-arginine deiminase type-6

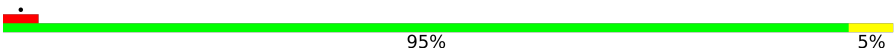
Chain x:

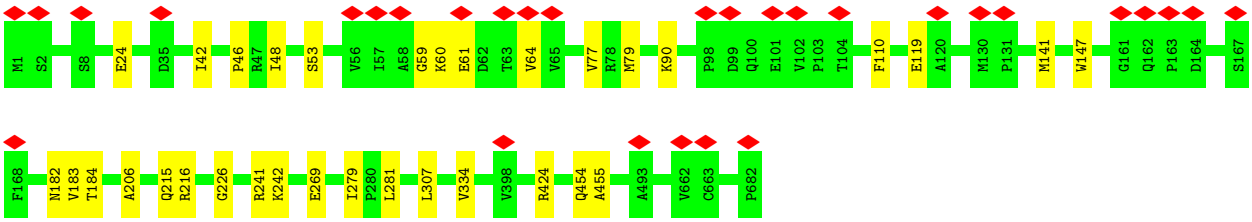




• Molecule 2: Inactive protein-arginine deiminase type-6

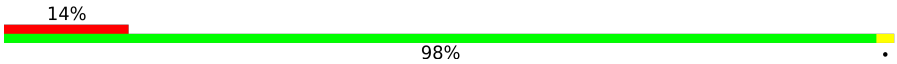
Chain y:

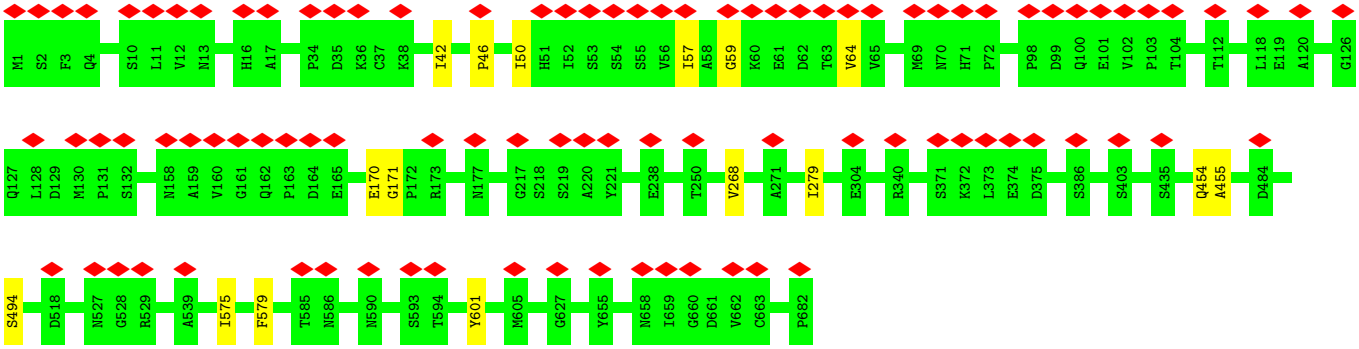




• Molecule 2: Inactive protein-arginine deiminase type-6

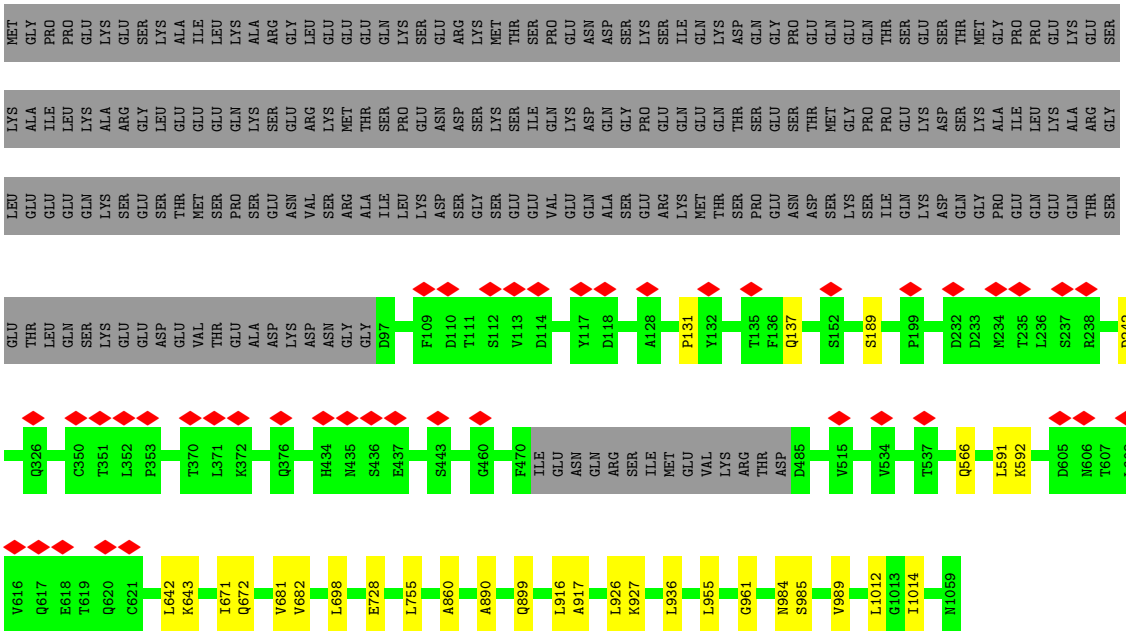
Chain z:





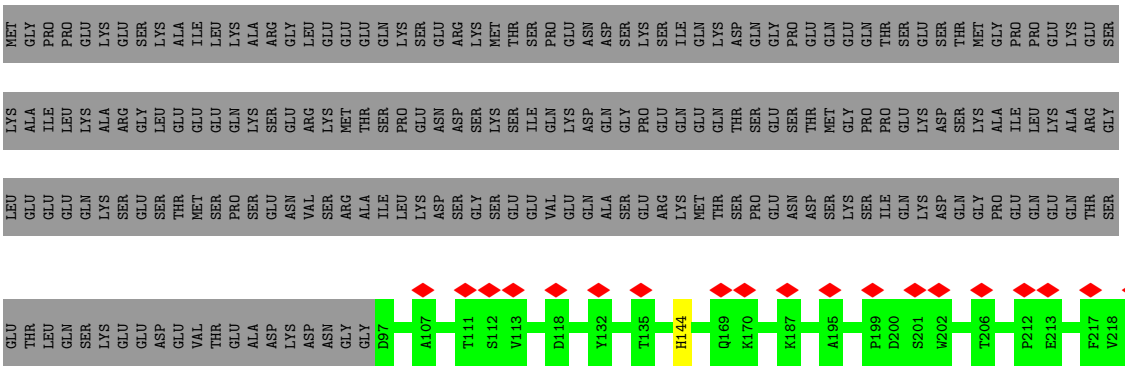
• Molecule 3: NACHT, LRR and PYD domains-containing protein 5

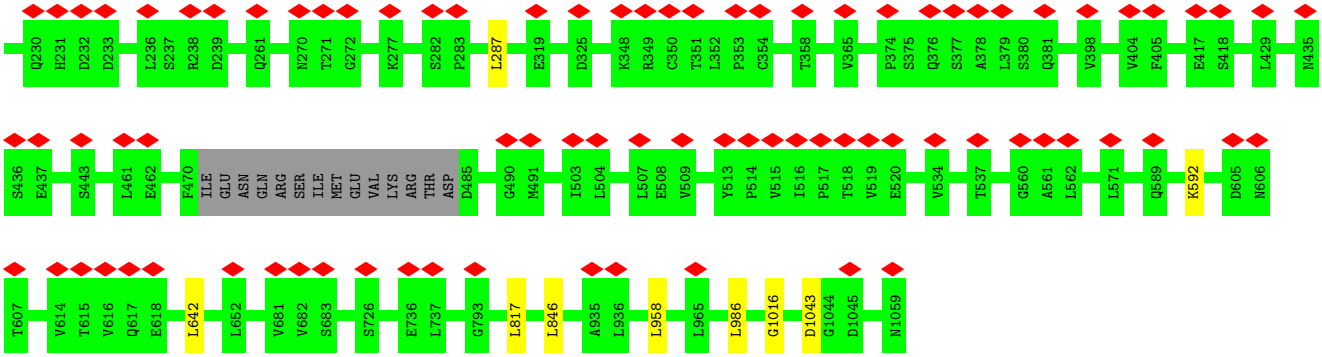
Chain 4:



• Molecule 3: NACHT, LRR and PYD domains-containing protein 5

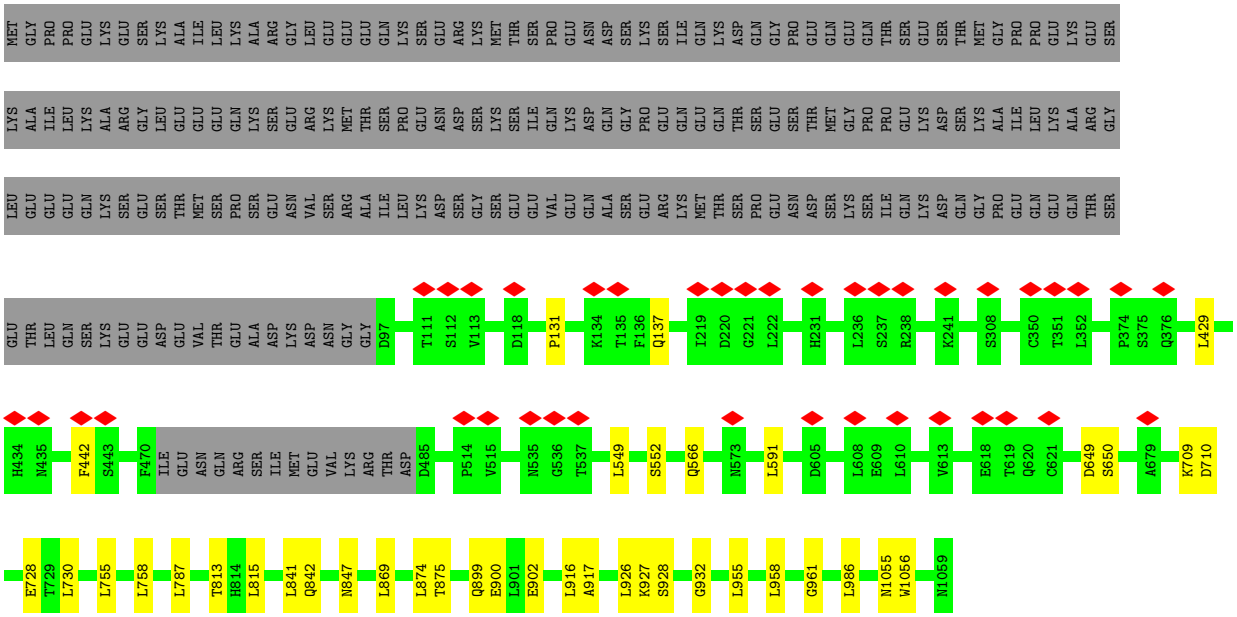
Chain 7:





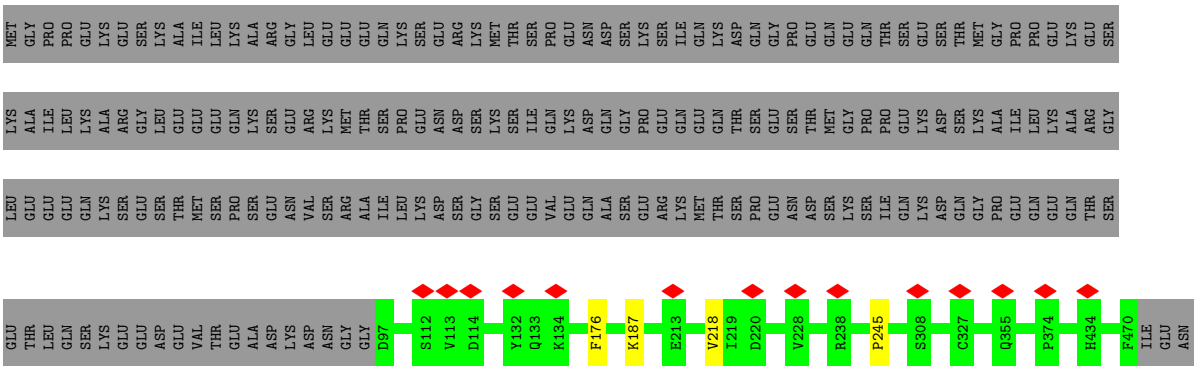
- Molecule 3: NACHT, LRR and PYD domains-containing protein 5

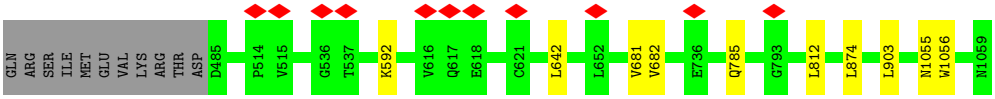
Chain M:



- Molecule 3: NACHT, LRR and PYD domains-containing protein 5

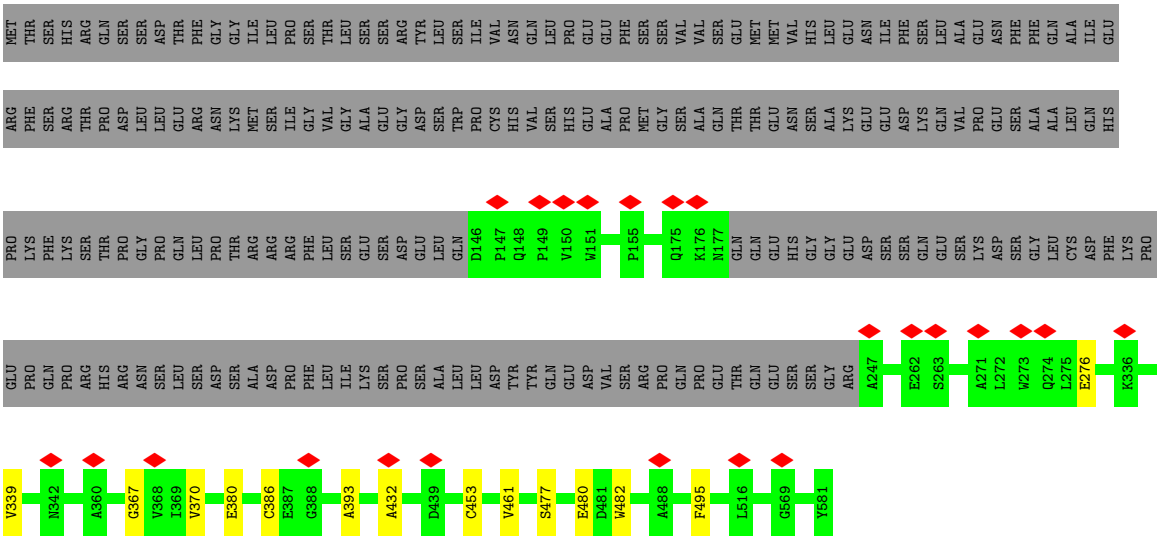
Chain P:





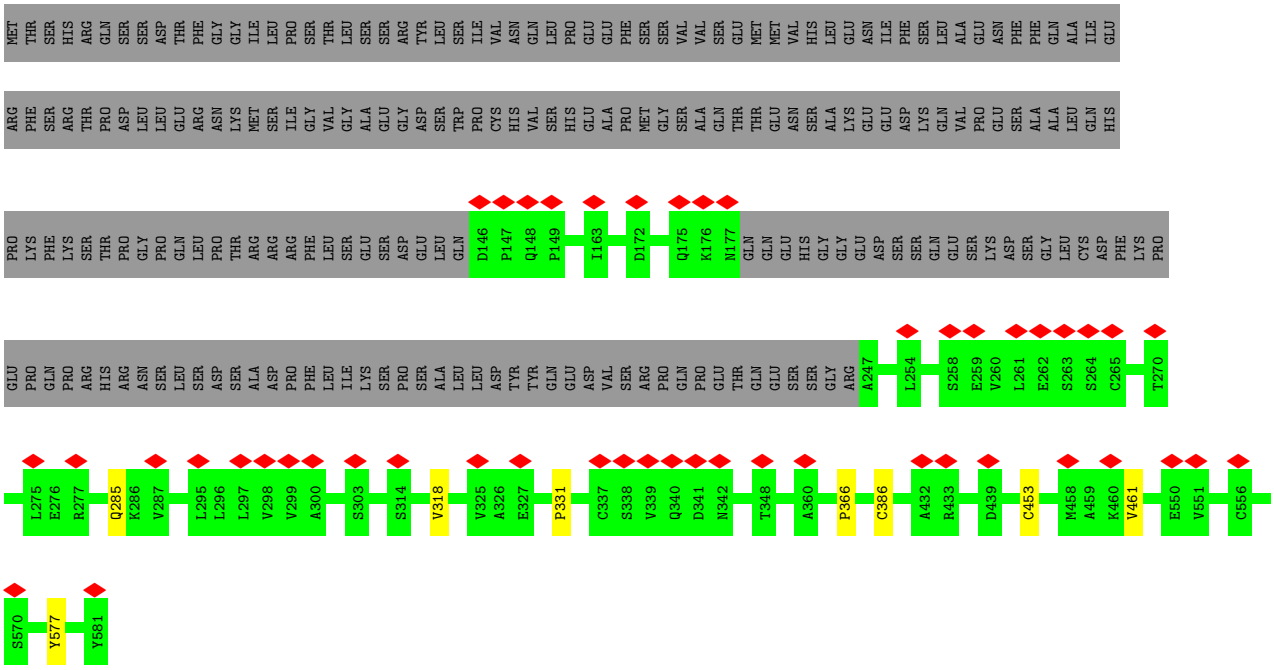
• Molecule 4: Transducin-like enhancer protein 6

Chain 5:



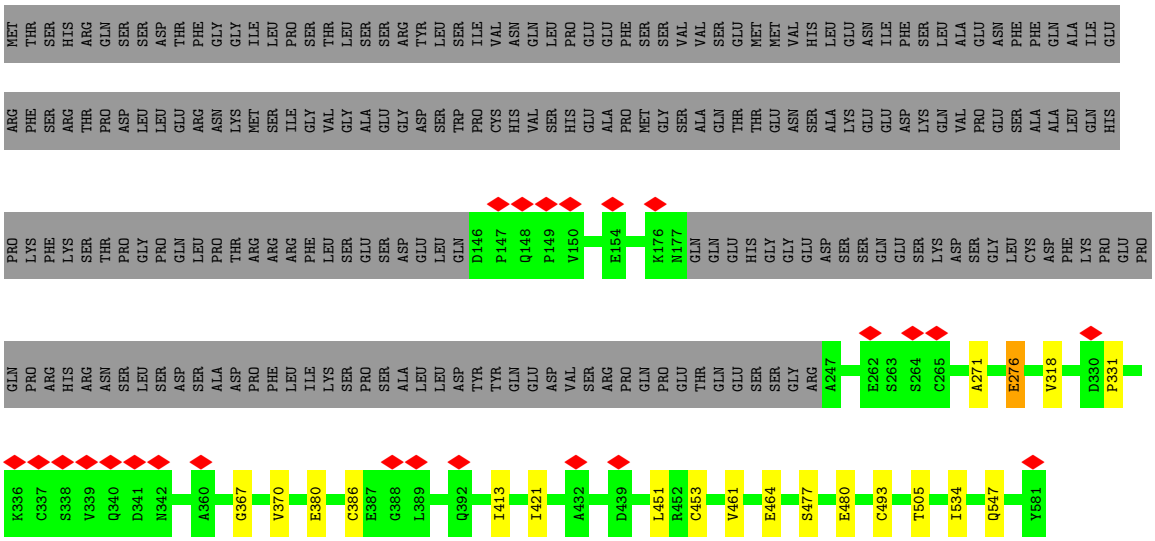
• Molecule 4: Transducin-like enhancer protein 6

Chain 8:



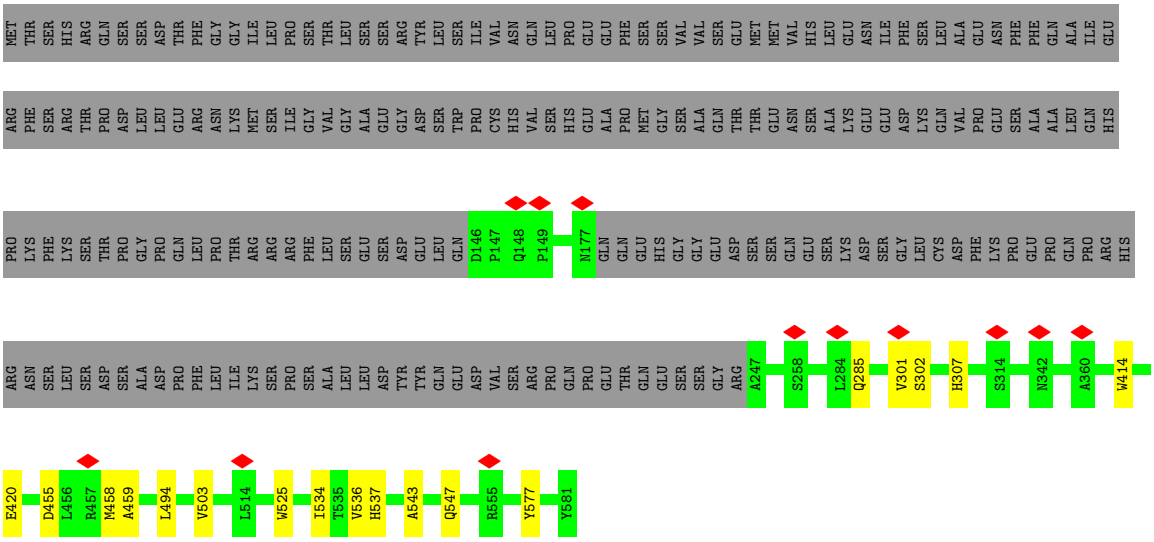
• Molecule 4: Transducin-like enhancer protein 6

Chain N:



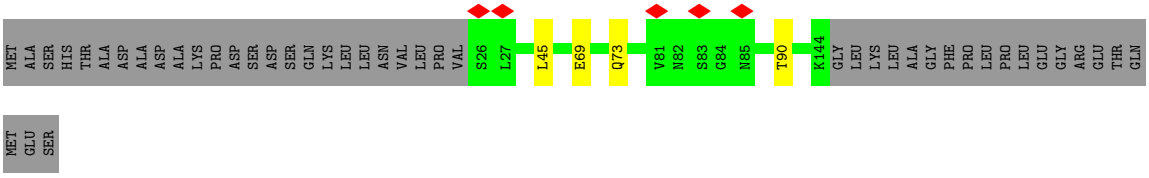
• Molecule 4: Transducin-like enhancer protein 6

Chain Q:



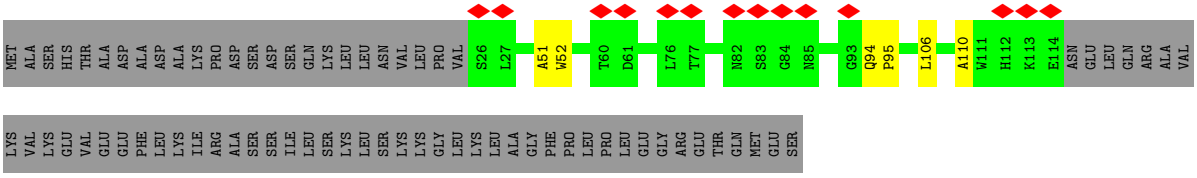
• Molecule 5: Oocyte-expressed protein homolog

Chain 6:



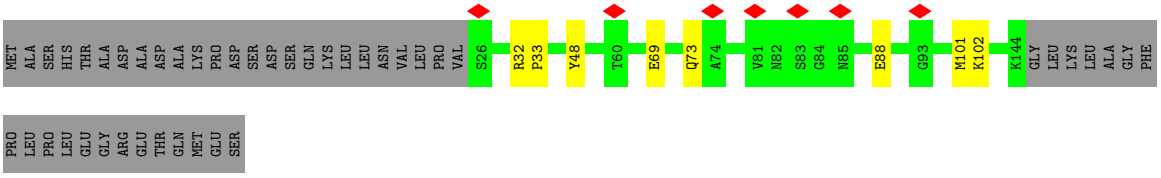
• Molecule 5: Oocyte-expressed protein homolog

Chain 9:



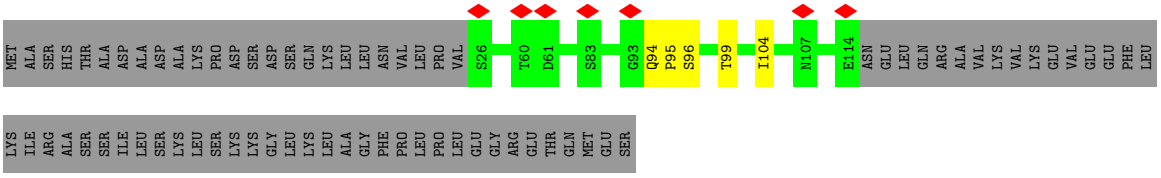
• Molecule 5: Oocyte-expressed protein homolog

Chain O:



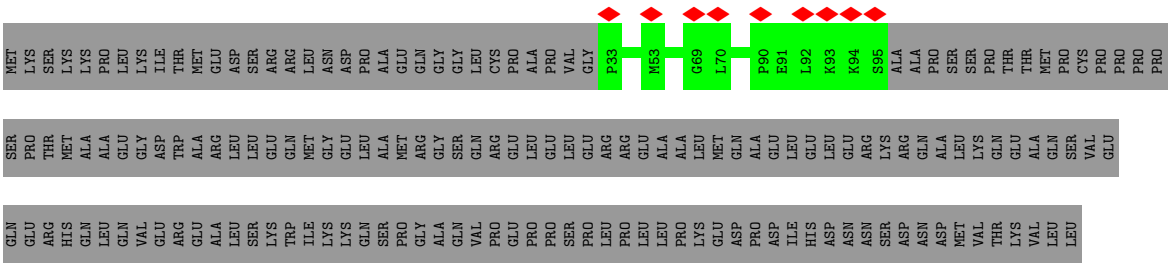
• Molecule 5: Oocyte-expressed protein homolog

Chain R:



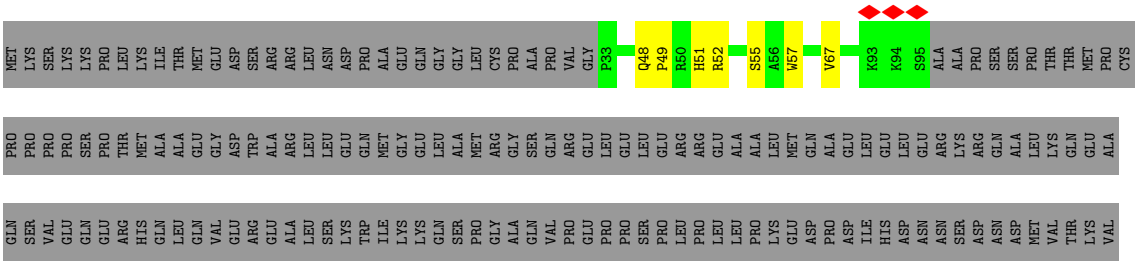
• Molecule 6: Zinc finger BED domain-containing protein 3

Chain AA:



• Molecule 6: Zinc finger BED domain-containing protein 3

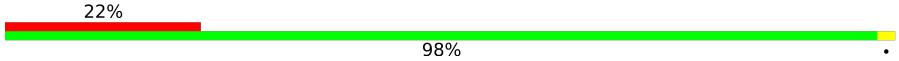
Chain T:



LEU
LEU

• Molecule 7: NLR family, pyrin domain containing 4F

Chain AE:



M1 A2 S3 F4 I5 S6 D7 F8 G9 L38 K39 Q40 K60 A86 A89 I90 VAL GLY N93 T106 H107 D108 C109 P110 K111 K122 I126 Q127 N128 D129 Y130 F133 E134 N135 L136 L137 I138 S139 K140 G141 T142 E143 R144 K145 G153 M154 S181 Q193 L194

K195 L199 A200 R205 S211 A212 P213 I214 L218 W236 D237 S243 E244 L245 C246 S276 E280 M285 E286 D287 A297 T298 A299 D315 E328 L332 G356 G357 D358 Q381 G404 D408 M435 L503 G513 G517 S521 K522

L528 C531 T534 L541 E558 D559 E560 A561 F562 L563 K578 A586 A587 Y588 S594 S602 T603 G610 S627 D634 I635 Q636 E637 L638 F645 N646 E647 P648 A649 K658 Y659 P660 S661 N665 V668 A669 N670 G675 D676 M677 H678 V679 L680

F681 N686 Q690 Y691 L692 S695 C696 S697 F698 L699 S700 H701 N702 E703 V704 L707 C708 D709 A714 E715 I718 E719 K720 L721 M722 I723 A724 S729 P730 D731 D732 C733 K734 I735 F736 G737 S738 K744 S745 L746 K747 V748 L749 N750 L751 N755 L756 N757 Q758 G759 I760

S761 S762 L763 C764 K765 P770 H771 C772 T773 L774 V778 S785 E786 Q787 Q798 T801 L802 S803 E815 G816 L817 R822 P827 Y828 C829 E832 T842 E843 R844 G845 C846 Q847 D848 L849 A850 E851 N855 L859 Y866 K870 D871 T872 G873 V874 C878

C886 H887 L888 K889 D890 T899 D900 A901 S902 N903 E914 T915 L921 N924 A925 F926 E927 V928 V932 F933 F934 F937

• Molecule 7: NLR family, pyrin domain containing 4F

Chain AF:

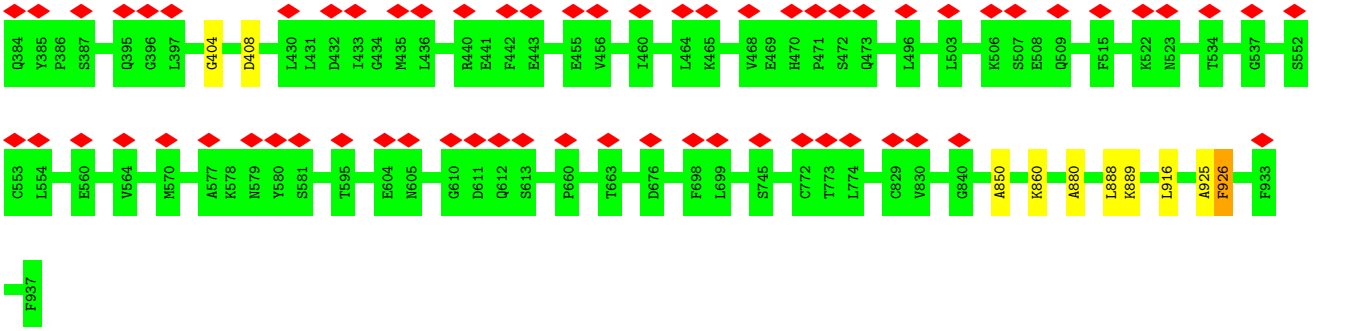
MET ALA SER PHE ILE SER ASP PHE GLY LEU ILE TRP TYR LEU ARG GLU LEU ASN LYS LYS GLU PHE MET LYS PHE LYS ASP PHE LEU ILE GLN GLU ILE LEU GLU LEU LYS LEU LYS GLN VAL SER SER THR LYS VAL LYS LYS ALA SER ARG GLU ASP LEU ALA ASN LEU LEU LEU LYS

CYS GLY GLU ASN GLN ALA TRP ASP MET THR PHE ARG ILE LEU GLN LYS ILE ASN ARG LYS ASP LEU THR GLU ARG ALA THR GLY ALA ILE VAL GLY N93 P94 N95 L96 H100 L101 K102 K103 K104 L105 T106 H107 D108 C109 P110 K111 V115 D119 F125 I126 Q127 N128 D129 Y130

D131 A132 F133 E134 N135 L136 L137 I138 S139 K140 G141 T142 E143 R144 K145 M148 V149 F150 G153 M154 A155 G156 V157 K164 N165 W170 S171 K172 G173 L174 Q177 N178 K179 Y182 A183 Q189 D190 V191 K192 Q193 L194 K195 T196 A197 S198 L199 A200 E201 L202 I203 S204 R205 E206

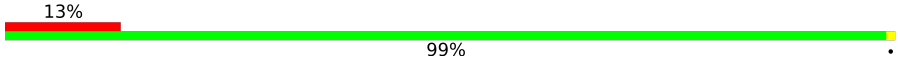
W207 P208 S209 P210 S211 A212 P213 I214 E215 E216 I217 L218 S219 Q220 L224 L225 D229 S230 G233 M234 E235 W236 D237 L238 T239 K240 Q241 E242 S243 E244 L245 C246 D247 D248 E251 K252 Q253 P254 V255 S256 T257 L258 L259 M267 S272 L273 L274 L275 P279 E280 K284

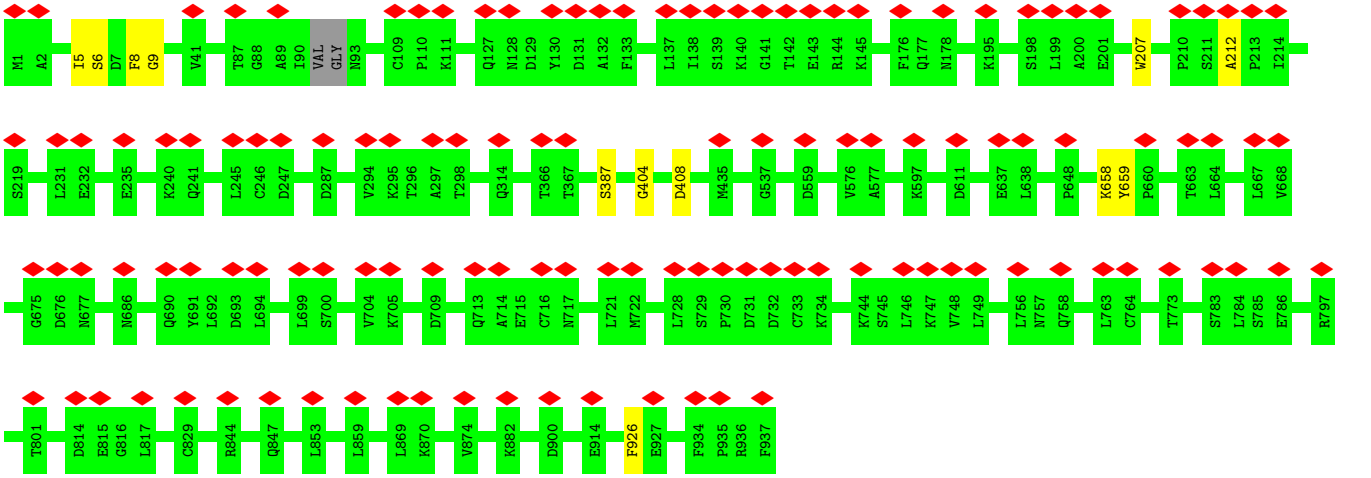
D293 V294 K295 T296 A297 T298 A299 E302 R303 S304 Y308 D315 R316 K317 R318 A322 F323 S324 L325 V326 R327 E328 P339 L340 L341 C342 V345 A346 T347 C348 E351 E352 I353 E354 K355 G356 G357 D358 P359 L362 C363 R364 R365 T366 T367 T371 I379 S382 A383



- Molecule 7: NLR family, pyrin domain containing 4F

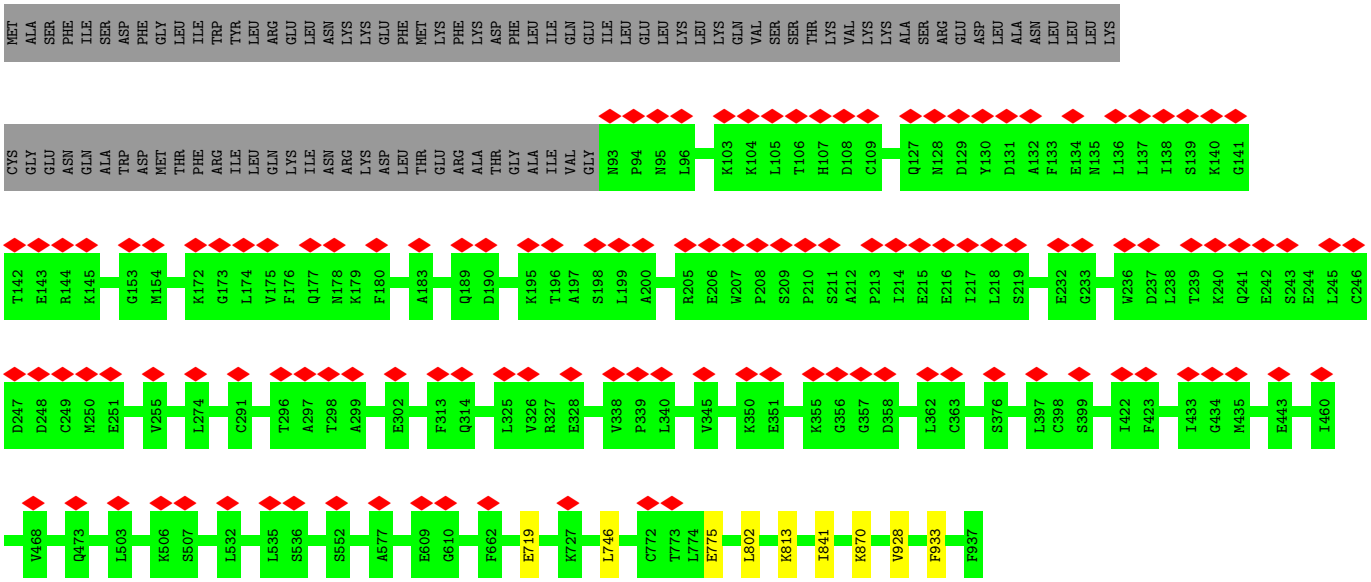
Chain X:





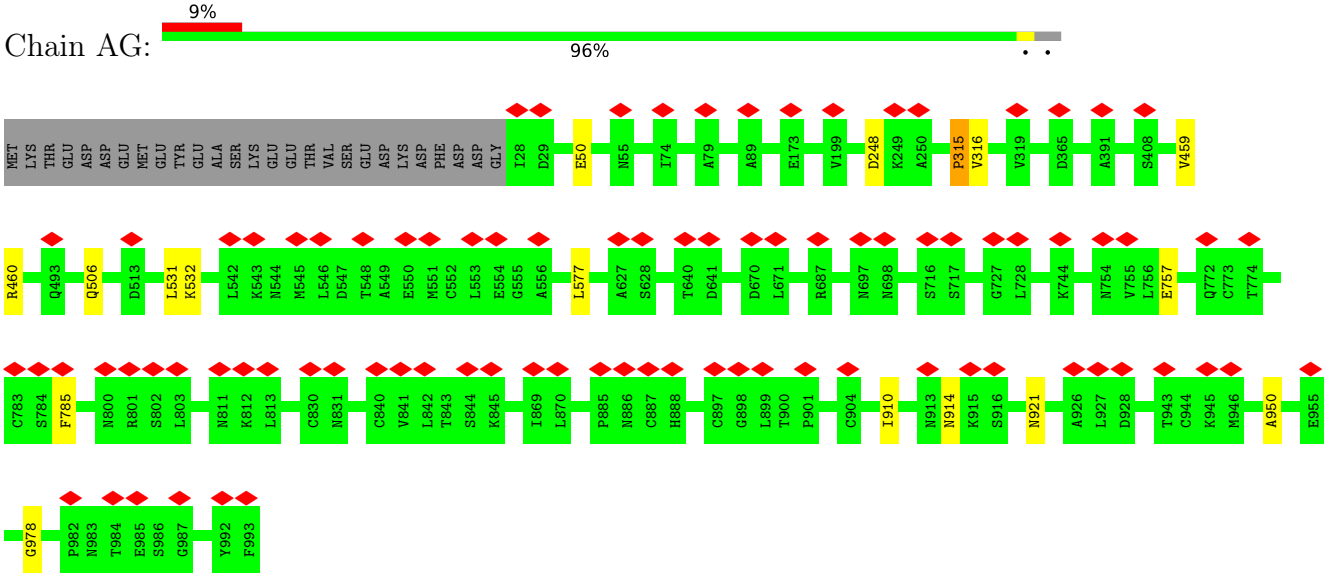
- Molecule 7: NLR family, pyrin domain containing 4F

Chain Y:



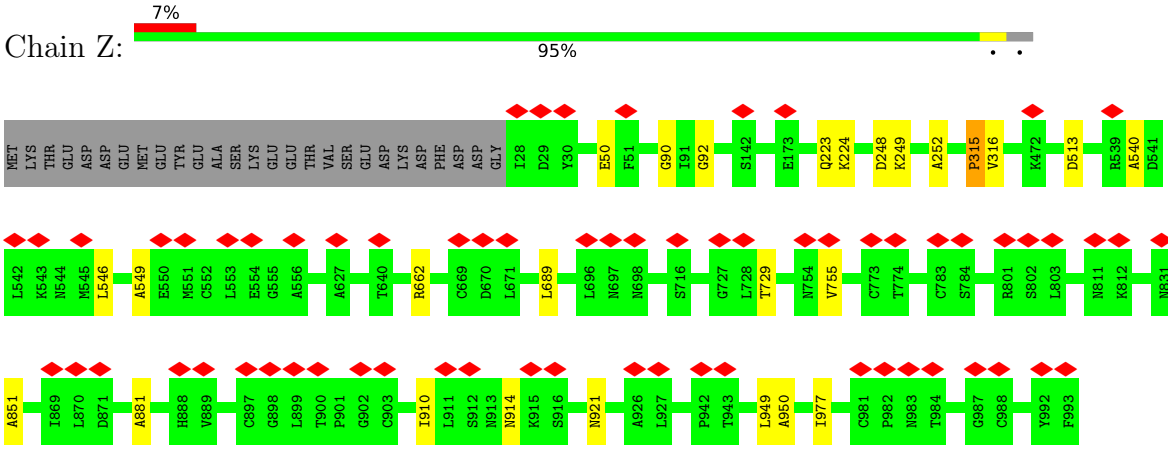
• Molecule 8: NACHT, LRR and PYD domains-containing protein 14

Chain AG:



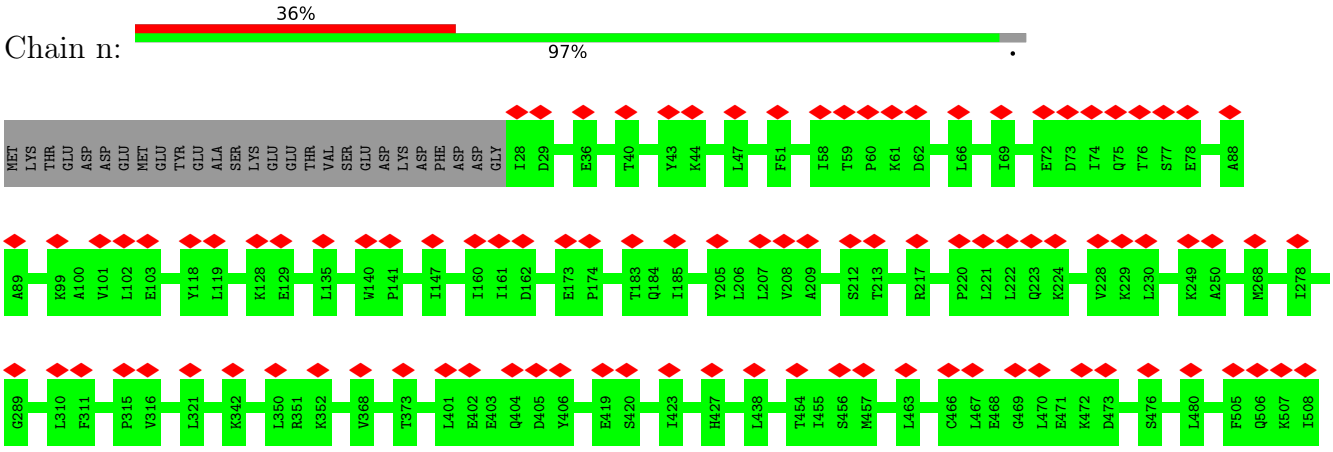
• Molecule 8: NACHT, LRR and PYD domains-containing protein 14

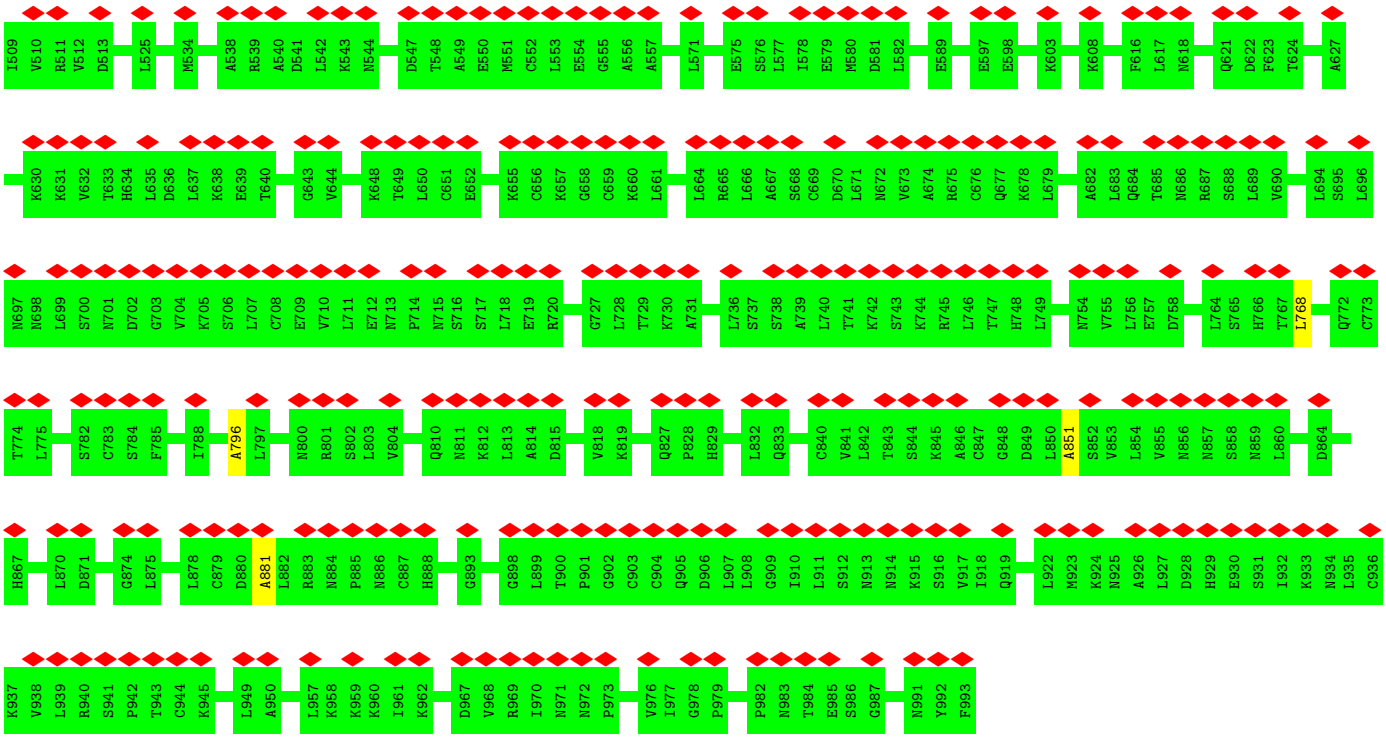
Chain Z:



• Molecule 8: NACHT, LRR and PYD domains-containing protein 14

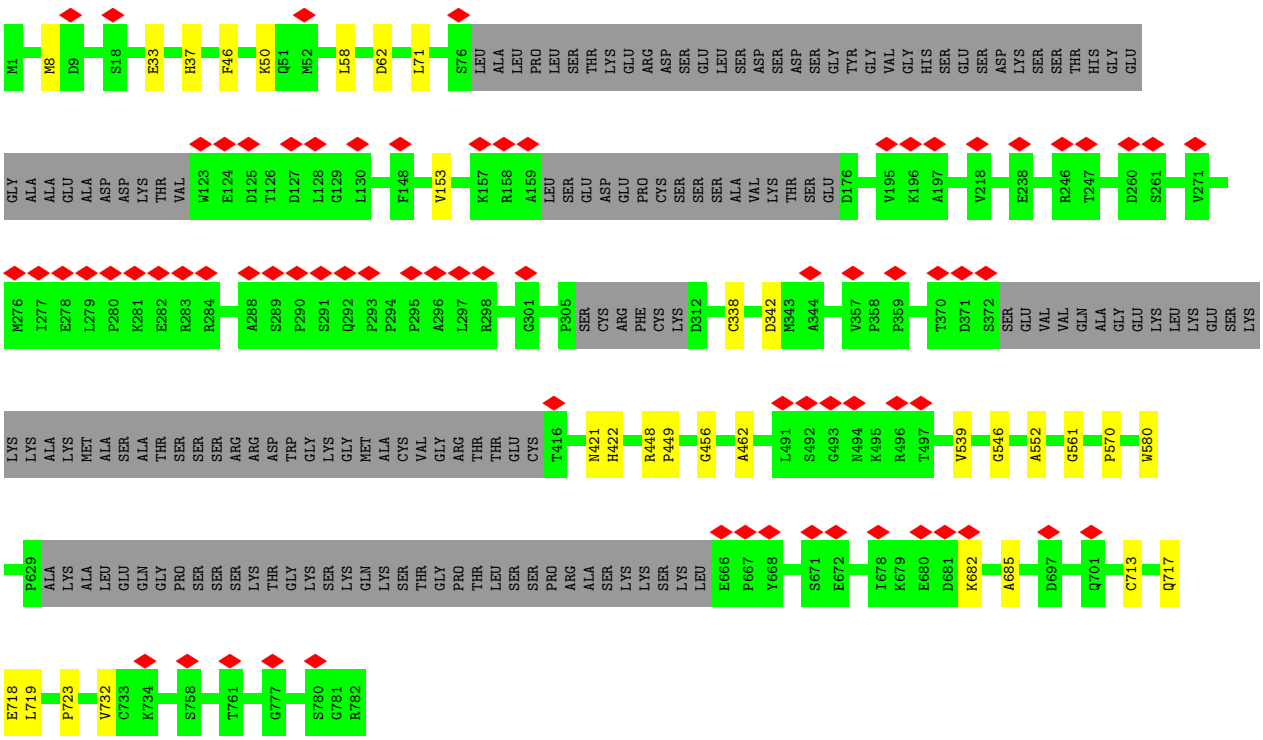
Chain n:





- Molecule 9: E3 ubiquitin-protein ligase UHRF1

Chain AH: 9% 77% 19%



- Molecule 9: E3 ubiquitin-protein ligase UHRF1

Chain a: 9% 78% • 19%

M1 M8 L71 S76 LEU ALA LEU PRO LEU SER THR LYS GLU ARG ASP SER GLU LEU SER ASP SER ASP SER GLY TYR GLY VAL GLY HIS SER GLU SER ASP LYS SER SER THR HIS GLY GLU GLY ALA ALA GLU ALA ASP ASP LYS THR VAL W123 E124 D125 T126 D127 R140

D141 N142 I143 F144 G145 A146 R158 A159 LEU SER GLU ASP GLU PRO CYS SER SER SER ALA VAL LYS THR SER GLU D176 D177 I178 M179 Y180 H181 V192 D193 I194 V195 K196 A197 R205 L213 E214 Q217 V218 R246 T247 I255 V271 M276 I277 E278 L279 P280 K281

E282 R283 R284 S289 P290 S291 Q292 P293 P294 P295 A296 L297 R298 N299 T300 G301 G304 P305 SER CYS ARG PHE CYS LYS D312 S372 SER GLU VAL VAL GLN ALA GLY GLU LYS LEU LYS GLU SER LYS LYS LYS ALA LYS MET ALA SER ALA THR SER SER SER ARG ARG ASP TRP GLY

LYS GLY MET ALA CYS VAL GLY ARG THR THR GLU CYS T416 G453 G456 A462 Y463 S464 L465 G469 L491 S492 G493 N494 K495 R496 T507 N508 R538 V539 G561 T595 R596 P629 ALA LYS ALA LEU GLU GLN GLY PRO SER SER SER LYS THR GLY LYS SER

LYS GLN LYS SER THR GLY PRO THR LEU SER SER PRO ARG ALA SER LYS LYS SER LYS LEU E666 E672 I678 K679 E680 P699 Q712 L719 P723 D756 H757 S758 S759 P760 T761 R762 V763 S780 G781 R782

• Molecule 9: E3 ubiquitin-protein ligase UHRF1

Chain o: 19% 79% • 19%

M1 D9 G10 K11 H14 N17 S18 E27 L28 K31 I32 E33 E34 V35 L45 Y61 R64 L65 V73 R74 Q75 S76 LEU ALA LEU PRO LEU SER THR LYS GLU ARG ASP SER GLU LEU SER ASP SER ASP SER GLY TYR GLY VAL GLY HIS SER GLU SER ASP

LYS SER SER THR HIS GLY GLU GLY ALA ALA GLU ALA ASP ASP LYS THR VAL W123 E124 D125 T126 D127 L128 G129 L130 Y131 K132 N142 I143 F144 E149 V153 Q154 V155 Q156 K157 R158 A159 LEU SER GLU ASP GLU PRO CYS SER SER SER ALA VAL LYS THR SER GLU D176 D177 I178

K183 Y184 D185 D186 Y187 P188 E189 H190 D193 I194 V195 K196 A197 K198 N199 V200 A204 R205 P209 W210 E211 N212 L213 E214 V215 G216 V219 M220 A221 N224 V225 D226 Y227 P228 R229 K230 R231 G232 F233 W234 Y235 D236 V237 E238 I239 C240 R241 T245 R246 T247 A248 R249 E250

N254 I255 R256 L257 D260 S261 Q262 L263 N264 N265 C266 R267 D272 E278 L279 P280 K281 E282 R283 R284 P285 L286 I287 A288 S289 P290 S291 Q292 P293 P294 P295 A296 L297 T300 G301 K302 P305 SER CYS ARG PHE CYS LYS D312 G318 A322 E333 T355 P359

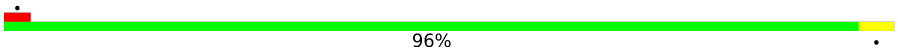
E360 P361 E362 T370 D371 S372 SER GLU VAL VAL GLN ALA GLY GLU LYS LEU LYS GLU SER LYS LYS LYS ALA LYS MET ALA SER ALA THR SER SER SER ARG ARG ASP TRP GLY LYS GLY MET ALA CYS VAL GLY ARG THR THR GLU CYS T416 S492 G493 N494 K495 R496 T497 T507

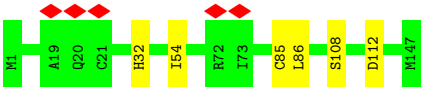
N508 I521 G525 V537 I562 W569 K574 R628 P629 ALA LYS ALA LEU GLU GLN GLY PRO SER SER SER LYS THR GLY LYS SER LYS GLN LYS SER THR GLY PRO THR LEU SER SER SER PRO ARG ALA SER LYS LYS SER LYS LEU E666 P667 Y668 Q673 Q674 K679

E680 K686 L692 T693 S694 L695 Q696 D697 A710 P760 P776 S780 G781 R782

• Molecule 10: Ubiquitin-conjugating enzyme E2 D3

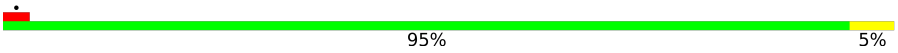
Chain AI:

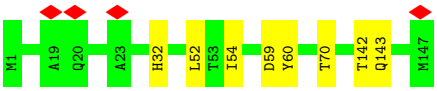




• Molecule 10: Ubiquitin-conjugating enzyme E2 D3

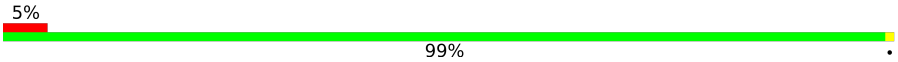
Chain b:

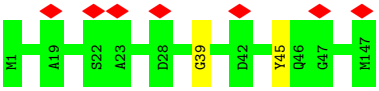




• Molecule 10: Ubiquitin-conjugating enzyme E2 D3

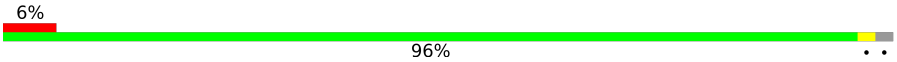
Chain p:

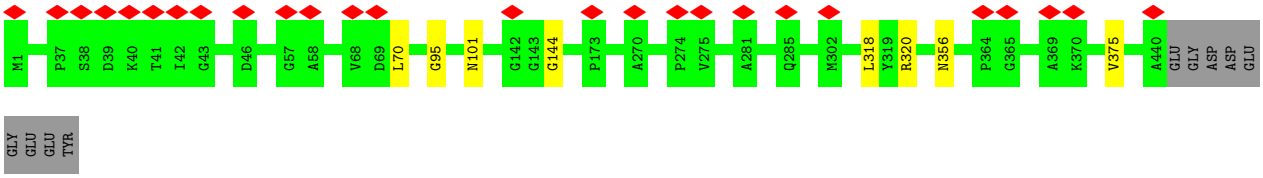




• Molecule 11: Tubulin alpha-1C chain

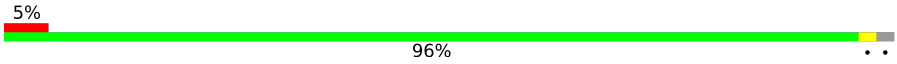
Chain AJ:

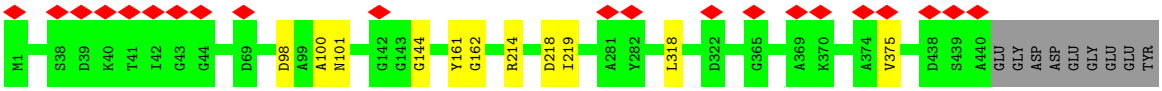




• Molecule 11: Tubulin alpha-1C chain

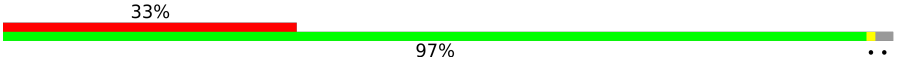
Chain c:

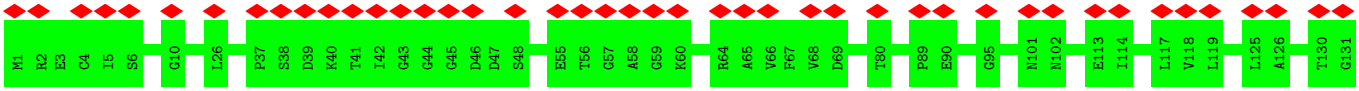


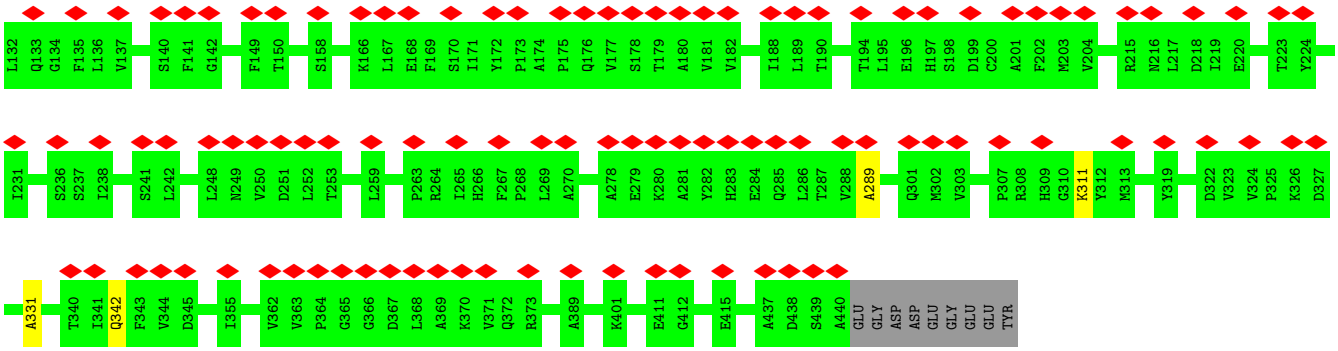


• Molecule 11: Tubulin alpha-1C chain

Chain q:

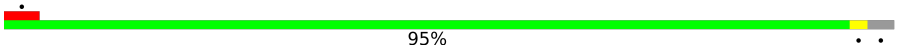


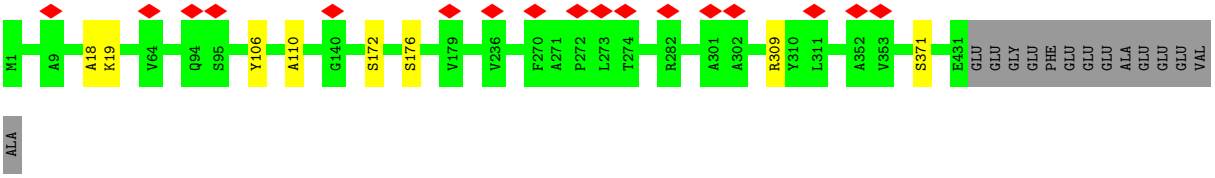




- Molecule 12: Tubulin beta-4B chain

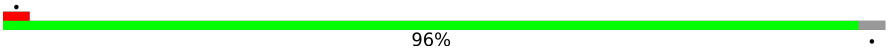
Chain AK:

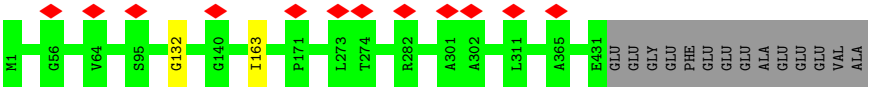




- Molecule 12: Tubulin beta-4B chain

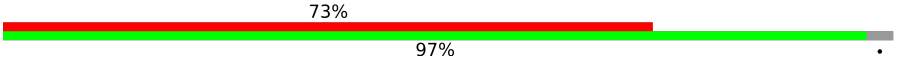
Chain d:

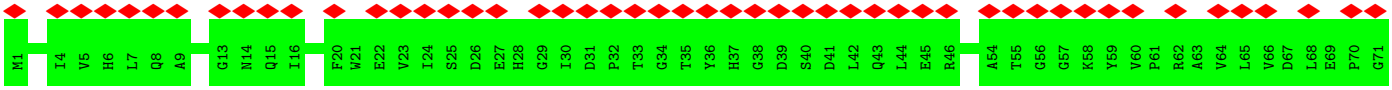


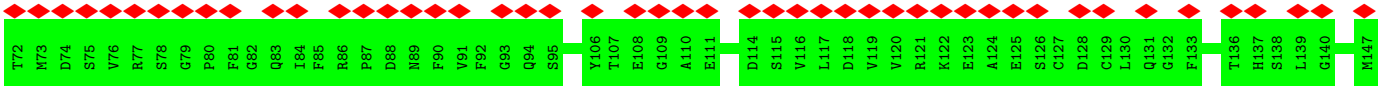


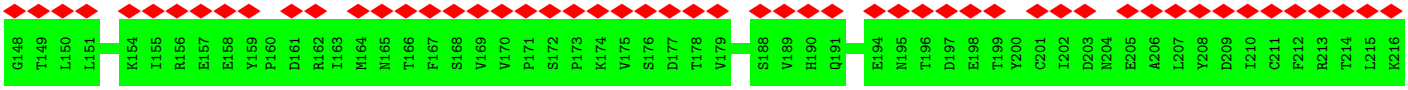
- Molecule 12: Tubulin beta-4B chain

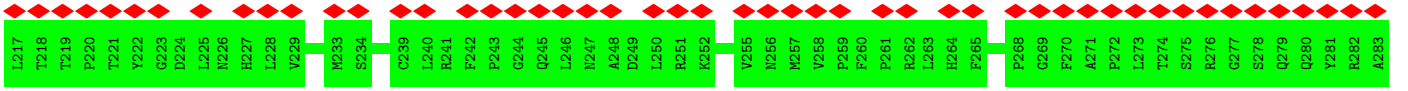
Chain r:

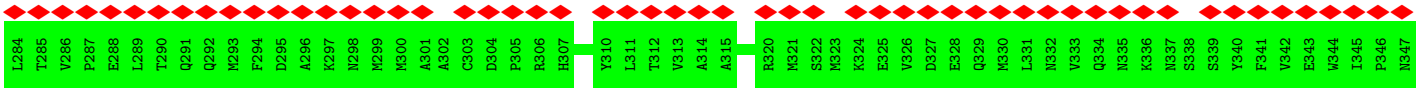


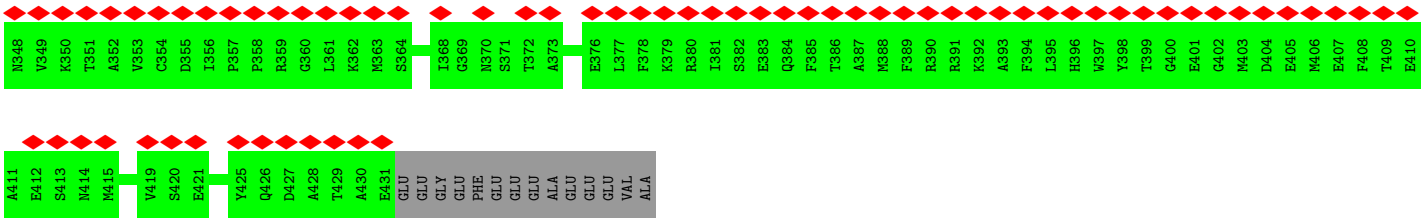






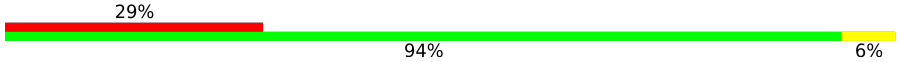


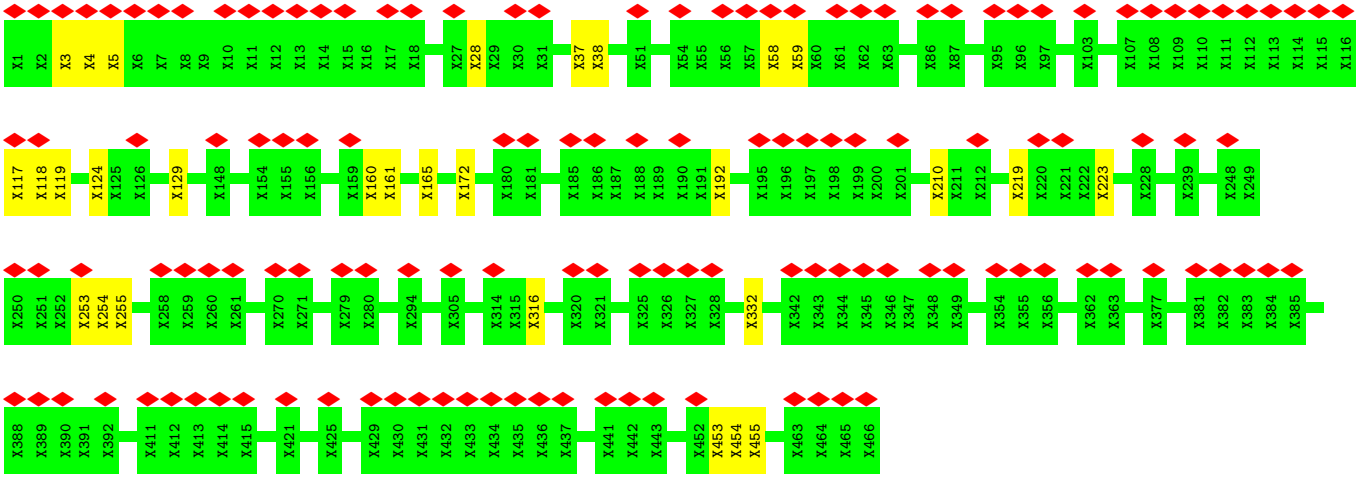




• Molecule 13: F-box/WD repeat-containing protein

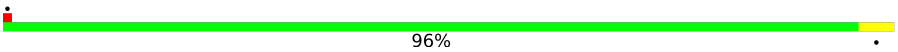
Chain AL:

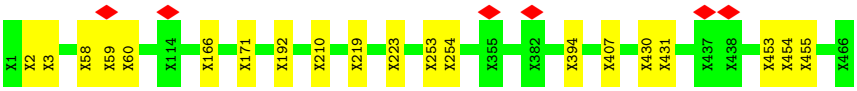




• Molecule 13: F-box/WD repeat-containing protein

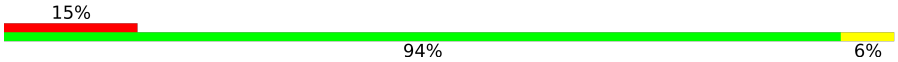
Chain AN:

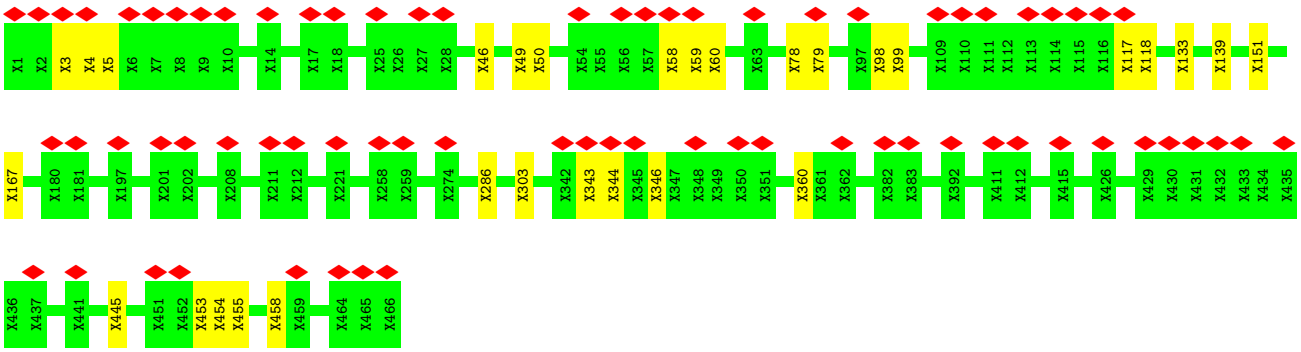




• Molecule 13: F-box/WD repeat-containing protein

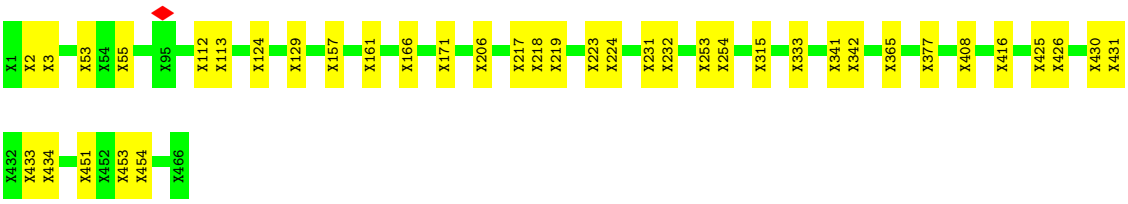
Chain e:





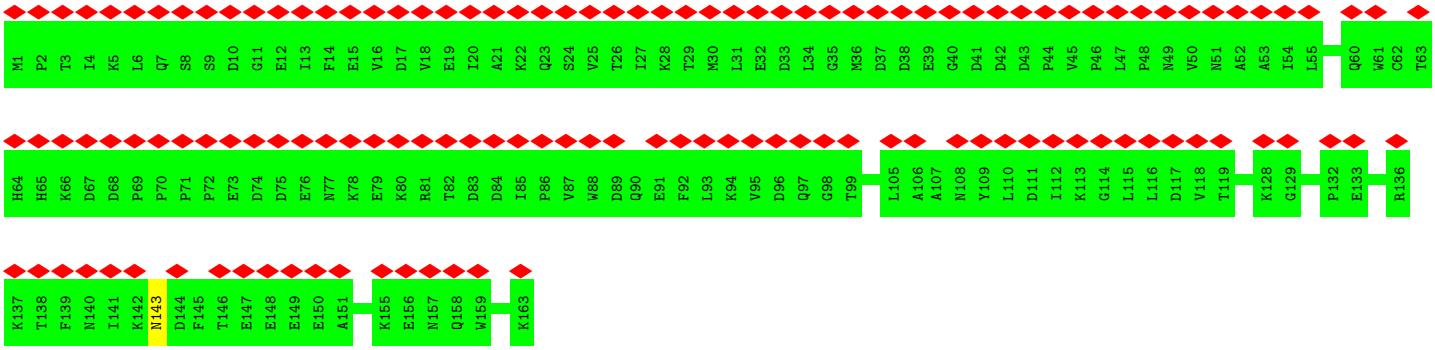
• Molecule 13: F-box/WD repeat-containing protein

Chain g: 92% 8%



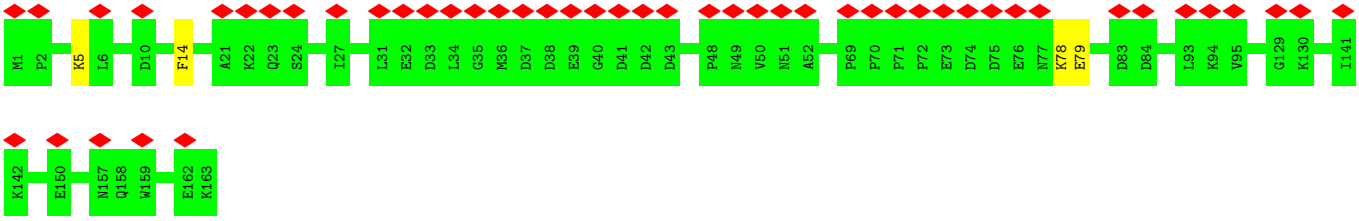
- Molecule 14: S-phase kinase-associated protein 1

Chain AM: 80% 99%



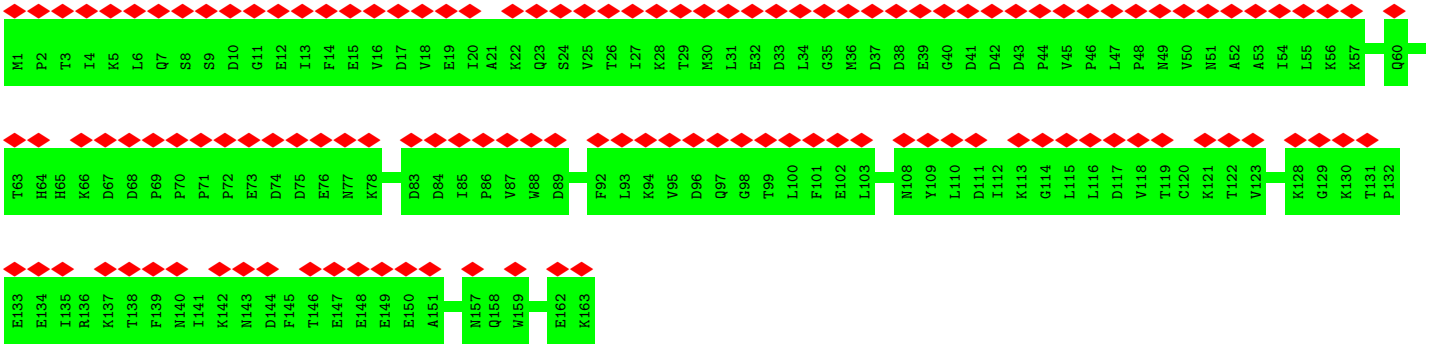
- Molecule 14: S-phase kinase-associated protein 1

Chain AO: 30% 98%



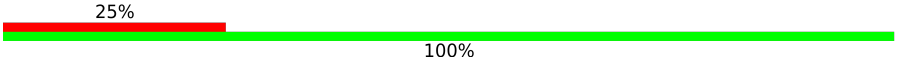
- Molecule 14: S-phase kinase-associated protein 1

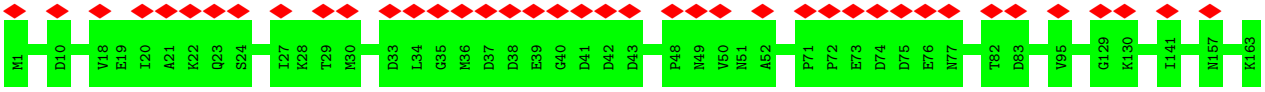
Chain f: 79% 100%



• Molecule 14: S-phase kinase-associated protein 1

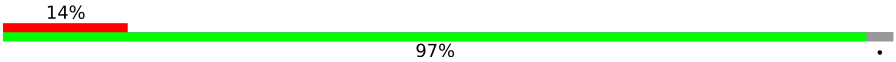
Chain h:

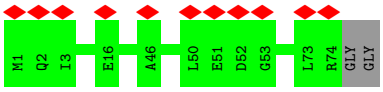




• Molecule 15: Polyubiquitin-C

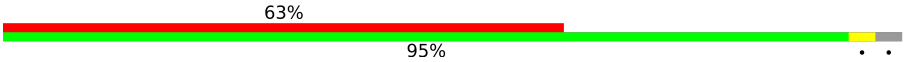
Chain U:

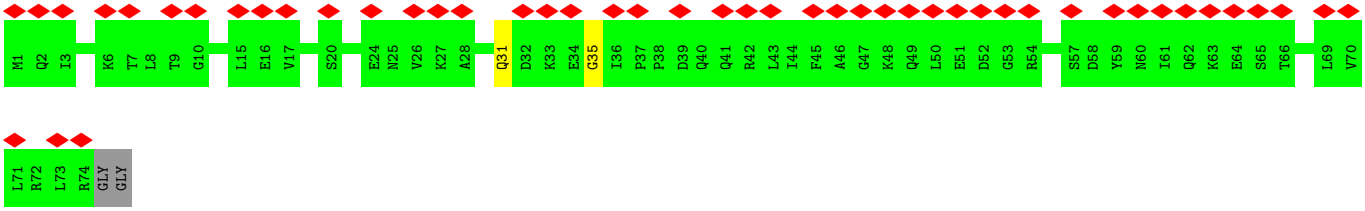




• Molecule 15: Polyubiquitin-C

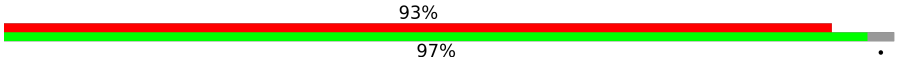
Chain V:

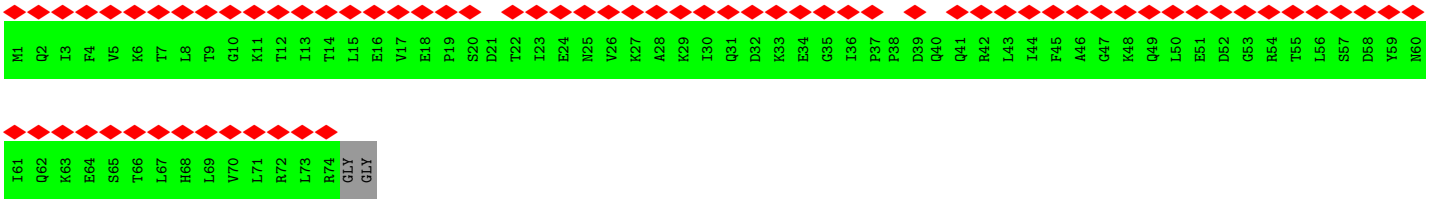




• Molecule 15: Polyubiquitin-C

Chain W:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	30490	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	115	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.227	Depositor
Minimum map value	-0.114	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.056	Depositor
Map size (Å)	606.72, 606.72, 606.72	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.37, 2.37, 2.37	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	0	0.21	0/672	0.38	0/935
1	S	0.20	0/672	0.38	0/935
2	1	0.22	0/3372	0.55	0/4697
2	2	0.11	0/3372	0.32	0/4697
2	3	0.12	0/3372	0.34	0/4697
2	A	0.22	0/3372	0.45	0/4697
2	B	0.20	0/3372	0.39	0/4697
2	C	0.17	0/3372	0.38	0/4697
2	D	0.17	0/3372	0.39	0/4697
2	E	0.15	0/3372	0.36	0/4697
2	F	0.15	0/3372	0.35	0/4697
2	G	0.24	0/3372	0.57	0/4697
2	H	0.18	0/3372	0.41	0/4697
2	I	0.19	0/3372	0.39	0/4697
2	J	0.19	0/3372	0.40	0/4697
2	K	0.11	0/3372	0.31	0/4697
2	L	0.14	0/3372	0.35	0/4697
2	m	0.21	0/3372	0.42	0/4697
2	s	0.19	0/3372	0.41	0/4697
2	t	0.17	0/3372	0.37	0/4697
2	u	0.20	0/3372	0.42	0/4697
2	v	0.16	0/3372	0.36	0/4697
2	w	0.16	0/3372	0.37	0/4697
2	x	0.21	0/3372	0.43	0/4697
2	y	0.17	0/3372	0.39	0/4697
2	z	0.17	0/3372	0.40	0/4697
3	4	0.20	0/4700	0.40	0/6551
3	7	0.17	0/4700	0.38	0/6551
3	M	0.21	0/4700	0.40	0/6551
3	P	0.21	0/4700	0.41	0/6551
4	5	0.16	0/1810	0.42	1/2517 (0.0%)
4	8	0.16	0/1810	0.42	0/2517
4	N	0.18	0/1810	0.41	0/2517
4	Q	0.18	0/1810	0.43	0/2517

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
5	6	0.22	0/591	0.39	0/824
5	9	0.18	0/441	0.47	0/614
5	O	0.22	0/591	0.41	0/824
5	R	0.22	0/441	0.49	0/614
6	AA	0.23	0/310	0.40	0/430
6	T	0.27	0/310	0.51	0/430
7	AE	0.15	0/4641	0.35	0/6475
7	AF	0.14	0/4195	0.35	0/5854
7	X	0.15	0/4641	0.35	0/6475
7	Y	0.15	0/4195	0.36	0/5854
8	AG	0.18	0/4793	0.37	0/6687
8	Z	0.19	0/4793	0.38	0/6687
8	n	0.14	0/4793	0.34	0/6687
9	AH	0.16	0/3125	0.36	0/4339
9	a	0.17	0/3125	0.38	0/4339
9	o	0.15	0/3125	0.37	0/4339
10	AI	0.22	0/728	0.39	0/1014
10	b	0.24	0/728	0.44	0/1014
10	p	0.19	0/728	0.40	0/1014
11	AJ	0.19	0/2166	0.36	0/3011
11	c	0.21	0/2166	0.40	0/3011
11	q	0.14	0/2166	0.31	0/3011
12	AK	0.21	0/2120	0.39	0/2946
12	d	0.23	0/2120	0.39	0/2946
12	r	0.13	0/2120	0.31	0/2946
14	AM	0.14	0/808	0.31	0/1126
14	AO	0.16	0/808	0.33	0/1126
14	f	0.15	0/808	0.30	0/1126
14	h	0.17	0/808	0.34	0/1126
15	U	0.18	0/365	0.31	0/507
15	V	0.15	0/365	0.31	0/507
15	W	0.15	0/365	0.33	0/507
All	All	0.18	0/171791	0.39	1/239280 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	1	0	2
2	A	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	2
2	J	0	1
2	K	0	2
2	m	0	1
2	s	0	1
2	y	0	1
3	4	0	1
5	R	0	1
7	Y	0	1
8	AG	0	3
8	Z	0	3
9	AH	0	1
All	All	0	21

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	5	339	VAL	N-CA-C	-5.20	107.34	111.81

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	565	LEU	Peptide
2	1	59	GLY	Peptide
3	4	936	LEU	Peptide
2	A	509	GLY	Peptide
8	AG	248	ASP	Peptide
8	AG	315	PRO	Peptide
8	AG	50	GLU	Peptide
9	AH	153	VAL	Peptide
2	G	223	LEU	Peptide
2	G	585	THR	Peptide
2	J	509	GLY	Peptide
2	K	96	PHE	Peptide
2	K	97	CYS	Peptide
5	R	104	ILE	Peptide
7	Y	933	PHE	Peptide
8	Z	248	ASP	Peptide
8	Z	315	PRO	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
8	Z	50	GLU	Peptide
2	m	215	GLN	Peptide
2	s	565	LEU	Peptide
2	y	281	LEU	Peptide

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	0	673	0	298	3	0
1	S	673	0	298	4	0
2	1	3373	0	1454	24	0
2	2	3373	0	1454	1	0
2	3	3373	0	1454	8	0
2	A	3373	0	1454	26	0
2	B	3373	0	1454	20	0
2	C	3373	0	1454	13	0
2	D	3373	0	1454	27	0
2	E	3373	0	1454	12	0
2	F	3373	0	1454	12	0
2	G	3373	0	1454	35	0
2	H	3373	0	1454	12	0
2	I	3373	0	1454	13	0
2	J	3373	0	1454	22	0
2	K	3373	0	1454	4	0
2	L	3373	0	1454	4	0
2	m	3373	0	1454	21	0
2	s	3373	0	1454	24	0
2	t	3373	0	1454	16	0
2	u	3373	0	1454	24	0
2	v	3373	0	1454	14	0
2	w	3373	0	1454	8	0
2	x	3373	0	1454	26	0
2	y	3373	0	1454	18	0
2	z	3373	0	1454	8	0
3	4	4702	0	2048	15	0
3	7	4702	0	2048	5	0
3	M	4702	0	2048	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	4702	0	2048	7	0
4	5	1812	0	802	6	0
4	8	1812	0	802	4	0
4	N	1812	0	802	11	0
4	Q	1812	0	802	10	0
5	6	592	0	266	2	0
5	9	442	0	200	3	0
5	O	592	0	266	4	0
5	R	442	0	200	3	0
6	AA	311	0	140	0	0
6	T	311	0	140	5	0
7	AE	4643	0	2005	7	0
7	AF	4196	0	1802	5	0
7	X	4643	0	2005	6	0
7	Y	4196	0	1802	3	0
8	AG	4794	0	2077	8	0
8	Z	4794	0	2077	12	0
8	n	4794	0	2077	2	0
9	AH	3131	0	1365	16	0
9	a	3131	0	1365	11	0
9	o	3131	0	1365	11	0
10	AI	729	0	314	3	0
10	b	729	0	314	4	0
10	p	729	0	314	1	0
11	AJ	2167	0	1009	4	0
11	c	2167	0	1009	6	0
11	q	2167	0	1009	2	0
12	AK	2121	0	962	4	0
12	d	2121	0	962	1	0
12	r	2121	0	962	0	0
13	AL	2312	0	499	17	0
13	AN	2312	0	500	11	0
13	e	2312	0	495	18	0
13	g	2312	0	502	20	0
14	AM	809	0	345	1	0
14	AO	809	0	345	2	0
14	f	809	0	345	0	0
14	h	809	0	345	0	0
15	U	366	0	157	0	0
15	V	366	0	157	1	0
15	W	366	0	157	0	0
All	All	181130	0	76746	664	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 3.

All (664) 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)
8:Z:921:ASN:HA	8:Z:950:ALA:HB3	1.78	0.66
8:Z:249:LYS:HA	8:Z:252:ALA:HB3	1.80	0.64
2:F:46:PRO:HA	2:F:60:LYS:HA	1.81	0.62
2:B:356:ALA:HB3	2:B:359:LYS:O	2.01	0.61
2:H:46:PRO:HA	2:H:60:LYS:HA	1.83	0.61
2:A:506:GLN:HA	2:A:511:GLY:N	2.18	0.59
2:w:46:PRO:HA	2:w:60:LYS:HA	1.84	0.59
2:1:356:ALA:HB3	2:1:359:LYS:O	2.04	0.58
2:x:271:ALA:HB2	2:x:278:GLU:N	2.18	0.58
3:4:566:GLN:HA	3:4:591:LEU:HA	1.85	0.57
2:I:268:VAL:HA	2:I:280:PRO:HA	1.86	0.57
2:G:170:GLU:HA	2:G:220:ALA:HB1	1.87	0.56
2:s:565:LEU:O	2:s:567:LEU:N	2.38	0.56
13:g:453:UNK:O	13:g:454:UNK:C	2.54	0.55
2:H:206:ALA:HB1	2:H:226:GLY:O	2.06	0.55
2:1:206:ALA:HB1	2:1:226:GLY:O	2.06	0.55
4:8:285:GLN:O	4:8:577:TYR:HA	2.07	0.55
2:w:30:SER:HA	2:w:33:ALA:HB3	1.88	0.55
2:1:565:LEU:O	2:1:567:LEU:N	2.41	0.54
2:D:271:ALA:HB2	2:D:278:GLU:N	2.21	0.54
2:t:46:PRO:HA	2:t:60:LYS:HA	1.88	0.54
2:C:46:PRO:HA	2:C:60:LYS:HA	1.90	0.54
2:v:46:PRO:HA	2:v:60:LYS:HA	1.90	0.53
7:X:8:PHE:O	7:X:9:GLY:C	2.51	0.53
12:d:132:GLY:HA3	12:d:163:ILE:O	2.09	0.53
13:g:231:UNK:O	13:g:232:UNK:C	2.57	0.53
9:o:257:LEU:H	9:o:260:ASP:HA	1.73	0.52
2:G:493:ALA:HA	2:G:575:ILE:O	2.08	0.52
2:x:44:GLY:O	2:x:62:ASP:HA	2.09	0.52
2:1:46:PRO:C	2:1:60:LYS:HA	2.34	0.52
4:Q:534:ILE:O	4:Q:547:GLN:HA	2.10	0.52
2:E:46:PRO:HA	2:E:60:LYS:HA	1.91	0.52
2:J:62:ASP:O	2:x:132:SER:HA	2.09	0.52
2:u:46:PRO:HA	2:u:60:LYS:O	2.10	0.52
13:AL:3:UNK:O	13:AL:4:UNK:C	2.58	0.52
9:a:453:GLY:O	9:a:465:LEU:HA	2.10	0.52
10:AI:32:HIS:HA	10:AI:54:ILE:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:46:PRO:O	2:H:60:LYS:HA	2.09	0.51
3:M:566:GLN:HA	3:M:591:LEU:HA	1.92	0.51
2:y:24:GLU:HA	2:y:77:VAL:O	2.11	0.51
13:AN:192:UNK:HA	13:AN:210:UNK:HA	1.92	0.51
2:y:46:PRO:HA	2:y:60:LYS:HA	1.92	0.51
7:AF:850:ALA:HB1	7:AF:880:ALA:HB2	1.92	0.51
2:A:356:ALA:HB3	2:A:359:LYS:O	2.10	0.51
8:AG:921:ASN:HA	8:AG:950:ALA:HB3	1.91	0.51
2:H:447:PHE:O	2:H:450:ALA:HB3	2.11	0.51
2:L:48:ILE:O	2:L:59:GLY:C	2.54	0.51
3:M:899:GLN:HA	3:M:926:LEU:HA	1.92	0.51
13:g:425:UNK:O	13:g:426:UNK:C	2.58	0.51
7:AE:86:ALA:O	7:AE:89:ALA:HB3	2.11	0.50
2:x:414:LYS:HA	2:x:419:ASP:HA	1.93	0.50
2:1:303:LEU:H	2:1:670:ARG:HA	1.76	0.50
2:D:217:GLY:O	2:D:218:SER:O	2.29	0.50
3:4:984:ASN:HA	3:4:1012:LEU:HA	1.94	0.50
7:AE:5:ILE:O	7:AE:6:SER:C	2.55	0.50
6:T:48:GLN:O	6:T:52:ARG:N	2.44	0.50
2:A:353:TYR:HA	2:A:362:SER:HA	1.94	0.50
13:AN:253:UNK:O	13:AN:254:UNK:C	2.59	0.50
2:D:46:PRO:HA	2:D:60:LYS:O	2.12	0.50
2:J:236:THR:O	2:J:237:PHE:C	2.55	0.50
2:s:626:ASN:C	2:s:628:THR:H	2.19	0.50
1:0:3:SER:N	1:0:77:VAL:O	2.45	0.49
2:1:42:ILE:O	2:1:64:VAL:HA	2.11	0.49
13:AL:4:UNK:O	13:AL:5:UNK:C	2.59	0.49
13:AL:253:UNK:O	13:AL:254:UNK:C	2.59	0.49
2:G:414:LYS:HA	2:G:419:ASP:HA	1.94	0.49
3:4:728:GLU:HA	3:4:755:LEU:HA	1.94	0.49
13:AN:453:UNK:O	13:AN:454:UNK:C	2.60	0.49
2:J:46:PRO:O	2:J:60:LYS:N	2.45	0.49
4:Q:285:GLN:O	4:Q:577:TYR:HA	2.12	0.49
2:m:46:PRO:C	2:m:60:LYS:HA	2.37	0.49
2:x:493:ALA:HA	2:x:575:ILE:O	2.13	0.49
2:m:115:GLU:O	2:m:185:VAL:HA	2.13	0.49
2:B:30:SER:HA	2:B:33:ALA:HB3	1.94	0.49
8:n:851:ALA:HB1	8:n:881:ALA:HB2	1.93	0.49
2:1:52:ILE:HA	2:1:75:ALA:HA	1.93	0.49
2:K:42:ILE:HA	2:K:92:LEU:O	2.12	0.49
5:O:48:TYR:HA	5:O:88:GLU:HA	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:39:SER:HA	2:A:68:SER:HA	1.95	0.49
2:m:429:GLY:O	2:m:460:PHE:HA	2.12	0.49
8:Z:910:ILE:O	8:Z:914:ASN:N	2.45	0.49
13:e:49:UNK:O	13:e:50:UNK:C	2.59	0.49
2:m:308:CYS:HA	2:m:334:VAL:O	2.13	0.49
2:A:442:LYS:O	2:A:443:GLY:C	2.55	0.48
2:F:149:ALA:O	2:F:288:PHE:HA	2.13	0.48
3:M:842:GLN:HA	3:M:869:LEU:HA	1.95	0.48
2:3:30:SER:HA	2:3:33:ALA:HB3	1.95	0.48
2:B:579:PHE:HA	2:B:600:PRO:HA	1.95	0.48
2:G:271:ALA:HB2	2:G:278:GLU:N	2.29	0.48
2:G:476:VAL:O	2:G:488:PHE:HA	2.13	0.48
3:M:549:LEU:O	3:M:552:SER:O	2.30	0.48
2:x:46:PRO:HA	2:x:59:GLY:O	2.13	0.48
3:4:927:LYS:HA	3:4:955:LEU:HA	1.95	0.48
2:C:476:VAL:O	2:C:488:PHE:HA	2.14	0.48
2:y:307:LEU:O	2:y:334:VAL:N	2.47	0.48
9:AH:546:GLY:HA2	9:AH:552:ALA:HB3	1.96	0.48
2:B:183:VAL:O	2:B:242:LYS:HA	2.13	0.48
2:y:46:PRO:HA	2:y:59:GLY:O	2.14	0.48
2:E:17:ALA:O	2:E:111:LEU:HA	2.13	0.48
8:n:768:LEU:CB	8:n:796:ALA:HB1	2.43	0.48
2:u:356:ALA:HB3	2:u:359:LYS:O	2.13	0.48
9:AH:8:MET:N	9:AH:71:LEU:O	2.47	0.48
2:y:48:ILE:HA	2:y:79:MET:HA	1.96	0.48
3:4:916:LEU:O	3:4:917:ALA:C	2.57	0.48
2:I:150:ILE:HA	2:I:289:ARG:O	2.14	0.48
2:m:39:SER:HA	2:m:68:SER:HA	1.96	0.48
11:q:289:ALA:HB2	11:q:331:ALA:HB2	1.96	0.48
2:u:42:ILE:O	2:u:64:VAL:HA	2.13	0.48
2:x:427:ILE:O	2:x:459:LEU:N	2.46	0.48
8:Z:851:ALA:HB1	8:Z:881:ALA:HB2	1.96	0.48
2:s:454:GLN:O	2:s:455:ALA:C	2.57	0.48
2:s:617:ILE:O	2:s:648:PHE:HA	2.14	0.48
4:N:271:ALA:HB3	4:N:276:GLU:HA	1.96	0.47
2:v:514:THR:HA	2:v:533:THR:HA	1.96	0.47
2:z:42:ILE:O	2:z:64:VAL:HA	2.14	0.47
2:B:429:GLY:O	2:B:460:PHE:HA	2.15	0.47
2:B:492:LEU:O	2:B:575:ILE:N	2.47	0.47
2:G:427:ILE:O	2:G:459:LEU:N	2.47	0.47
2:H:454:GLN:O	2:H:455:ALA:C	2.57	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:268:VAL:HA	2:A:280:PRO:HA	1.96	0.47
2:H:424:ARG:HA	2:H:454:GLN:O	2.14	0.47
2:I:427:ILE:O	2:I:459:LEU:N	2.48	0.47
2:D:45:SER:O	2:D:60:LYS:HA	2.14	0.47
2:m:130:MET:O	2:u:61:GLU:O	2.33	0.47
7:AE:670:ASN:HA	7:AE:695:SER:O	2.15	0.47
2:E:153:VAL:HA	2:E:249:ALA:O	2.14	0.47
11:c:214:ARG:O	11:c:218:ASP:HA	2.14	0.47
2:B:39:SER:HA	2:B:68:SER:HA	1.96	0.47
4:Q:525:TRP:O	4:Q:536:VAL:HA	2.15	0.47
2:y:206:ALA:HB1	2:y:226:GLY:O	2.15	0.47
2:G:43:ARG:O	2:G:91:VAL:HA	2.15	0.47
13:e:4:UNK:O	13:e:5:UNK:C	2.62	0.47
2:s:513:VAL:O	2:s:533:THR:HA	2.15	0.47
2:x:42:ILE:O	2:x:64:VAL:HA	2.15	0.47
2:x:492:LEU:O	2:x:575:ILE:N	2.48	0.47
7:AE:8:PHE:O	7:AE:9:GLY:C	2.56	0.47
2:B:617:ILE:O	2:B:648:PHE:HA	2.15	0.47
2:E:353:TYR:HA	2:E:362:SER:HA	1.97	0.47
2:s:427:ILE:O	2:s:459:LEU:N	2.48	0.47
2:u:45:SER:O	2:u:60:LYS:HA	2.15	0.47
2:A:198:ILE:O	2:A:265:LEU:HA	2.15	0.46
9:AH:539:VAL:N	9:AH:561:GLY:HA3	2.31	0.46
2:J:214:SER:HA	2:J:220:ALA:O	2.14	0.46
2:J:356:ALA:HB3	2:J:359:LYS:O	2.15	0.46
1:S:3:SER:N	1:S:77:VAL:O	2.48	0.46
13:AL:454:UNK:O	13:AL:455:UNK:C	2.63	0.46
14:AO:5:LYS:HA	14:AO:14:PHE:O	2.15	0.46
7:Y:813:LYS:O	7:Y:841:ILE:HA	2.15	0.46
2:v:214:SER:O	2:v:215:GLN:C	2.57	0.46
4:5:370:VAL:O	4:5:380:GLU:HA	2.15	0.46
2:G:236:THR:O	2:G:237:PHE:C	2.57	0.46
2:J:143:GLY:HA2	2:J:678:TRP:O	2.15	0.46
4:N:534:ILE:O	4:N:547:GLN:HA	2.16	0.46
5:O:101:MET:O	5:O:102:LYS:C	2.56	0.46
2:s:442:LYS:O	2:s:443:GLY:C	2.58	0.46
2:u:494:SER:N	2:u:575:ILE:O	2.48	0.46
2:A:493:ALA:HA	2:A:575:ILE:O	2.15	0.46
13:AL:58:UNK:O	13:AL:59:UNK:C	2.63	0.46
2:E:46:PRO:O	2:E:60:LYS:N	2.48	0.46
4:N:453:CYS:O	4:N:461:VAL:HA	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:562:LYS:O	2:1:566:GLY:HA2	2.16	0.46
13:g:253:UNK:O	13:g:254:UNK:C	2.64	0.46
2:x:429:GLY:O	2:x:460:PHE:HA	2.16	0.46
3:4:860:ALA:HB1	3:4:890:ALA:HB2	1.96	0.46
2:B:267:LEU:O	2:B:280:PRO:HA	2.15	0.46
2:D:494:SER:N	2:D:575:ILE:O	2.49	0.46
4:5:453:CYS:O	4:5:461:VAL:HA	2.16	0.46
2:H:183:VAL:O	2:H:242:LYS:HA	2.16	0.46
3:M:728:GLU:HA	3:M:755:LEU:HA	1.98	0.46
9:a:723:PRO:O	9:a:763:VAL:HA	2.15	0.46
5:9:51:ALA:O	5:9:52:TRP:C	2.58	0.46
8:AG:506:GLN:HA	8:AG:531:LEU:HA	1.98	0.46
13:AL:453:UNK:O	13:AL:454:UNK:C	2.64	0.46
2:B:153:VAL:HA	2:B:249:ALA:HB3	1.97	0.46
2:G:80:VAL:O	2:G:81:ALA:C	2.59	0.46
4:N:477:SER:O	4:N:480:GLU:O	2.34	0.46
7:Y:775:GLU:HA	7:Y:802:LEU:HA	1.98	0.46
2:t:46:PRO:O	2:t:60:LYS:N	2.48	0.46
2:t:579:PHE:HA	2:t:600:PRO:HA	1.98	0.46
2:v:170:GLU:O	2:v:171:GLY:C	2.59	0.46
2:y:424:ARG:HA	2:y:454:GLN:O	2.15	0.46
2:D:30:SER:HA	2:D:33:ALA:HB3	1.98	0.45
2:D:424:ARG:HA	2:D:454:GLN:O	2.16	0.45
2:I:424:ARG:HA	2:I:454:GLN:O	2.16	0.45
3:M:649:ASP:O	3:M:650:SER:C	2.60	0.45
3:M:730:LEU:O	3:M:758:LEU:HA	2.15	0.45
9:a:181:HIS:HA	9:a:193:ASP:O	2.16	0.45
2:s:562:LYS:O	2:s:566:GLY:HA2	2.15	0.45
2:1:37:CYS:HA	2:1:97:CYS:HA	1.98	0.45
7:AF:925:ALA:O	7:AF:926:PHE:O	2.34	0.45
9:AH:338:CYS:O	9:AH:342:ASP:HA	2.17	0.45
11:AJ:101:ASN:C	11:AJ:144:GLY:HA3	2.42	0.45
4:N:367:GLY:HA2	4:N:386:CYS:H	1.80	0.45
11:c:214:ARG:HA	11:c:219:ILE:O	2.16	0.45
13:g:124:UNK:HA	13:g:129:UNK:O	2.17	0.45
2:u:424:ARG:HA	2:u:454:GLN:O	2.16	0.45
8:AG:459:VAL:O	8:AG:460:ARG:C	2.59	0.45
9:AH:546:GLY:CA	9:AH:552:ALA:HB3	2.46	0.45
3:M:958:LEU:O	3:M:986:LEU:HA	2.16	0.45
3:4:899:GLN:HA	3:4:926:LEU:HA	1.97	0.45
5:9:94:GLN:O	5:9:95:PRO:C	2.59	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:44:GLY:O	2:G:62:ASP:HA	2.16	0.45
2:J:39:SER:HA	2:J:68:SER:HA	1.99	0.45
3:M:787:LEU:O	3:M:815:LEU:HA	2.17	0.45
2:s:492:LEU:O	2:s:575:ILE:N	2.49	0.45
2:x:97:CYS:O	2:x:98:PRO:C	2.58	0.45
2:y:119:GLU:N	2:y:182:ASN:O	2.50	0.45
2:1:656:LEU:O	2:1:657:ALA:C	2.60	0.45
4:5:482:TRP:HA	4:5:495:PHE:O	2.17	0.45
2:A:427:ILE:O	2:A:459:LEU:N	2.49	0.45
2:G:43:ARG:HA	2:G:63:THR:O	2.16	0.45
9:a:539:VAL:N	9:a:561:GLY:HA3	2.32	0.45
2:u:263:LEU:O	2:u:285:THR:HA	2.15	0.45
2:x:424:ARG:HA	2:x:454:GLN:O	2.17	0.45
2:D:211:VAL:O	2:D:223:LEU:HA	2.16	0.45
2:K:97:CYS:O	2:K:98:PRO:C	2.59	0.45
1:S:73:ILE:HA	1:S:87:TRP:O	2.17	0.45
2:u:170:GLU:O	2:u:171:GLY:C	2.59	0.45
2:u:268:VAL:HA	2:u:280:PRO:HA	1.98	0.45
13:AN:58:UNK:O	13:AN:59:UNK:C	2.65	0.45
2:G:492:LEU:O	2:G:575:ILE:N	2.49	0.45
4:Q:414:TRP:HA	4:Q:420:GLU:O	2.16	0.45
7:X:404:GLY:O	7:X:408:ASP:N	2.49	0.45
13:g:219:UNK:O	13:g:223:UNK:HA	2.16	0.45
2:m:25:ILE:O	2:m:76:LEU:HA	2.17	0.45
13:AL:316:UNK:HA	13:AL:332:UNK:O	2.17	0.45
2:B:493:ALA:HA	2:B:575:ILE:O	2.17	0.45
2:G:46:PRO:HA	2:G:59:GLY:O	2.16	0.45
9:a:507:THR:O	9:a:508:ASN:C	2.60	0.45
13:e:343:UNK:O	13:e:344:UNK:C	2.65	0.45
13:e:453:UNK:O	13:e:454:UNK:C	2.64	0.45
4:5:477:SER:O	4:5:480:GLU:O	2.35	0.45
2:E:30:SER:HA	2:E:33:ALA:HB3	1.99	0.45
2:x:30:SER:HA	2:x:33:ALA:HB3	1.98	0.45
2:x:211:VAL:O	2:x:223:LEU:HA	2.17	0.45
2:G:143:GLY:HA2	2:G:679:LYS:O	2.17	0.45
2:H:494:SER:N	2:H:575:ILE:O	2.50	0.45
2:I:494:SER:N	2:I:575:ILE:O	2.50	0.45
2:m:23:MET:O	2:m:78:ARG:HA	2.16	0.45
2:t:578:LEU:O	2:t:600:PRO:HA	2.17	0.45
2:u:101:GLU:O	2:u:102:VAL:C	2.59	0.45
2:y:90:LYS:HA	2:y:110:PHE:HA	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AH:718:GLU:O	9:AH:719:LEU:C	2.61	0.44
2:B:119:GLU:N	2:B:182:ASN:O	2.51	0.44
2:E:183:VAL:O	2:E:242:LYS:HA	2.17	0.44
2:K:424:ARG:HA	2:K:454:GLN:O	2.16	0.44
2:t:478:THR:H	2:t:488:PHE:HA	1.82	0.44
2:x:170:GLU:O	2:x:171:GLY:C	2.59	0.44
2:A:212:TYR:HA	2:A:222:GLU:O	2.17	0.44
2:A:623:PRO:O	2:A:629:CYS:HA	2.17	0.44
2:F:617:ILE:O	2:F:648:PHE:HA	2.18	0.44
2:w:170:GLU:O	2:w:171:GLY:C	2.60	0.44
2:x:447:PHE:O	2:x:450:ALA:HB3	2.17	0.44
2:y:141:MET:O	2:y:147:TRP:O	2.34	0.44
2:z:494:SER:N	2:z:575:ILE:O	2.50	0.44
2:C:39:SER:HA	2:C:68:SER:HA	1.99	0.44
2:C:454:GLN:O	2:C:455:ALA:C	2.61	0.44
2:C:473:MET:HA	2:C:491:LEU:O	2.17	0.44
2:G:408:MET:O	2:G:425:VAL:HA	2.17	0.44
5:O:32:ARG:O	5:O:33:PRO:C	2.59	0.44
4:Q:455:ASP:O	4:Q:459:ALA:HA	2.17	0.44
6:T:57:TRP:HA	6:T:67:VAL:O	2.17	0.44
2:s:211:VAL:O	2:s:223:LEU:HA	2.17	0.44
2:z:454:GLN:O	2:z:455:ALA:C	2.60	0.44
4:5:367:GLY:HA2	4:5:386:CYS:H	1.83	0.44
2:C:424:ARG:HA	2:C:454:GLN:O	2.17	0.44
2:D:195:TYR:HA	2:D:268:VAL:O	2.17	0.44
2:x:184:THR:HA	2:x:241:ARG:O	2.18	0.44
3:4:961:GLY:HA2	3:4:989:VAL:O	2.18	0.44
9:AH:46:PHE:HA	9:AH:50:LYS:O	2.18	0.44
13:AL:254:UNK:O	13:AL:255:UNK:C	2.66	0.44
2:D:116:ILE:HA	2:D:184:THR:O	2.18	0.44
2:F:454:GLN:O	2:F:455:ALA:C	2.60	0.44
2:G:51:HIS:HA	2:G:55:SER:O	2.17	0.44
4:Q:494:LEU:O	4:Q:503:VAL:HA	2.18	0.44
7:X:5:ILE:O	7:X:6:SER:C	2.60	0.44
9:a:456:GLY:HA2	9:a:462:ALA:HA	2.00	0.44
13:g:157:UNK:O	13:g:161:UNK:N	2.50	0.44
2:s:152:LEU:O	2:s:249:ALA:HB3	2.18	0.44
2:u:45:SER:N	2:u:59:GLY:O	2.50	0.44
2:u:100:GLN:O	2:u:102:VAL:N	2.51	0.44
3:4:592:LYS:HA	3:4:642:LEU:HA	1.99	0.44
2:A:306:TYR:O	2:A:666:ALA:HB1	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AH:682:LYS:HA	9:AH:685:ALA:HB2	1.98	0.44
2:L:45:SER:O	2:L:59:GLY:O	2.35	0.44
4:N:413:ILE:O	4:N:421:ILE:HA	2.18	0.44
2:s:153:VAL:HA	2:s:249:ALA:O	2.17	0.44
2:t:30:SER:HA	2:t:33:ALA:HB3	1.99	0.44
2:1:52:ILE:O	2:1:54:SER:N	2.51	0.44
2:1:144:MET:C	2:1:146:GLY:H	2.26	0.44
5:9:106:LEU:O	5:9:110:ALA:N	2.51	0.44
8:AG:910:ILE:O	8:AG:914:ASN:N	2.50	0.44
13:AN:59:UNK:O	13:AN:60:UNK:C	2.65	0.44
2:D:184:THR:HA	2:D:241:ARG:O	2.18	0.44
2:u:414:LYS:HA	2:u:419:ASP:HA	1.99	0.44
7:AF:889:LYS:HA	7:AF:916:LEU:HA	1.99	0.44
2:I:42:ILE:O	2:I:64:VAL:HA	2.17	0.44
13:g:53:UNK:O	13:g:55:UNK:N	2.51	0.44
13:g:206:UNK:O	13:g:217:UNK:HA	2.18	0.44
2:m:472:PHE:O	2:m:492:LEU:HA	2.18	0.44
3:4:131:PRO:HA	3:4:137:GLN:HA	2.00	0.44
5:6:69:GLU:O	5:6:73:GLN:N	2.50	0.44
8:AG:532:LYS:HA	8:AG:577:LEU:HA	2.00	0.44
13:AN:2:UNK:O	13:AN:3:UNK:C	2.66	0.44
2:D:214:SER:HA	2:D:220:ALA:O	2.17	0.44
2:J:24:GLU:HA	2:J:77:VAL:O	2.17	0.44
2:J:51:HIS:HA	2:J:56:VAL:HA	2.00	0.44
7:X:658:LYS:O	7:X:659:TYR:C	2.61	0.44
2:v:17:ALA:O	2:v:111:LEU:HA	2.17	0.44
2:3:44:GLY:O	2:3:62:ASP:HA	2.18	0.43
3:4:189:SER:HA	3:4:242:ASP:O	2.18	0.43
2:B:212:TYR:HA	2:B:222:GLU:O	2.18	0.43
4:N:370:VAL:O	4:N:380:GLU:HA	2.18	0.43
9:o:507:THR:O	9:o:508:ASN:C	2.61	0.43
2:A:95:TYR:O	2:A:103:PRO:HA	2.19	0.43
2:G:402:ASP:HA	2:G:440:MET:HA	1.99	0.43
2:s:46:PRO:HA	2:s:60:LYS:HA	1.99	0.43
2:1:37:CYS:HA	2:1:96:PHE:O	2.19	0.43
2:G:353:TYR:HA	2:G:362:SER:HA	2.00	0.43
2:t:267:LEU:O	2:t:280:PRO:HA	2.18	0.43
2:A:472:PHE:O	2:A:492:LEU:HA	2.19	0.43
2:A:494:SER:O	2:A:576:PRO:HA	2.18	0.43
2:A:566:GLY:O	2:A:567:LEU:O	2.36	0.43
8:AG:950:ALA:HA	8:AG:978:GLY:O	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AK:309:ARG:O	12:AK:371:SER:HA	2.18	0.43
2:s:578:LEU:O	2:s:600:PRO:HA	2.18	0.43
2:v:153:VAL:HA	2:v:249:ALA:O	2.18	0.43
2:1:211:VAL:O	2:1:223:LEU:HA	2.19	0.43
8:AG:757:GLU:O	8:AG:785:PHE:CB	2.67	0.43
9:AH:58:LEU:O	9:AH:62:ASP:N	2.52	0.43
13:AN:454:UNK:O	13:AN:455:UNK:C	2.66	0.43
2:B:424:ARG:HA	2:B:454:GLN:O	2.18	0.43
2:D:271:ALA:HB2	2:D:278:GLU:H	1.83	0.43
13:g:341:UNK:O	13:g:342:UNK:C	2.65	0.43
2:s:476:VAL:O	2:s:488:PHE:HA	2.18	0.43
2:u:324:SER:O	2:u:328:LYS:N	2.51	0.43
2:w:602:PHE:O	2:w:603:PRO:C	2.61	0.43
2:x:513:VAL:O	2:x:533:THR:HA	2.18	0.43
3:7:592:LYS:HA	3:7:642:LEU:HA	2.00	0.43
7:AF:404:GLY:O	7:AF:408:ASP:N	2.51	0.43
2:F:210:ARG:O	2:F:247:VAL:HA	2.18	0.43
2:J:52:ILE:O	2:J:54:SER:N	2.52	0.43
3:M:131:PRO:HA	3:M:137:GLN:HA	2.00	0.43
9:a:8:MET:N	9:a:71:LEU:O	2.52	0.43
2:s:424:ARG:HA	2:s:454:GLN:O	2.19	0.43
2:x:46:PRO:HA	2:x:60:LYS:HA	2.01	0.43
7:AE:404:GLY:O	7:AE:408:ASP:N	2.52	0.43
9:AH:723:PRO:HA	9:AH:732:VAL:O	2.19	0.43
2:G:150:ILE:HA	2:G:289:ARG:O	2.18	0.43
2:J:42:ILE:HA	2:J:92:LEU:O	2.19	0.43
3:M:429:LEU:HA	3:M:442:PHE:HA	1.99	0.43
3:M:709:LYS:O	3:M:710:ASP:C	2.61	0.43
5:O:69:GLU:O	5:O:73:GLN:N	2.52	0.43
3:P:1055:ASN:O	3:P:1056:TRP:C	2.60	0.43
9:o:237:VAL:HA	9:o:254:ASN:O	2.19	0.43
2:t:294:ILE:O	2:t:352:CYS:HA	2.19	0.43
2:y:183:VAL:O	2:y:242:LYS:HA	2.18	0.43
2:D:602:PHE:O	2:D:603:PRO:C	2.61	0.43
2:F:427:ILE:O	2:F:459:LEU:N	2.52	0.43
6:T:52:ARG:HA	6:T:55:SER:O	2.18	0.43
8:Z:223:GLN:O	8:Z:224:LYS:C	2.62	0.43
8:Z:315:PRO:O	8:Z:316:VAL:C	2.61	0.43
8:Z:729:THR:HA	8:Z:755:VAL:O	2.19	0.43
9:a:712:GLN:HA	9:a:719:LEU:HA	2.00	0.43
2:1:30:SER:HA	2:1:33:ALA:HB3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AH:570:PRO:HA	9:AH:580:TRP:HA	2.01	0.43
2:F:424:ARG:HA	2:F:454:GLN:O	2.19	0.43
2:F:514:THR:HA	2:F:533:THR:HA	2.00	0.43
2:I:59:GLY:C	2:I:61:GLU:H	2.27	0.43
2:I:356:ALA:HB3	2:I:359:LYS:O	2.19	0.43
3:P:874:LEU:O	3:P:903:LEU:HA	2.19	0.43
4:Q:301:VAL:O	4:Q:307:HIS:O	2.36	0.43
1:S:121:ALA:CB	7:X:387:SER:HA	2.49	0.43
10:b:142:THR:O	10:b:143:GLN:C	2.61	0.43
2:m:215:GLN:O	2:m:218:SER:N	2.52	0.43
2:s:25:ILE:O	2:s:76:LEU:HA	2.18	0.43
2:u:447:PHE:O	2:u:450:ALA:HB3	2.19	0.43
3:4:681:VAL:O	3:4:682:VAL:C	2.62	0.43
13:AL:28:UNK:O	14:AM:143:ASN:HA	2.19	0.43
13:AN:394:UNK:HA	13:AN:407:UNK:O	2.19	0.43
2:J:493:ALA:HA	2:J:575:ILE:O	2.19	0.43
2:J:581:LEU:HA	2:J:597:PHE:O	2.18	0.43
9:o:537:VAL:O	9:o:562:ILE:HA	2.19	0.43
2:s:473:MET:HA	2:s:491:LEU:O	2.19	0.43
2:s:494:SER:N	2:s:575:ILE:O	2.51	0.43
2:t:494:SER:N	2:t:575:ILE:O	2.52	0.43
2:2:617:ILE:O	2:2:648:PHE:HA	2.19	0.42
13:AL:192:UNK:HA	13:AL:210:UNK:HA	2.00	0.42
11:c:161:TYR:O	11:c:162:GLY:C	2.62	0.42
13:e:151:UNK:HA	13:e:167:UNK:HA	1.99	0.42
9:o:224:ASN:HA	9:o:232:GLY:HA3	2.01	0.42
2:s:217:GLY:O	2:s:218:SER:O	2.36	0.42
11:AJ:70:LEU:O	11:AJ:95:GLY:C	2.62	0.42
13:AL:160:UNK:O	13:AL:161:UNK:C	2.67	0.42
2:G:536:GLN:O	2:G:539:ALA:HB3	2.19	0.42
2:H:602:PHE:O	2:H:603:PRO:C	2.62	0.42
5:R:95:PRO:O	5:R:96:SER:C	2.62	0.42
6:T:51:HIS:O	6:T:55:SER:O	2.37	0.42
13:e:454:UNK:O	13:e:455:UNK:C	2.65	0.42
13:g:365:UNK:O	13:g:377:UNK:HA	2.19	0.42
13:g:430:UNK:O	13:g:431:UNK:C	2.65	0.42
2:u:212:TYR:HA	2:u:222:GLU:O	2.20	0.42
2:z:268:VAL:HA	2:z:279:ILE:O	2.18	0.42
7:AE:513:GLY:HA2	7:AE:517:GLY:HA2	2.00	0.42
2:E:268:VAL:HA	2:E:280:PRO:HA	2.01	0.42
2:G:98:PRO:C	2:G:100:GLN:H	2.28	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:324:SER:O	2:H:328:LYS:N	2.52	0.42
2:J:153:VAL:HA	2:J:249:ALA:HB3	2.01	0.42
2:J:494:SER:N	2:J:575:ILE:O	2.52	0.42
2:A:254:SER:O	2:A:257:PHE:O	2.37	0.42
2:C:236:THR:O	2:C:237:PHE:C	2.62	0.42
2:F:45:SER:O	2:F:59:GLY:HA3	2.19	0.42
2:H:90:LYS:HA	2:H:110:PHE:HA	2.01	0.42
7:Y:719:GLU:HA	7:Y:746:LEU:HA	2.01	0.42
9:o:260:ASP:O	9:o:262:GLN:N	2.52	0.42
9:o:260:ASP:O	9:o:261:SER:C	2.62	0.42
2:w:41:THR:O	2:w:93:VAL:HA	2.19	0.42
9:AH:713:CYS:O	9:AH:717:GLN:HA	2.19	0.42
13:AN:430:UNK:O	13:AN:431:UNK:C	2.67	0.42
2:D:24:GLU:HA	2:D:77:VAL:O	2.19	0.42
13:e:58:UNK:O	13:e:59:UNK:C	2.66	0.42
13:e:59:UNK:O	13:e:60:UNK:C	2.67	0.42
13:g:451:UNK:C	13:g:453:UNK:N	2.81	0.42
1:0:73:ILE:HA	1:0:87:TRP:O	2.20	0.42
3:4:672:GLN:HA	3:4:698:LEU:HA	2.01	0.42
5:6:45:LEU:O	5:6:90:THR:HA	2.20	0.42
2:C:414:LYS:HA	2:C:419:ASP:HA	2.02	0.42
2:D:133:ASP:O	2:D:136:ALA:HB3	2.20	0.42
2:E:50:ILE:N	2:E:57:ILE:O	2.52	0.42
2:G:172:PRO:O	2:G:173:ARG:C	2.61	0.42
10:b:52:LEU:HA	10:b:70:THR:H	1.85	0.42
2:w:45:SER:O	2:w:46:PRO:C	2.63	0.42
2:y:184:THR:HA	2:y:241:ARG:O	2.20	0.42
2:1:143:GLY:HA2	2:1:678:TRP:O	2.19	0.42
4:8:453:CYS:O	4:8:461:VAL:HA	2.20	0.42
12:AK:106:TYR:O	12:AK:110:ALA:HB2	2.20	0.42
2:m:494:SER:N	2:m:575:ILE:O	2.52	0.42
11:q:311:LYS:HA	11:q:342:GLN:O	2.20	0.42
2:t:454:GLN:O	2:t:455:ALA:C	2.62	0.42
2:u:39:SER:HA	2:u:68:SER:HA	2.02	0.42
2:x:267:LEU:O	2:x:280:PRO:HA	2.20	0.42
2:y:215:GLN:O	2:y:216:ARG:C	2.62	0.42
4:8:366:PRO:C	4:8:386:CYS:O	2.62	0.42
13:AL:37:UNK:O	13:AL:38:UNK:C	2.67	0.42
3:M:813:THR:HA	3:M:841:LEU:HA	2.01	0.42
3:M:900:GLU:HA	3:M:928:SER:O	2.19	0.42
5:R:95:PRO:O	5:R:99:THR:CB	2.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:32:HIS:HA	10:b:54:ILE:O	2.19	0.42
2:v:89:ASP:O	2:v:111:LEU:N	2.53	0.42
3:7:958:LEU:O	3:7:986:LEU:HA	2.20	0.42
2:A:43:ARG:HA	2:A:63:THR:O	2.20	0.42
9:AH:421:ASN:O	9:AH:422:HIS:C	2.63	0.42
2:D:82:PRO:HA	2:D:113:GLY:C	2.44	0.42
2:G:271:ALA:HB2	2:G:278:GLU:H	1.84	0.42
2:G:462:ASP:O	2:G:463:TRP:C	2.62	0.42
2:H:260:LEU:HA	2:H:288:PHE:O	2.20	0.42
2:J:50:ILE:N	2:J:57:ILE:O	2.53	0.42
9:a:595:THR:O	9:a:596:ARG:C	2.63	0.42
2:t:268:VAL:HA	2:t:280:PRO:HA	2.01	0.42
2:u:303:LEU:H	2:u:670:ARG:HA	1.85	0.42
2:v:23:MET:O	2:v:78:ARG:HA	2.20	0.42
2:z:170:GLU:O	2:z:171:GLY:C	2.62	0.42
2:3:39:SER:HA	2:3:68:SER:HA	2.01	0.42
2:A:271:ALA:HB2	2:A:278:GLU:N	2.35	0.42
2:B:427:ILE:O	2:B:459:LEU:N	2.52	0.42
2:G:513:VAL:O	2:G:533:THR:HA	2.20	0.42
2:J:130:MET:O	2:x:61:GLU:O	2.38	0.42
2:J:447:PHE:O	2:J:450:ALA:HB3	2.20	0.42
2:s:169:GLN:O	2:s:222:GLU:HA	2.20	0.42
2:y:454:GLN:O	2:y:455:ALA:C	2.63	0.42
2:1:49:LEU:O	2:1:78:ARG:O	2.38	0.41
2:3:454:GLN:O	2:3:455:ALA:C	2.63	0.41
2:A:37:CYS:HA	2:A:97:CYS:HA	2.00	0.41
2:A:45:SER:O	2:A:59:GLY:O	2.38	0.41
2:A:473:MET:HA	2:A:491:LEU:O	2.20	0.41
13:AN:166:UNK:HA	13:AN:171:UNK:O	2.19	0.41
2:F:211:VAL:HA	2:F:246:TYR:O	2.20	0.41
2:J:617:ILE:O	2:J:648:PHE:HA	2.20	0.41
3:M:927:LYS:HA	3:M:955:LEU:HA	2.02	0.41
4:N:318:VAL:O	4:N:331:PRO:HA	2.19	0.41
4:N:367:GLY:HA2	4:N:386:CYS:N	2.35	0.41
3:P:592:LYS:HA	3:P:642:LEU:HA	2.02	0.41
13:e:346:UNK:HA	13:e:360:UNK:C	2.50	0.41
13:g:166:UNK:HA	13:g:171:UNK:O	2.20	0.41
2:m:50:ILE:N	2:m:57:ILE:O	2.53	0.41
9:o:318:CYS:O	9:o:322:ALA:HB3	2.20	0.41
2:s:356:ALA:HB3	2:s:359:LYS:O	2.20	0.41
2:s:429:GLY:O	2:s:460:PHE:HA	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:t:261:ILE:O	2:t:288:PHE:N	2.53	0.41
2:u:30:SER:HA	2:u:33:ALA:HB3	2.02	0.41
2:x:200:HIS:O	2:x:264:SER:O	2.38	0.41
3:7:817:LEU:O	3:7:846:LEU:HA	2.20	0.41
13:AN:219:UNK:O	13:AN:223:UNK:HA	2.21	0.41
2:B:454:GLN:O	2:B:455:ALA:C	2.63	0.41
8:Z:90:GLY:C	8:Z:92:GLY:H	2.28	0.41
9:o:255:ILE:O	9:o:262:GLN:HA	2.20	0.41
2:u:454:GLN:O	2:u:455:ALA:C	2.63	0.41
2:w:93:VAL:O	2:w:106:THR:HA	2.20	0.41
2:x:294:ILE:O	2:x:352:CYS:HA	2.19	0.41
2:1:452:GLN:O	2:1:453:VAL:C	2.63	0.41
13:AL:124:UNK:HA	13:AL:129:UNK:O	2.20	0.41
2:B:27:LEU:O	2:B:74:VAL:HA	2.21	0.41
2:B:353:TYR:HA	2:B:362:SER:HA	2.03	0.41
4:N:493:CYS:HA	4:N:505:THR:HA	2.01	0.41
13:e:445:UNK:HA	13:e:458:UNK:O	2.21	0.41
2:z:50:ILE:N	2:z:57:ILE:O	2.53	0.41
4:8:318:VAL:O	4:8:331:PRO:CB	2.68	0.41
5:R:94:GLN:O	5:R:95:PRO:C	2.64	0.41
11:c:318:LEU:O	11:c:375:VAL:HA	2.20	0.41
13:e:117:UNK:O	13:e:118:UNK:C	2.69	0.41
9:o:525:GLY:HA3	9:o:569:TRP:HA	2.03	0.41
2:v:411:PRO:O	2:v:423:GLY:HA2	2.21	0.41
2:v:447:PHE:O	2:v:450:ALA:HB3	2.20	0.41
2:3:90:LYS:HA	2:3:109:LEU:O	2.21	0.41
2:3:602:PHE:O	2:3:603:PRO:C	2.64	0.41
4:5:393:ALA:HB2	4:5:432:ALA:O	2.21	0.41
2:B:476:VAL:O	2:B:488:PHE:HA	2.20	0.41
7:X:207:TRP:CB	7:X:212:ALA:HB2	2.50	0.41
13:g:2:UNK:O	13:g:3:UNK:C	2.68	0.41
2:t:473:MET:HA	2:t:491:LEU:O	2.21	0.41
2:v:212:TYR:HA	2:v:223:LEU:HA	2.03	0.41
2:1:142:TRP:O	2:1:146:GLY:HA3	2.20	0.41
2:1:153:VAL:HA	2:1:249:ALA:O	2.21	0.41
3:4:643:LYS:HA	3:4:671:ILE:HA	2.02	0.41
3:7:144:HIS:O	3:7:287:LEU:HA	2.19	0.41
10:AI:108:SER:O	10:AI:112:ASP:N	2.54	0.41
2:D:40:PHE:O	2:D:66:TRP:HA	2.20	0.41
2:D:51:HIS:O	2:D:75:ALA:HA	2.21	0.41
2:G:7:LEU:O	2:G:27:LEU:HA	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:617:ILE:O	2:K:648:PHE:HA	2.21	0.41
3:M:1055:ASN:O	3:M:1056:TRP:C	2.64	0.41
3:P:187:LYS:HA	3:P:245:PRO:HA	2.02	0.41
4:Q:301:VAL:O	4:Q:302:SER:C	2.64	0.41
13:e:133:UNK:HA	13:e:139:UNK:O	2.20	0.41
13:e:286:UNK:HA	13:e:303:UNK:CB	2.50	0.41
13:g:408:UNK:O	13:g:416:UNK:HA	2.21	0.41
2:u:217:GLY:O	2:u:218:SER:O	2.39	0.41
2:y:42:ILE:O	2:y:64:VAL:HA	2.21	0.41
2:y:46:PRO:O	2:y:60:LYS:HA	2.19	0.41
2:1:486:LYS:C	2:1:488:PHE:H	2.29	0.41
11:AJ:318:LEU:O	11:AJ:375:VAL:HA	2.21	0.41
12:AK:172:SER:O	12:AK:176:SER:N	2.54	0.41
2:C:200:HIS:HA	2:C:230:PRO:O	2.20	0.41
2:G:61:GLU:O	2:G:62:ASP:C	2.64	0.41
1:S:55:PHE:O	1:S:58:ASP:O	2.38	0.41
8:Z:546:LEU:O	8:Z:549:ALA:O	2.39	0.41
9:a:140:ARG:HA	9:a:146:ALA:O	2.19	0.41
13:g:218:UNK:HA	13:g:224:UNK:O	2.21	0.41
2:u:259:GLY:O	2:u:289:ARG:HA	2.21	0.41
2:v:48:ILE:H	2:v:59:GLY:HA3	1.86	0.41
2:1:182:ASN:HA	2:1:243:GLU:O	2.20	0.41
7:AE:658:LYS:O	7:AE:659:TYR:C	2.63	0.41
3:P:176:PHE:HA	3:P:218:VAL:O	2.20	0.41
13:e:46:UNK:O	13:e:49:UNK:O	2.39	0.41
2:m:581:LEU:HA	2:m:597:PHE:O	2.21	0.41
2:t:602:PHE:O	2:t:603:PRO:C	2.62	0.41
2:1:579:PHE:HA	2:1:600:PRO:HA	2.02	0.41
3:4:985:SER:HA	3:4:1014:ILE:O	2.20	0.41
8:AG:315:PRO:O	8:AG:316:VAL:C	2.64	0.41
9:AH:33:GLU:O	9:AH:37:HIS:HA	2.21	0.41
13:AL:118:UNK:O	13:AL:119:UNK:C	2.67	0.41
13:AL:165:UNK:O	13:AL:172:UNK:HA	2.20	0.41
2:B:473:MET:HA	2:B:491:LEU:O	2.21	0.41
2:C:579:PHE:HA	2:C:601:TYR:H	1.85	0.41
2:D:41:THR:O	2:D:93:VAL:HA	2.21	0.41
2:E:212:TYR:HA	2:E:223:LEU:HA	2.02	0.41
2:F:264:SER:HA	2:F:284:ASP:O	2.21	0.41
2:G:356:ALA:O	2:G:357:PRO:C	2.64	0.41
3:M:932:GLY:HA2	3:M:961:GLY:O	2.21	0.41
8:Z:949:LEU:O	8:Z:977:ILE:HA	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:c:101:ASN:HA	11:c:144:GLY:HA3	2.03	0.41
13:e:3:UNK:O	13:e:4:UNK:C	2.68	0.41
13:g:433:UNK:O	13:g:434:UNK:CB	2.68	0.41
2:m:212:TYR:HA	2:m:222:GLU:O	2.20	0.41
2:m:212:TYR:HA	2:m:223:LEU:HA	2.03	0.41
2:m:261:ILE:O	2:m:288:PHE:N	2.54	0.41
2:s:472:PHE:O	2:s:492:LEU:HA	2.21	0.41
2:t:50:ILE:N	2:t:57:ILE:O	2.53	0.41
2:v:130:MET:O	2:y:61:GLU:O	2.39	0.41
2:x:43:ARG:HA	2:x:63:THR:O	2.21	0.41
1:0:43:ARG:HA	1:0:86:ILE:O	2.20	0.41
2:3:424:ARG:HA	2:3:454:GLN:O	2.22	0.41
3:7:1016:GLY:HA2	3:7:1043:ASP:O	2.21	0.41
9:AH:456:GLY:HA3	9:AH:462:ALA:HA	2.02	0.41
12:AK:18:ALA:O	12:AK:19:LYS:C	2.62	0.41
2:D:353:TYR:HA	2:D:362:SER:HA	2.03	0.41
2:G:46:PRO:HA	2:G:60:LYS:HA	2.03	0.41
3:M:847:ASN:HA	3:M:875:THR:O	2.21	0.41
15:V:31:GLN:O	15:V:35:GLY:N	2.54	0.41
10:b:59:ASP:O	10:b:60:TYR:C	2.63	0.41
13:g:315:UNK:O	13:g:333:UNK:HA	2.21	0.41
2:A:602:PHE:O	2:A:603:PRO:C	2.63	0.40
2:C:23:MET:O	2:C:78:ARG:HA	2.21	0.40
2:D:50:ILE:N	2:D:57:ILE:O	2.54	0.40
2:G:51:HIS:O	2:G:75:ALA:HB1	2.21	0.40
2:G:565:LEU:O	2:G:566:GLY:C	2.63	0.40
2:G:585:THR:O	2:G:587:VAL:N	2.54	0.40
2:I:206:ALA:HB1	2:I:226:GLY:O	2.21	0.40
2:I:454:GLN:O	2:I:455:ALA:C	2.62	0.40
2:I:613:LYS:O	2:I:645:LYS:N	2.54	0.40
2:J:37:CYS:HA	2:J:97:CYS:HA	2.03	0.40
2:L:24:GLU:HA	2:L:77:VAL:O	2.21	0.40
3:M:874:LEU:O	3:M:902:GLU:O	2.39	0.40
4:N:451:LEU:O	4:N:464:GLU:HA	2.21	0.40
2:m:215:GLN:O	2:m:216:ARG:C	2.64	0.40
9:o:493:GLY:C	9:o:495:LYS:H	2.29	0.40
2:v:494:SER:N	2:v:575:ILE:O	2.54	0.40
2:z:46:PRO:HA	2:z:59:GLY:HA3	2.03	0.40
2:3:129:ASP:O	2:3:130:MET:C	2.65	0.40
2:A:454:GLN:O	2:A:455:ALA:C	2.64	0.40
2:A:514:THR:HA	2:A:532:LYS:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AH:448:ARG:O	9:AH:449:PRO:C	2.64	0.40
2:C:46:PRO:O	2:C:60:LYS:N	2.54	0.40
2:D:45:SER:N	2:D:59:GLY:O	2.54	0.40
2:E:37:CYS:HA	2:E:97:CYS:HA	2.02	0.40
2:I:353:TYR:HA	2:I:362:SER:HA	2.03	0.40
4:Q:537:HIS:HA	4:Q:543:ALA:O	2.20	0.40
13:e:78:UNK:O	13:e:79:UNK:C	2.68	0.40
13:e:98:UNK:O	13:e:99:UNK:C	2.68	0.40
2:m:268:VAL:HA	2:m:280:PRO:HA	2.02	0.40
2:m:353:TYR:HA	2:m:362:SER:HA	2.03	0.40
2:y:269:GLU:N	2:y:279:ILE:O	2.54	0.40
2:1:36:LYS:O	2:1:97:CYS:HA	2.21	0.40
2:A:349:MET:HA	2:A:365:LEU:O	2.21	0.40
10:AI:85:CYS:O	10:AI:86:LEU:C	2.65	0.40
14:AO:78:LYS:O	14:AO:79:GLU:C	2.64	0.40
2:D:43:ARG:CB	2:D:63:THR:O	2.69	0.40
2:E:269:GLU:O	2:E:278:GLU:HA	2.21	0.40
2:J:206:ALA:HB1	2:J:226:GLY:O	2.21	0.40
3:M:916:LEU:O	3:M:917:ALA:C	2.64	0.40
4:Q:458:MET:O	4:Q:459:ALA:C	2.64	0.40
6:T:48:GLN:O	6:T:49:PRO:C	2.64	0.40
13:e:346:UNK:HA	13:e:360:UNK:O	2.21	0.40
2:m:45:SER:O	2:m:59:GLY:C	2.64	0.40
2:m:624:LYS:O	2:m:625:ILE:C	2.65	0.40
7:AF:860:LYS:HA	7:AF:888:LEU:HA	2.03	0.40
13:AL:219:UNK:O	13:AL:223:UNK:HA	2.21	0.40
2:C:324:SER:O	2:C:328:LYS:N	2.54	0.40
2:D:80:VAL:O	2:D:81:ALA:HB2	2.22	0.40
2:D:206:ALA:HB1	2:D:226:GLY:O	2.21	0.40
2:G:170:GLU:O	2:G:171:GLY:C	2.65	0.40
2:G:265:LEU:O	2:G:283:LYS:HA	2.21	0.40
2:G:267:LEU:O	2:G:280:PRO:CB	2.69	0.40
2:I:23:MET:O	2:I:78:ARG:HA	2.22	0.40
2:J:514:THR:HA	2:J:532:LYS:O	2.21	0.40
2:L:602:PHE:O	2:L:603:PRO:C	2.64	0.40
3:P:681:VAL:O	3:P:682:VAL:C	2.65	0.40
3:P:785:GLN:HA	3:P:812:LEU:HA	2.03	0.40
8:Z:513:ASP:HA	8:Z:540:ALA:HB2	2.03	0.40
9:a:464:SER:HA	9:a:538:ARG:O	2.22	0.40
11:c:98:ASP:C	11:c:100:ALA:H	2.30	0.40
13:g:112:UNK:O	13:g:113:UNK:C	2.69	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:p:39:GLY:HA3	10:p:45:TYR:O	2.21	0.40
2:t:153:VAL:HA	2:t:249:ALA:O	2.22	0.40
2:w:651:ASP:O	2:w:652:PHE:C	2.63	0.40
2:x:49:LEU:O	2:x:77:VAL:HA	2.22	0.40
11:AJ:320:ARG:HA	11:AJ:356:ASN:O	2.22	0.40
13:AL:117:UNK:O	13:AL:118:UNK:C	2.68	0.40
2:D:217:GLY:O	2:D:218:SER:C	2.64	0.40
2:F:353:TYR:HA	2:F:362:SER:HA	2.03	0.40
8:Z:662:ARG:HA	8:Z:689:LEU:HA	2.03	0.40
2:u:602:PHE:O	2:u:603:PRO:C	2.65	0.40
2:x:50:ILE:O	2:x:57:ILE:N	2.55	0.40
2:z:579:PHE:HA	2:z:601:TYR:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	134/440 (30%)	127 (95%)	7 (5%)	0	100	100
1	S	134/440 (30%)	128 (96%)	6 (4%)	0	100	100
2	1	680/682 (100%)	601 (88%)	76 (11%)	3 (0%)	30	67
2	2	680/682 (100%)	651 (96%)	29 (4%)	0	100	100
2	3	680/682 (100%)	643 (95%)	37 (5%)	0	100	100
2	A	680/682 (100%)	616 (91%)	63 (9%)	1 (0%)	48	83
2	B	680/682 (100%)	631 (93%)	48 (7%)	1 (0%)	48	83
2	C	680/682 (100%)	631 (93%)	49 (7%)	0	100	100
2	D	680/682 (100%)	621 (91%)	58 (8%)	1 (0%)	48	83
2	E	680/682 (100%)	637 (94%)	43 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	680/682 (100%)	632 (93%)	47 (7%)	1 (0%)	48	83
2	G	680/682 (100%)	602 (88%)	78 (12%)	0	100	100
2	H	680/682 (100%)	632 (93%)	48 (7%)	0	100	100
2	I	680/682 (100%)	630 (93%)	49 (7%)	1 (0%)	48	83
2	J	680/682 (100%)	617 (91%)	61 (9%)	2 (0%)	36	72
2	K	680/682 (100%)	656 (96%)	24 (4%)	0	100	100
2	L	680/682 (100%)	656 (96%)	24 (4%)	0	100	100
2	m	680/682 (100%)	624 (92%)	55 (8%)	1 (0%)	48	83
2	s	680/682 (100%)	613 (90%)	65 (10%)	2 (0%)	36	72
2	t	680/682 (100%)	642 (94%)	37 (5%)	1 (0%)	48	83
2	u	680/682 (100%)	607 (89%)	72 (11%)	1 (0%)	48	83
2	v	680/682 (100%)	626 (92%)	53 (8%)	1 (0%)	48	83
2	w	680/682 (100%)	635 (93%)	44 (6%)	1 (0%)	48	83
2	x	680/682 (100%)	620 (91%)	59 (9%)	1 (0%)	48	83
2	y	680/682 (100%)	630 (93%)	49 (7%)	1 (0%)	48	83
2	z	680/682 (100%)	638 (94%)	42 (6%)	0	100	100
3	4	945/1163 (81%)	859 (91%)	86 (9%)	0	100	100
3	7	945/1163 (81%)	874 (92%)	71 (8%)	0	100	100
3	M	945/1163 (81%)	865 (92%)	80 (8%)	0	100	100
3	P	945/1163 (81%)	855 (90%)	90 (10%)	0	100	100
4	5	363/581 (62%)	330 (91%)	32 (9%)	1 (0%)	36	72
4	8	363/581 (62%)	331 (91%)	32 (9%)	0	100	100
4	N	363/581 (62%)	321 (88%)	41 (11%)	1 (0%)	36	72
4	Q	363/581 (62%)	314 (86%)	49 (14%)	0	100	100
5	6	117/164 (71%)	111 (95%)	6 (5%)	0	100	100
5	9	87/164 (53%)	74 (85%)	13 (15%)	0	100	100
5	O	117/164 (71%)	113 (97%)	4 (3%)	0	100	100
5	R	87/164 (53%)	75 (86%)	12 (14%)	0	100	100
6	AA	61/228 (27%)	56 (92%)	5 (8%)	0	100	100
6	T	61/228 (27%)	58 (95%)	3 (5%)	0	100	100
7	AE	931/937 (99%)	860 (92%)	69 (7%)	2 (0%)	43	78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AF	843/937 (90%)	797 (94%)	45 (5%)	1 (0%)	48	83
7	X	931/937 (99%)	889 (96%)	41 (4%)	1 (0%)	48	83
7	Y	843/937 (90%)	793 (94%)	48 (6%)	2 (0%)	43	78
8	AG	964/993 (97%)	892 (92%)	72 (8%)	0	100	100
8	Z	964/993 (97%)	892 (92%)	72 (8%)	0	100	100
8	n	964/993 (97%)	901 (94%)	63 (6%)	0	100	100
9	AH	623/782 (80%)	578 (93%)	45 (7%)	0	100	100
9	a	623/782 (80%)	577 (93%)	46 (7%)	0	100	100
9	o	623/782 (80%)	568 (91%)	55 (9%)	0	100	100
10	AI	145/147 (99%)	128 (88%)	17 (12%)	0	100	100
10	b	145/147 (99%)	130 (90%)	15 (10%)	0	100	100
10	p	145/147 (99%)	133 (92%)	12 (8%)	0	100	100
11	AJ	438/449 (98%)	409 (93%)	29 (7%)	0	100	100
11	c	438/449 (98%)	409 (93%)	29 (7%)	0	100	100
11	q	438/449 (98%)	422 (96%)	16 (4%)	0	100	100
12	AK	429/445 (96%)	408 (95%)	21 (5%)	0	100	100
12	d	429/445 (96%)	405 (94%)	24 (6%)	0	100	100
12	r	429/445 (96%)	416 (97%)	13 (3%)	0	100	100
14	AM	161/163 (99%)	157 (98%)	4 (2%)	0	100	100
14	AO	161/163 (99%)	150 (93%)	11 (7%)	0	100	100
14	f	161/163 (99%)	157 (98%)	4 (2%)	0	100	100
14	h	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
15	U	72/76 (95%)	69 (96%)	3 (4%)	0	100	100
15	V	72/76 (95%)	69 (96%)	3 (4%)	0	100	100
15	W	72/76 (95%)	68 (94%)	4 (6%)	0	100	100
All	All	34555/38412 (90%)	32013 (93%)	2515 (7%)	27 (0%)	49	83

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	567	LEU
7	AF	926	PHE
2	D	218	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	Y	870	LYS
2	s	218	SER
2	x	80	VAL
2	1	53	SER
2	1	453	VAL
2	1	566	GLY
2	J	625	ILE
7	Y	928	VAL
2	s	566	GLY
2	u	218	SER
2	I	567	LEU
2	J	53	SER
7	X	926	PHE
2	v	53	SER
2	w	53	SER
2	B	625	ILE
2	F	53	SER
4	N	276	GLU
2	t	53	SER
2	y	53	SER
2	m	53	SER
4	5	276	GLU
7	AE	926	PHE
7	AE	928	VAL

5.3.2 Protein sidechains (i)

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

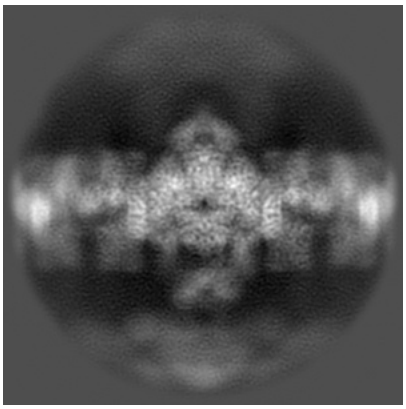
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-55607. These allow visual inspection of the internal detail of the map and identification of artifacts.

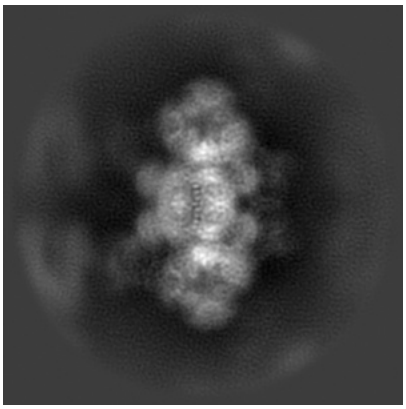
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

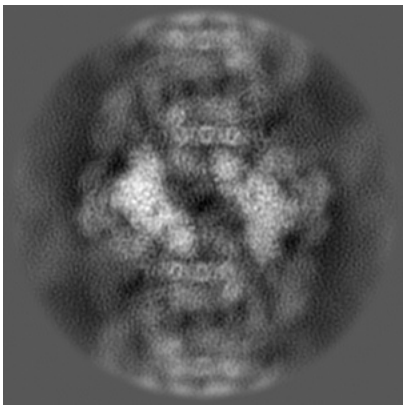
6.1.1 Primary map



X

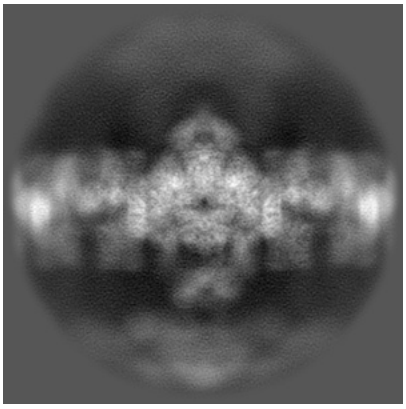


Y

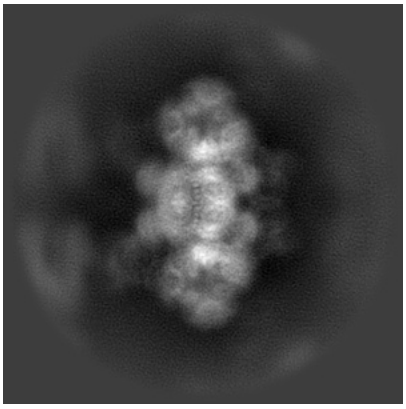


Z

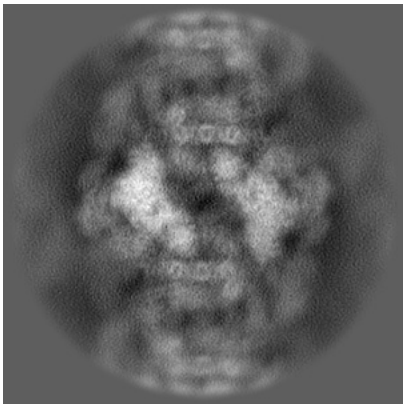
6.1.2 Raw map



X



Y

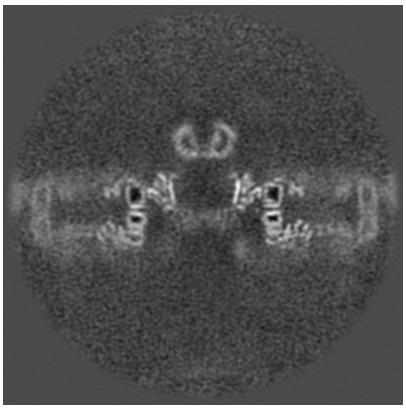


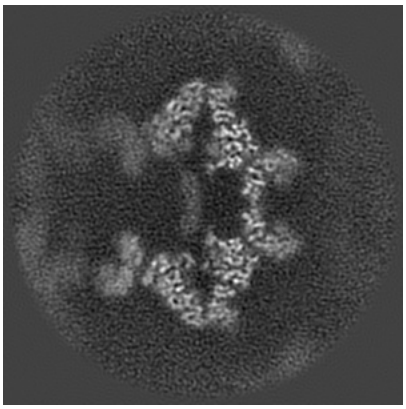
Z

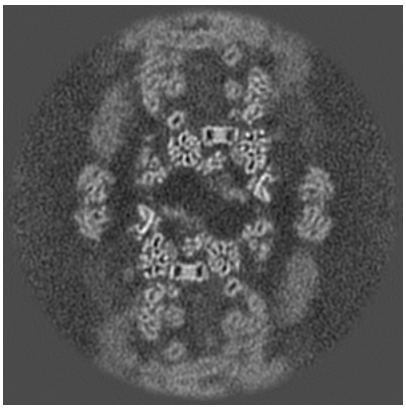
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

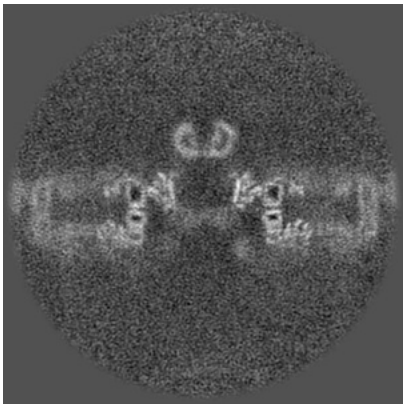
6.2.1 Primary map

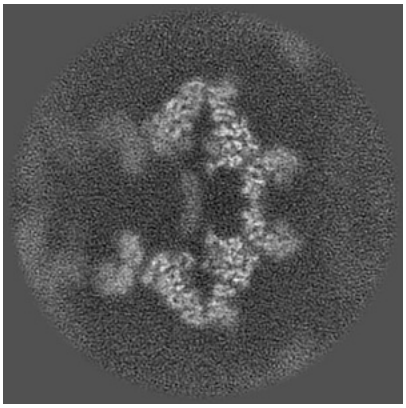

X Index: 128

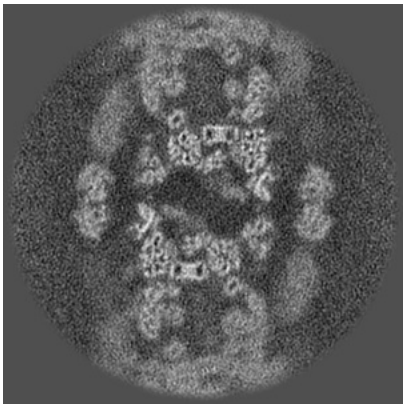

Y Index: 128


Z Index: 128

6.2.2 Raw map


X Index: 128

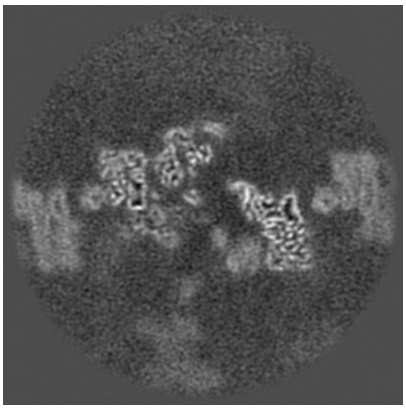

Y Index: 128

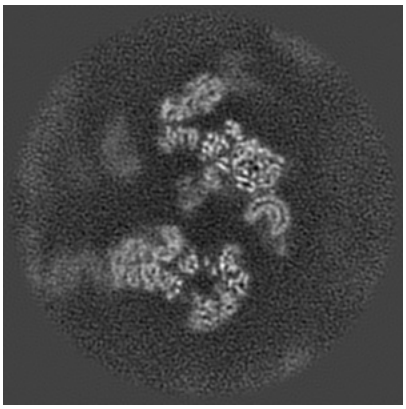

Z Index: 128

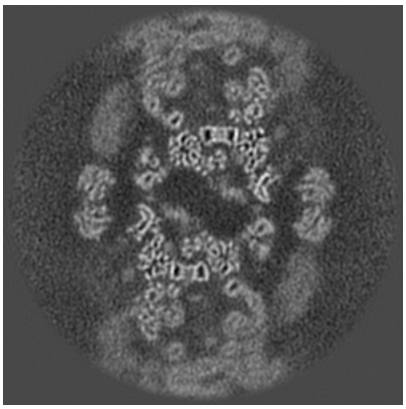
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

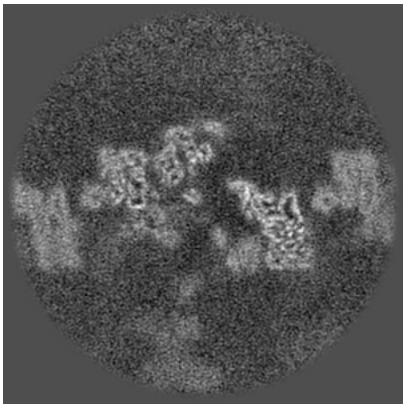
6.3.1 Primary map

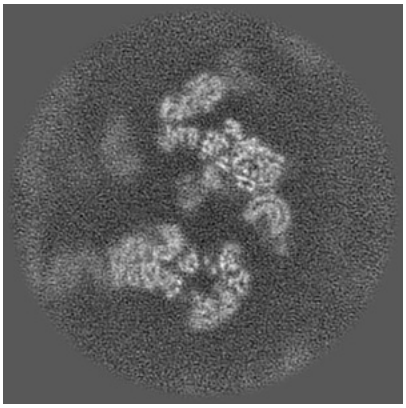

X Index: 111

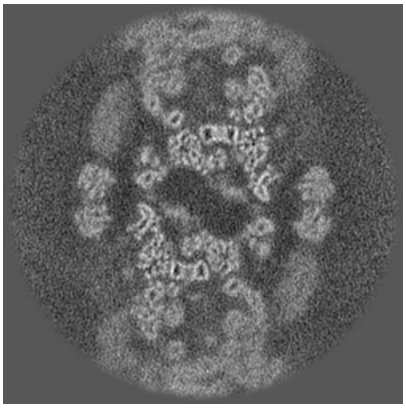

Y Index: 138


Z Index: 129

6.3.2 Raw map


X Index: 111

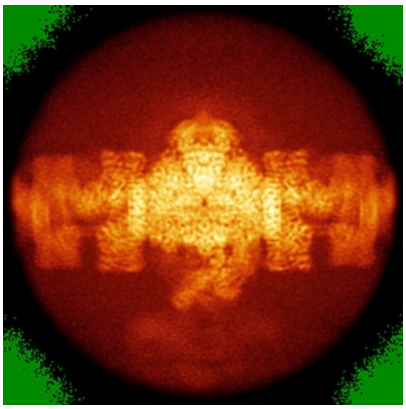

Y Index: 138

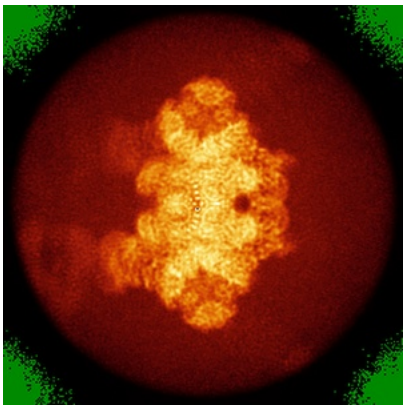

Z Index: 129

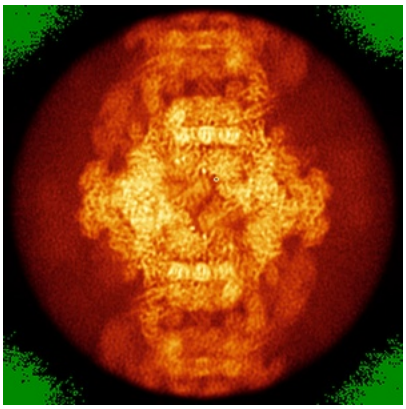
The images above show the largest variance slices of the map in three orthogonal directions.

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

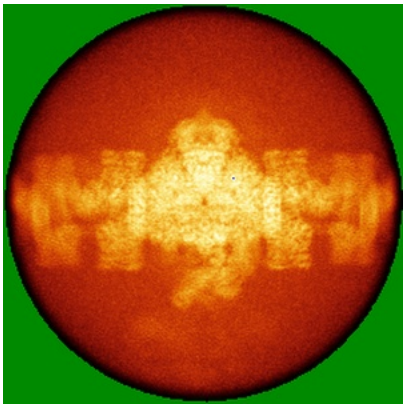
6.4.1 Primary map

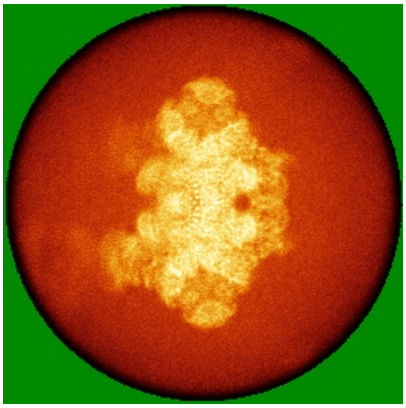

X

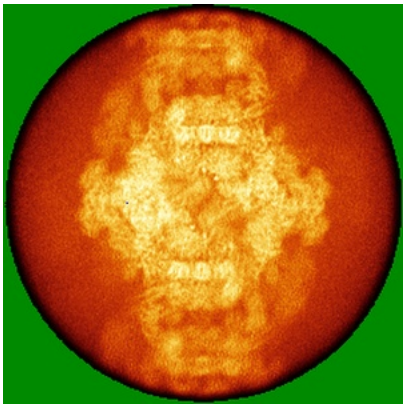

Y


Z

6.4.2 Raw map


X

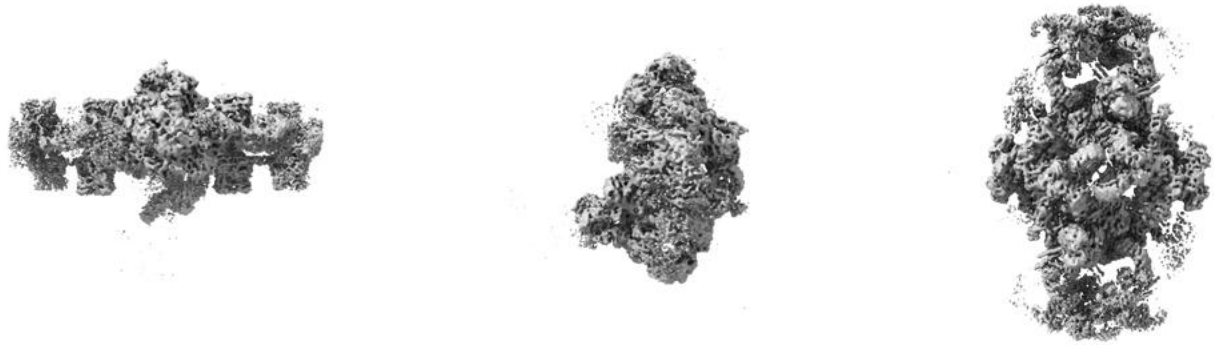

Y


Z

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

6.5 Orthogonal surface views (i)

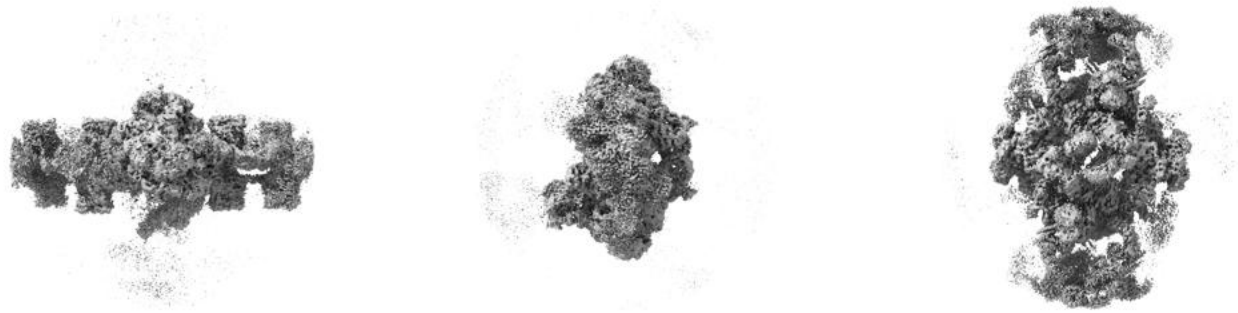
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.056. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

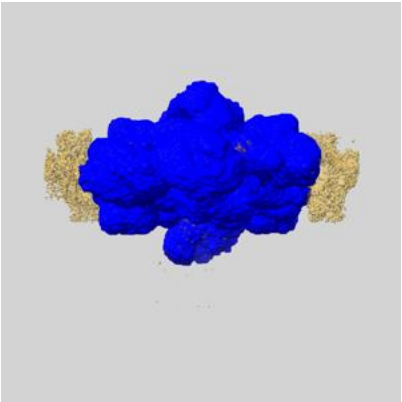
6.6 Mask visualisation (i)

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

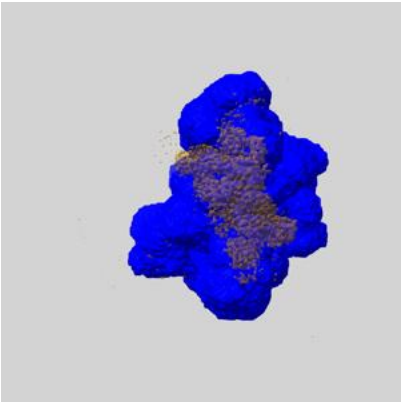
A mask typically either:

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

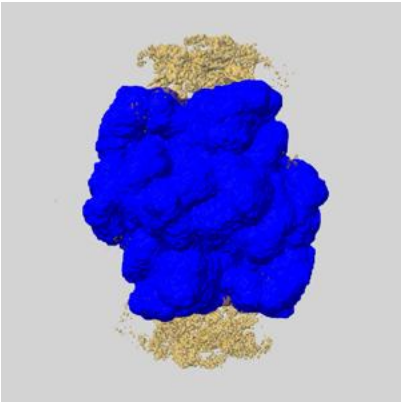
6.6.1 emd_55607_msk_1.map (i)



X



Y

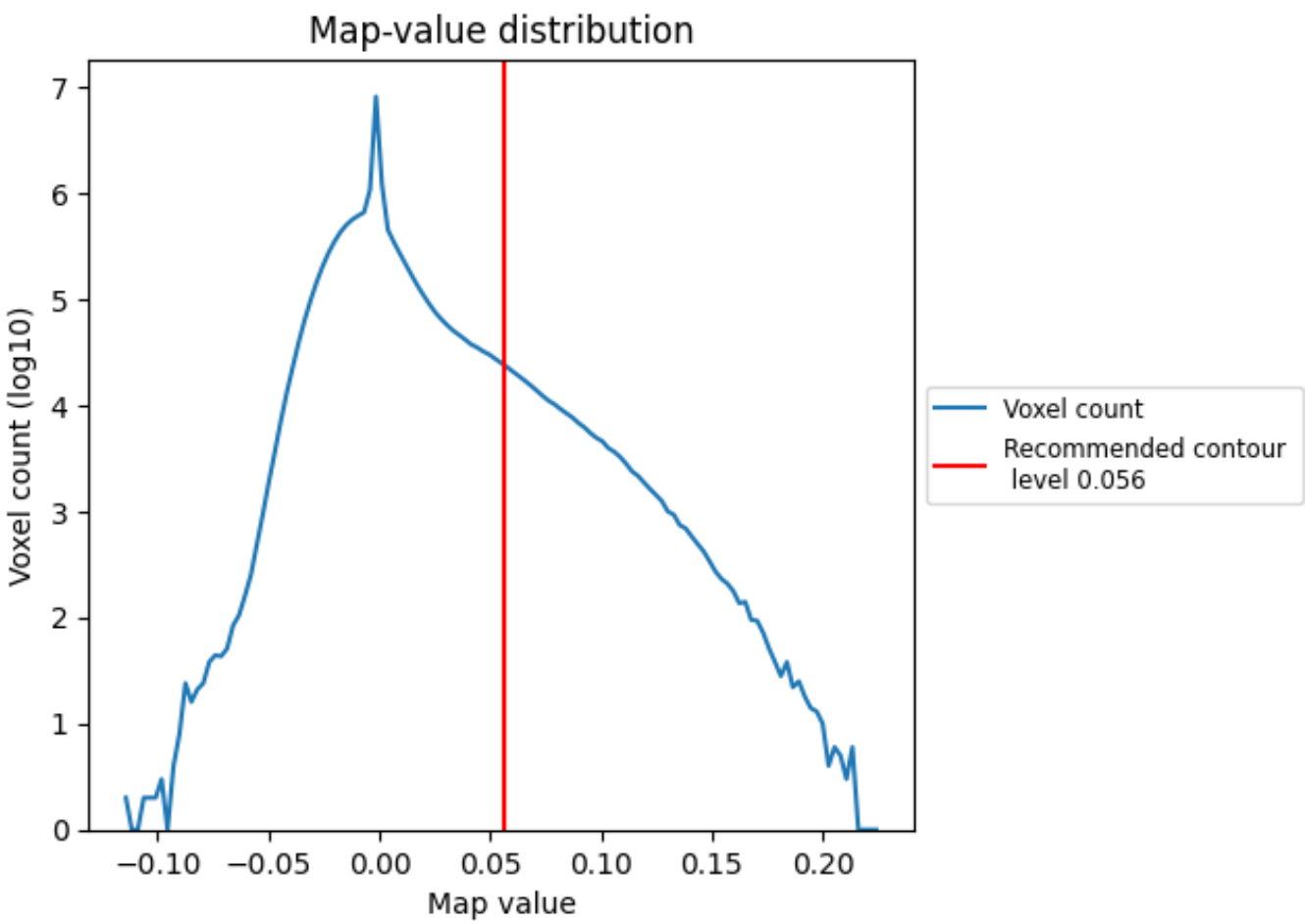


Z

7 Map analysis (i)

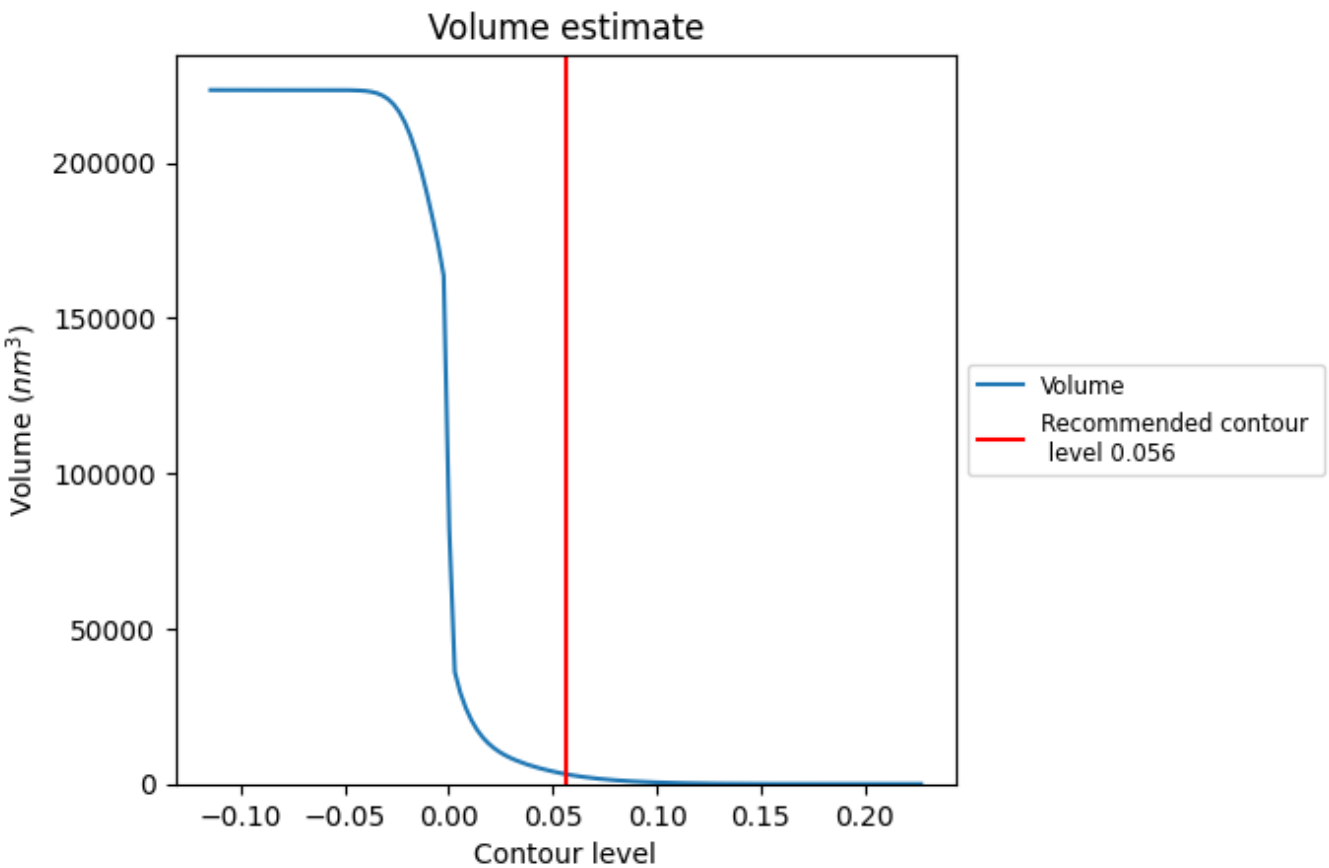
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

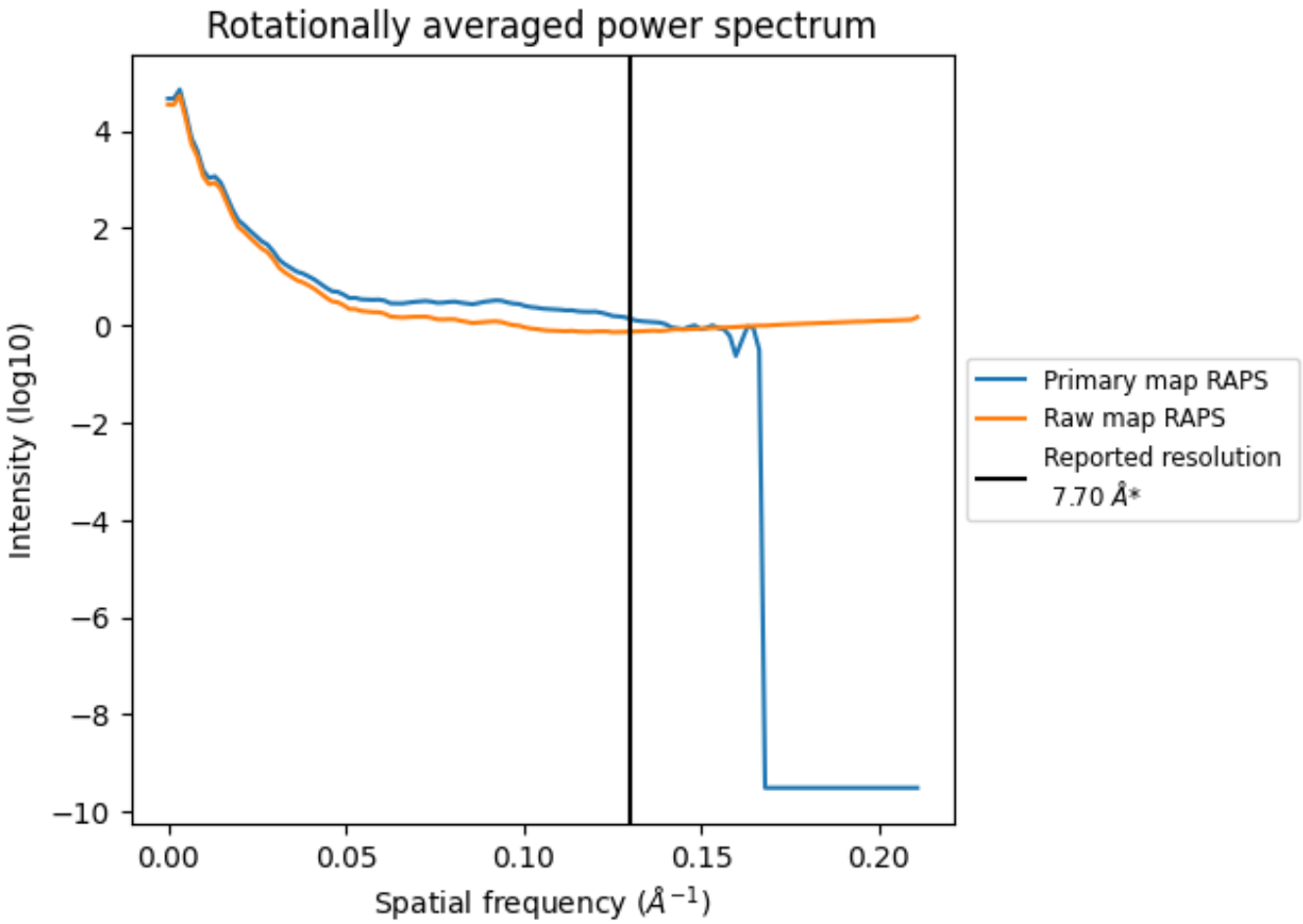
7.2 Volume estimate (i)



The volume at the recommended contour level is 3204 nm^3; this corresponds to an approximate mass of 2894 kDa.

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

7.3 Rotationally averaged power spectrum (i)

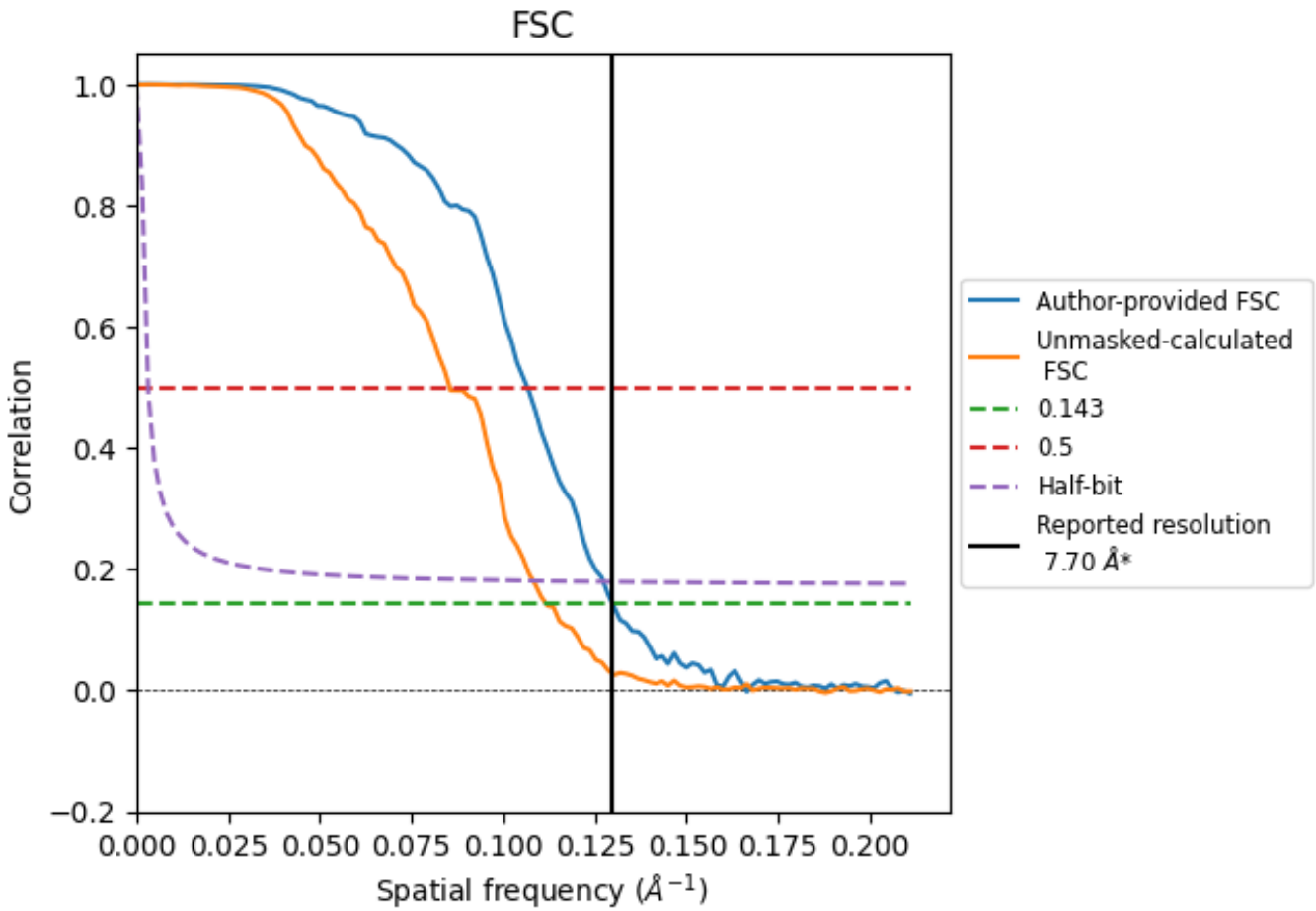


*Reported resolution corresponds to spatial frequency of 0.130 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.130 Å^{-1}

8.2 Resolution estimates (i)

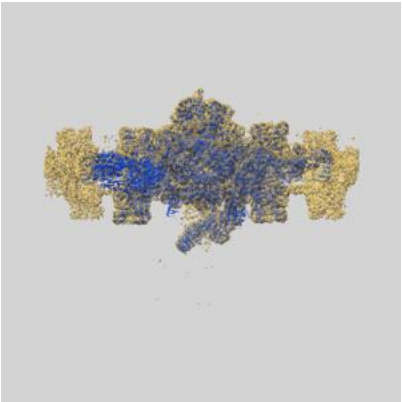
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.70	-	-
Author-provided FSC curve	7.70	9.38	7.86
Unmasked-calculated*	8.95	11.70	9.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.95 differs from the reported value 7.7 by more than 10 %

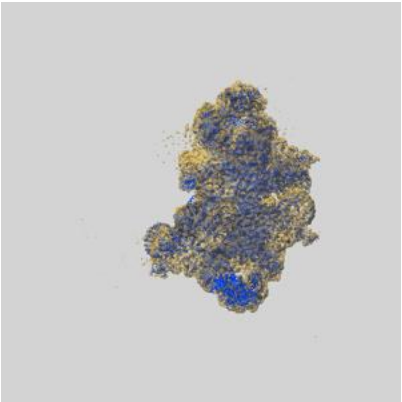
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-55607 and PDB model 9T67. Per-residue inclusion information can be found in section 3 on page 11.

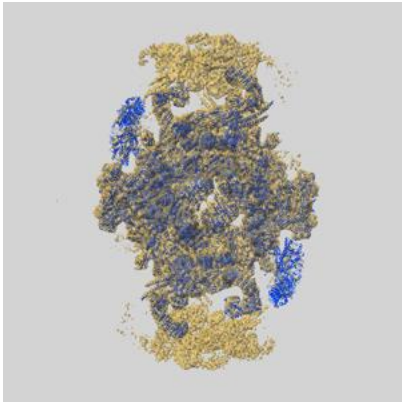
9.1 Map-model overlay (i)



X



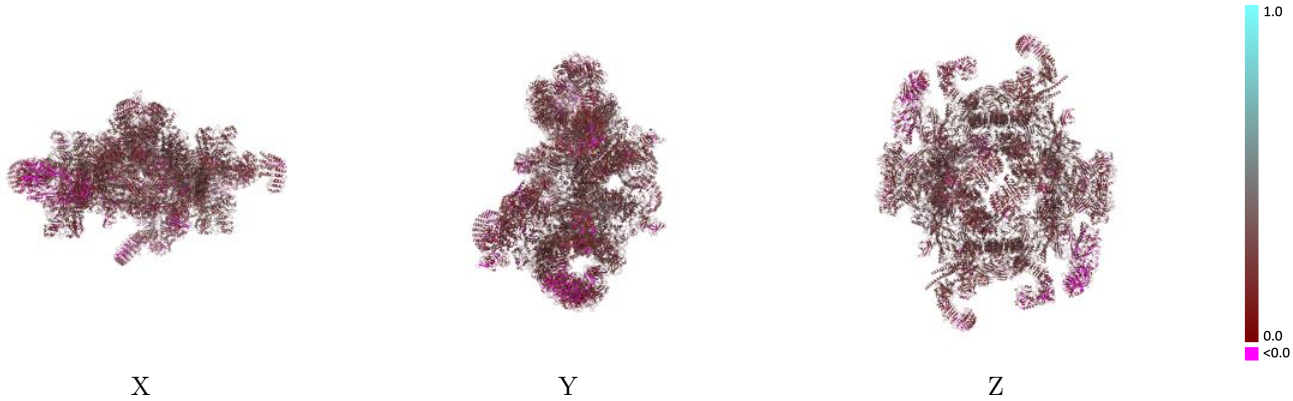
Y



Z

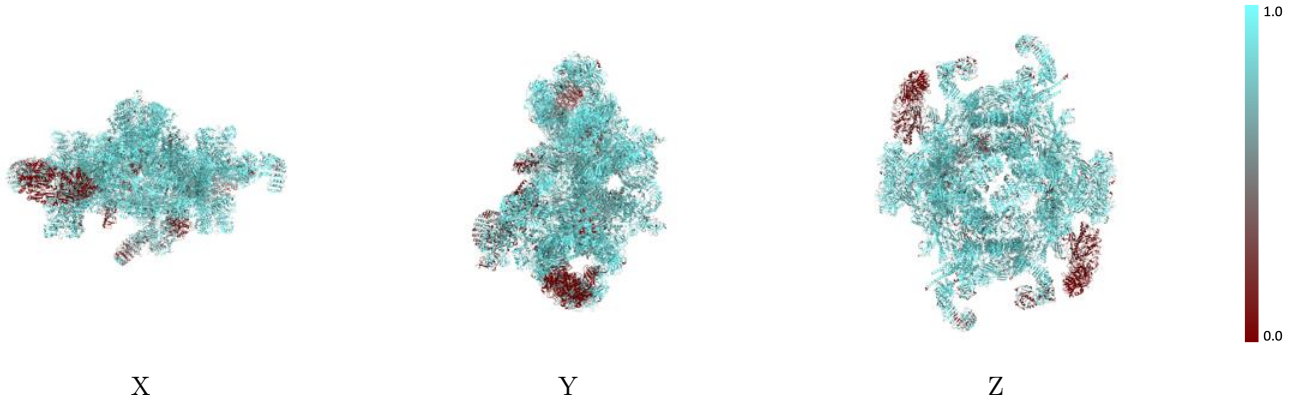
The images above show the 3D surface view of the map at the recommended contour level 0.056 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



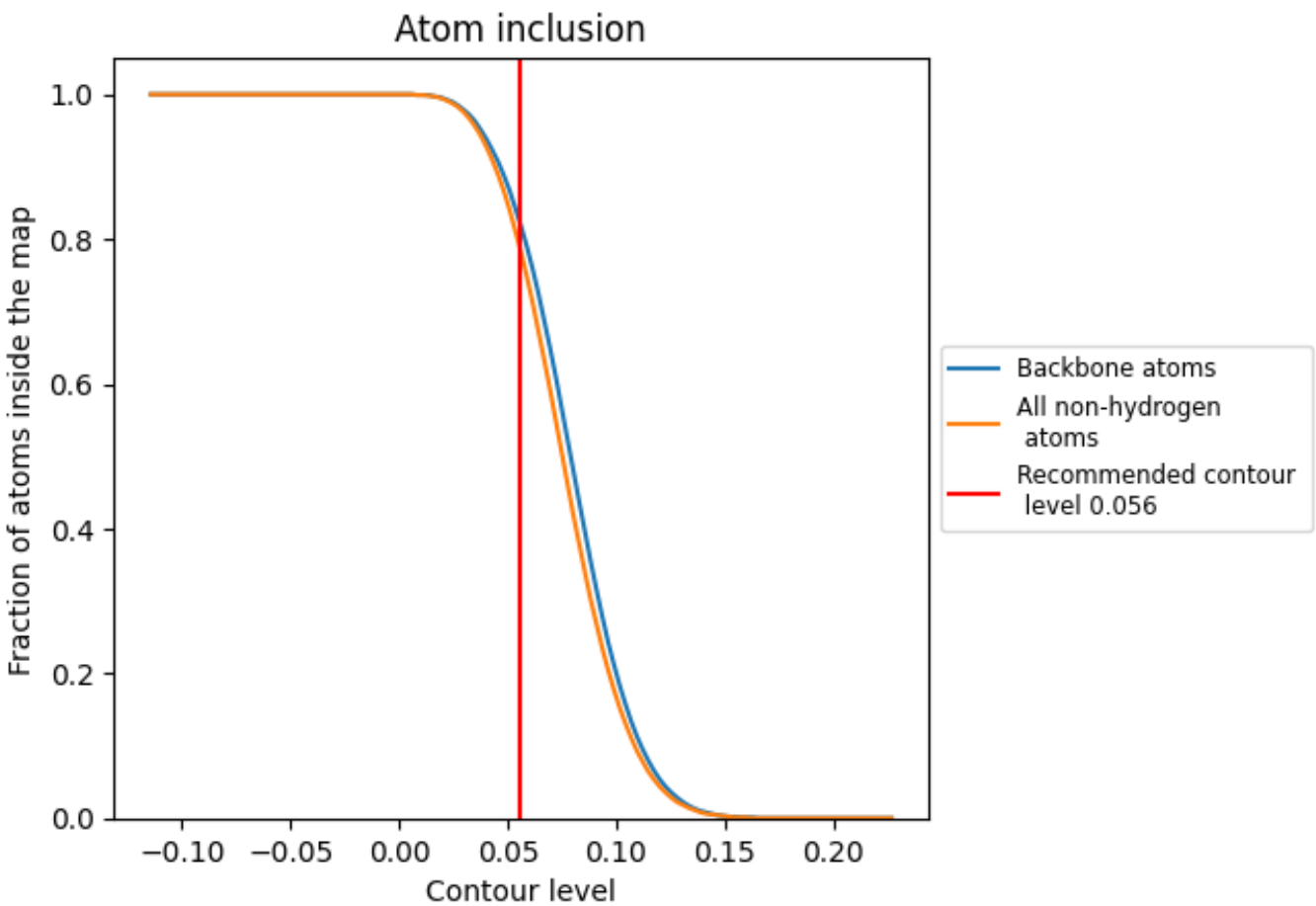
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.056).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.056) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7850	0.2360
0	0.8810	0.2510
1	0.8690	0.2590
2	0.0300	0.1110
3	0.0740	0.0930
4	0.9080	0.2630
5	0.8800	0.2470
6	0.9050	0.2750
7	0.8480	0.2360
8	0.8080	0.2180
9	0.7900	0.2390
A	0.9280	0.2870
AA	0.8330	0.2260
AE	0.7420	0.2110
AF	0.7030	0.2050
AG	0.8780	0.2460
AH	0.8480	0.2350
AI	0.9510	0.2720
AJ	0.8960	0.2480
AK	0.9100	0.2500
AL	0.6600	0.2250
AM	0.2050	0.1600
AN	0.9250	0.2630
AO	0.6720	0.2270
B	0.9050	0.2830
C	0.8870	0.2500
D	0.8750	0.2480
E	0.8350	0.2280
F	0.8310	0.2260
G	0.9150	0.2790
H	0.9170	0.2740
I	0.8840	0.2610
J	0.9170	0.2810
K	0.0880	0.1300
L	0.1500	0.1350

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
M	0.9210	0.2680
N	0.8970	0.2550
O	0.8950	0.2770
P	0.9340	0.2710
Q	0.9190	0.2650
R	0.8820	0.2630
S	0.9030	0.2820
T	0.9070	0.2560
U	0.7320	0.2880
V	0.3630	0.2800
W	0.0850	0.2510
X	0.8220	0.2220
Y	0.8210	0.2250
Z	0.8960	0.2500
a	0.8600	0.2370
b	0.9490	0.2710
c	0.9110	0.2670
d	0.9290	0.2710
e	0.7720	0.2470
f	0.2260	0.1690
g	0.9500	0.2870
h	0.7380	0.2360
m	0.9270	0.2890
n	0.6060	0.1610
o	0.7410	0.1840
p	0.9180	0.2600
q	0.6250	0.1910
r	0.2620	0.1130
s	0.9040	0.2750
t	0.9140	0.2670
u	0.9110	0.2730
v	0.8610	0.2350
w	0.8640	0.2340
x	0.9180	0.2820
y	0.9150	0.2680
z	0.8280	0.2330