wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 03:07 am GMT

PDB ID	:	6GSR
EMDB ID	:	EMD-0046
Title	:	Single Particle Cryo-EM map of human Transferrin receptor 1 - H-Ferritin complex at 5.5 Angstrom resolution.
Authors	:	Testi, C.; Montemiglio, L.C.; Vallone, B.; Des Georges, A.; Boffi, A.; Mancia, F.; Baiocco, P.
Deposited on	:	2018-06-15
Resolution	:	5.50 Å(reported)

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

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

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

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

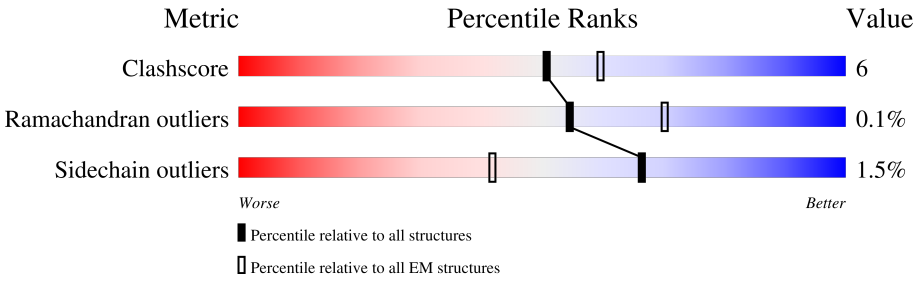
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	Aa	182	95% 93% · 5%
1	Ac	182	95% 93% · 5%
1	Ad	182	95% 93% · 5%
1	Ae	182	95% 93% · 5%
1	Af	182	95% 93% · 5%
1	Ag	182	95% 93% · 5%
1	Ah	182	95% 93% · 5%
1	Ai	182	95% 93% · 5%

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Mol	Chain	Length	Quality of chain
1	Aj	182	95% 93% • 5%
1	Ak	182	95% 93% • 5%
1	Al	182	95% 93% • 5%
1	Am	182	95% 93% • 5%
1	An	182	95% 93% • 5%
1	Ao	182	95% 93% • 5%
1	Ap	182	95% 93% • 5%
1	Ar	182	95% 93% • 5%
1	As	182	95% 93% • 5%
1	At	182	95% 93% • 5%
1	Au	182	95% 93% • 5%
1	Av	182	95% 93% • 5%
1	Aw	182	95% 93% • 5%
1	Ax	182	95% 93% • 5%
1	Ay	182	95% 93% • 5%
1	Az	182	95% 93% • 5%
2	Ab	640	99% 97% ••
2	Aq	640	99% 97% ••

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 45308 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 Ferritin heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Ac	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Ad	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Ae	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Af	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Ag	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Ah	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Ai	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Aj	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Ak	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Al	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Am	172	Total	C	N	O	S	10	0
			1431	903	244	275	9		
1	An	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Ao	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Ap	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Ar	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	As	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	At	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Au	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Av	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Aw	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Ax	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Ay	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Az	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		

- Molecule 2 is a protein called Transferrin receptor protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ab	633	Total	C	N	O	S	0	0
			4994	3201	843	936	14		
2	Aq	633	Total	C	N	O	S	0	0
			5004	3210	843	937	14		

There are 2 discrepancies between the modelled and reference sequences:

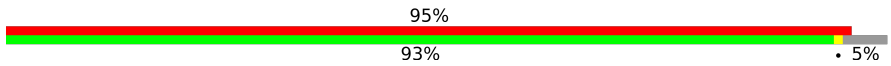
Chain	Residue	Modelled	Actual	Comment	Reference
Ab	142	SER	GLY	conflict	UNP P02786
Aq	142	SER	GLY	conflict	UNP P02786

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.

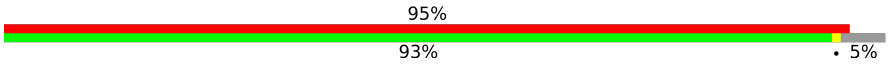
• Molecule 1: Ferritin heavy chain

Chain Aa:



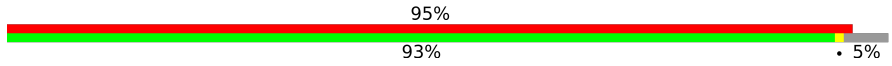
• Molecule 1: Ferritin heavy chain

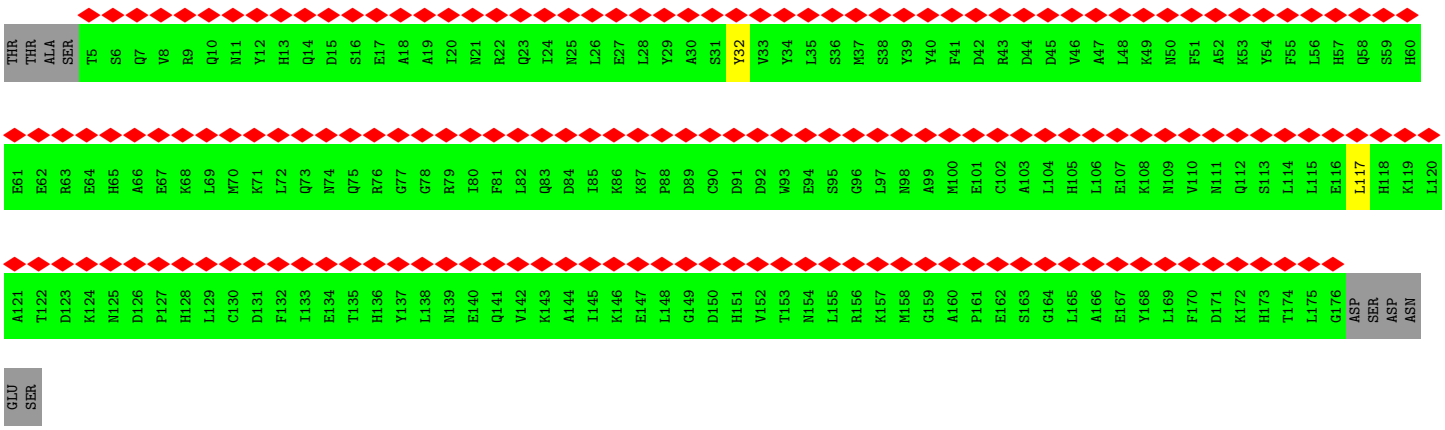
Chain Ac:



• Molecule 1: Ferritin heavy chain

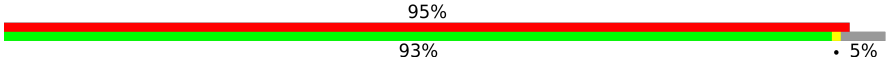
Chain Ad:

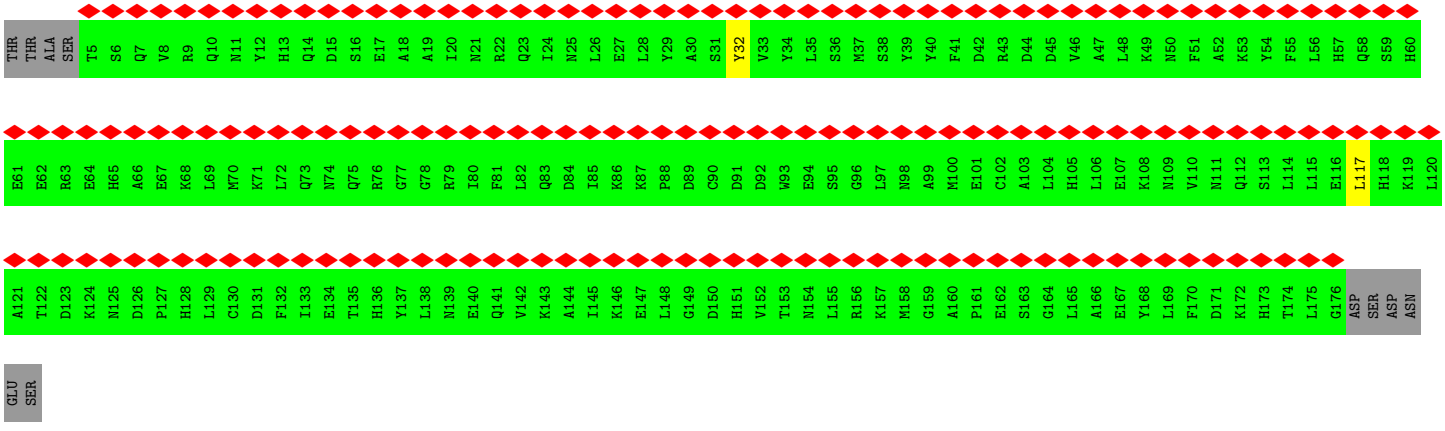




• Molecule 1: Ferritin heavy chain

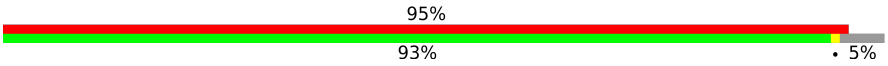
Chain Ae:

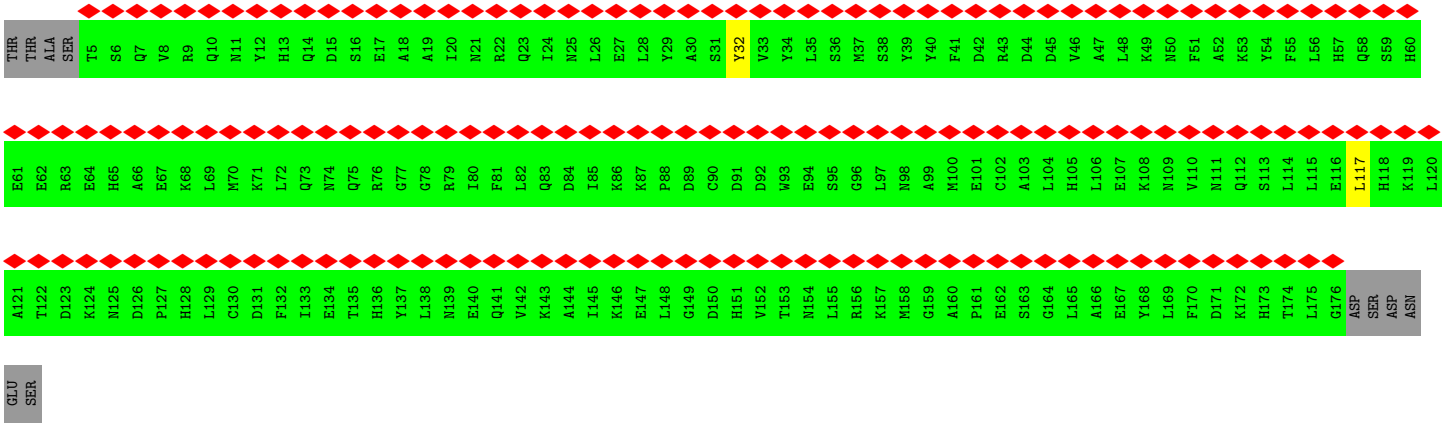




• Molecule 1: Ferritin heavy chain

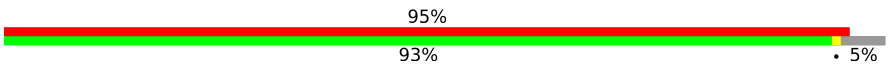
Chain Af:

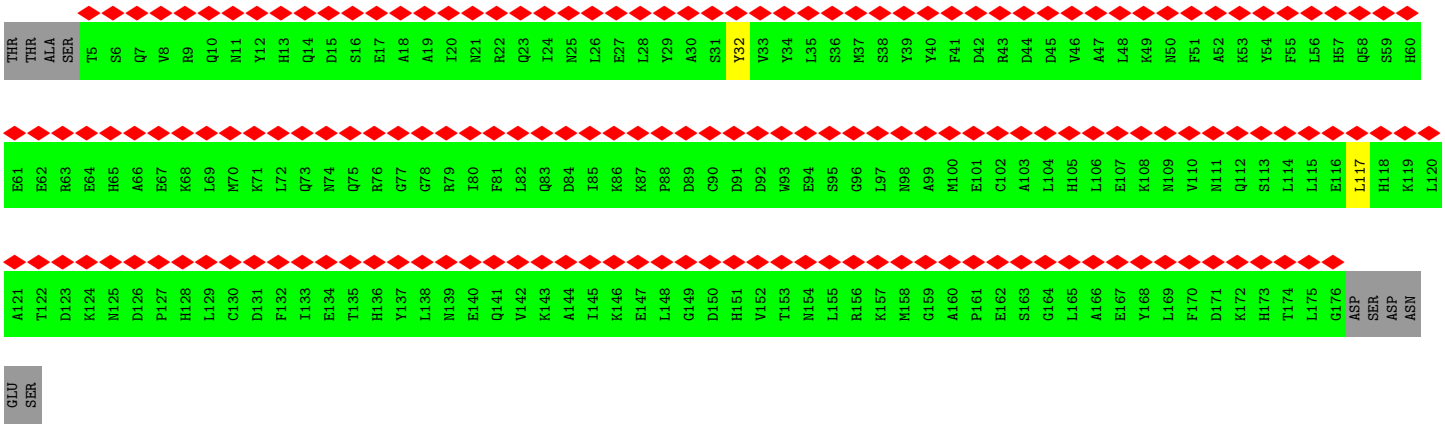




• Molecule 1: Ferritin heavy chain

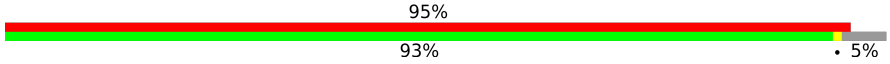
Chain Ag:

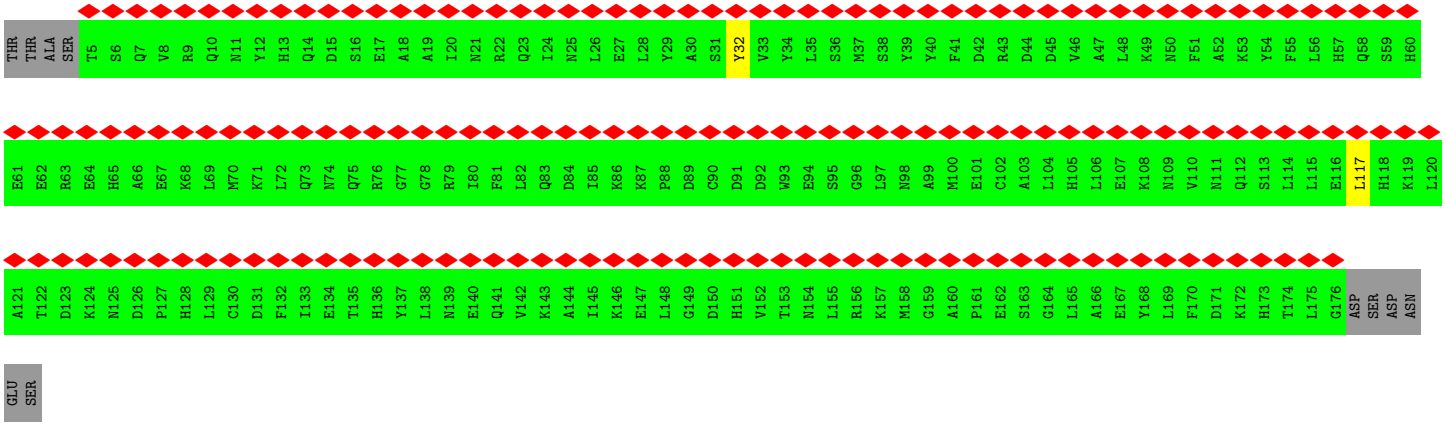




• Molecule 1: Ferritin heavy chain

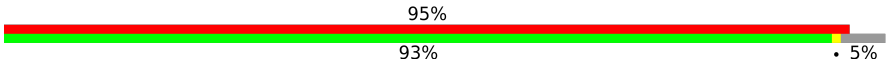
Chain Ah:

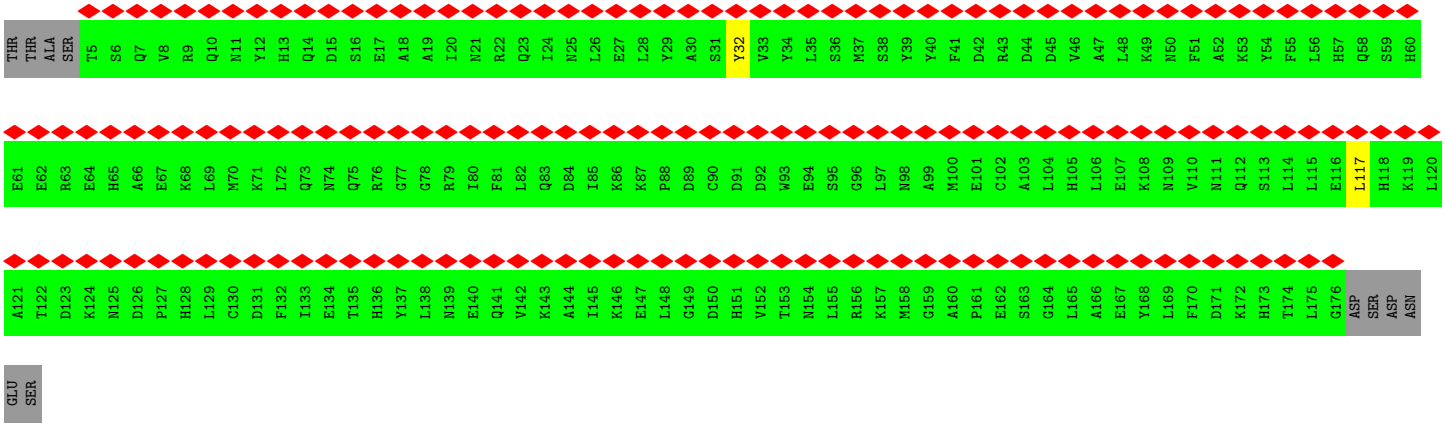




• Molecule 1: Ferritin heavy chain

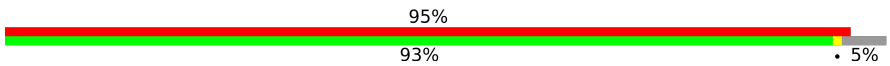
Chain Ai:

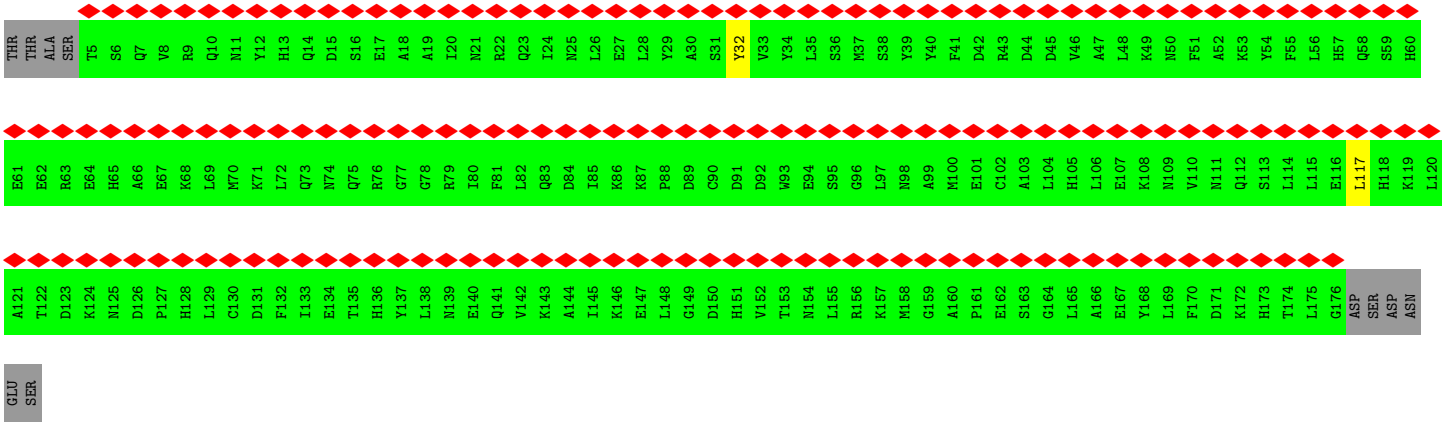




• Molecule 1: Ferritin heavy chain

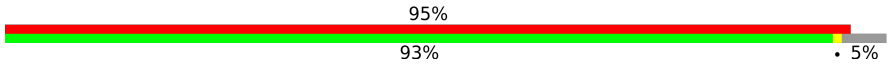
Chain Aj:

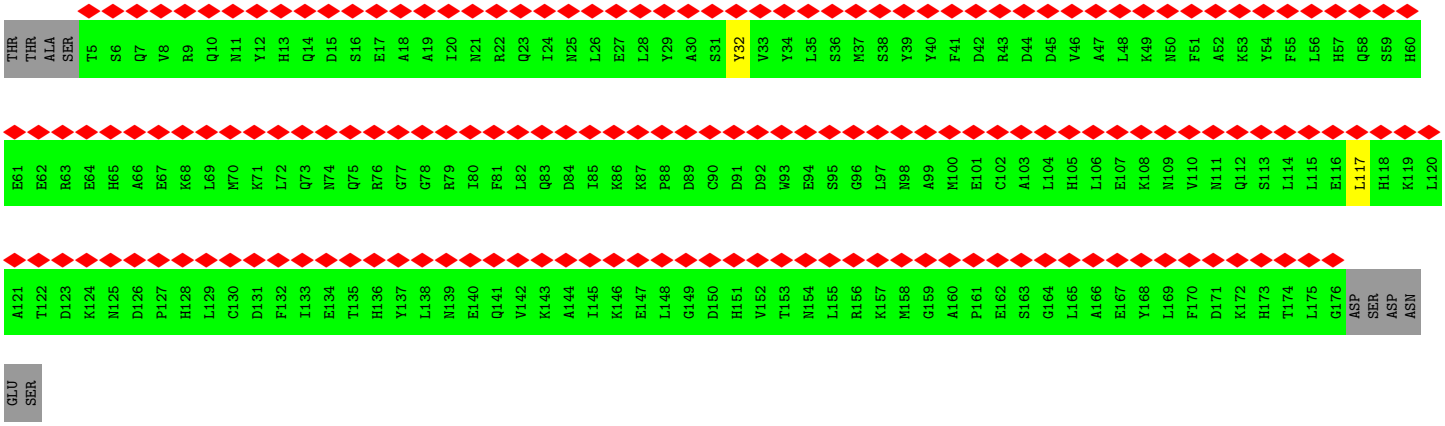




• Molecule 1: Ferritin heavy chain

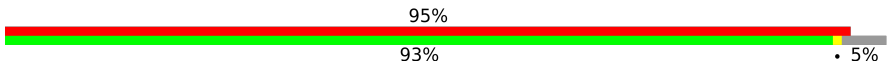
Chain Ak:

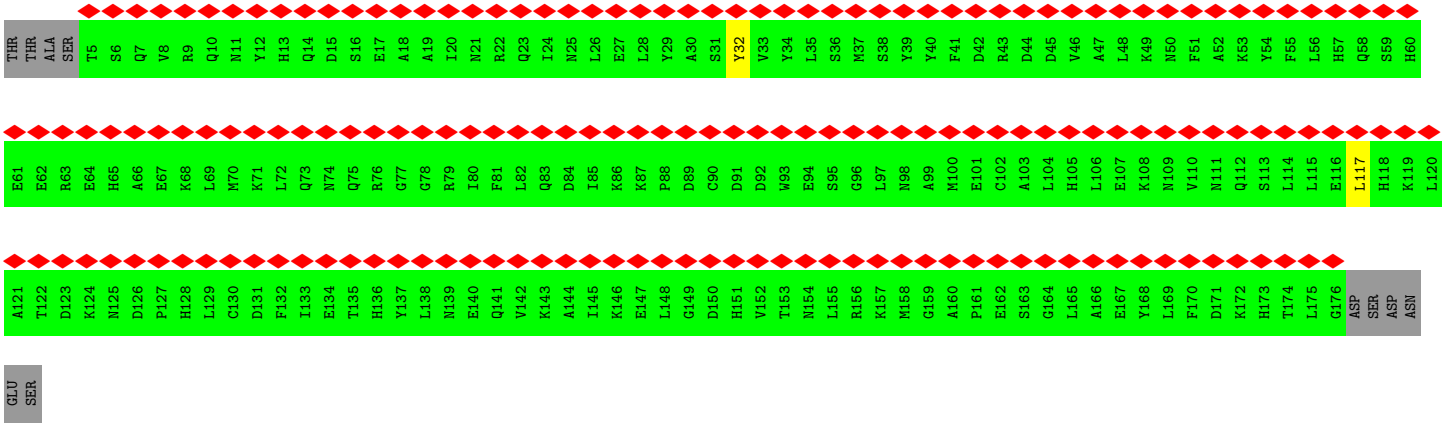




• Molecule 1: Ferritin heavy chain

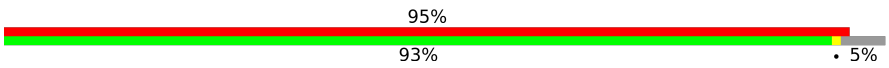
Chain Al:

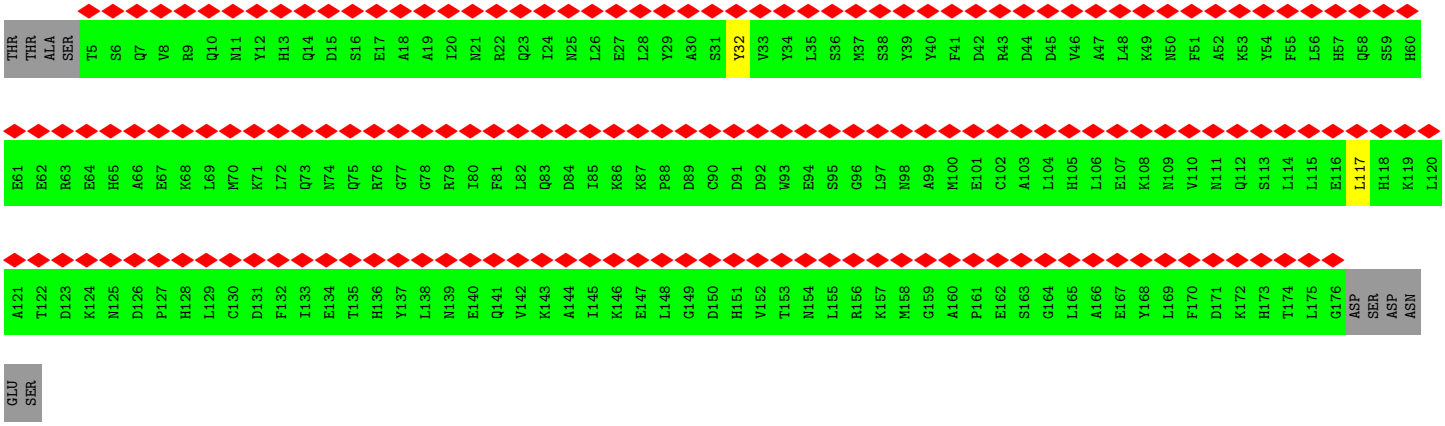




• Molecule 1: Ferritin heavy chain

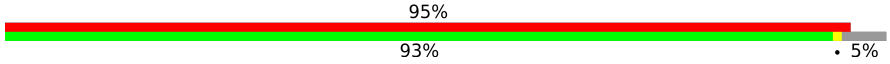
Chain Am:

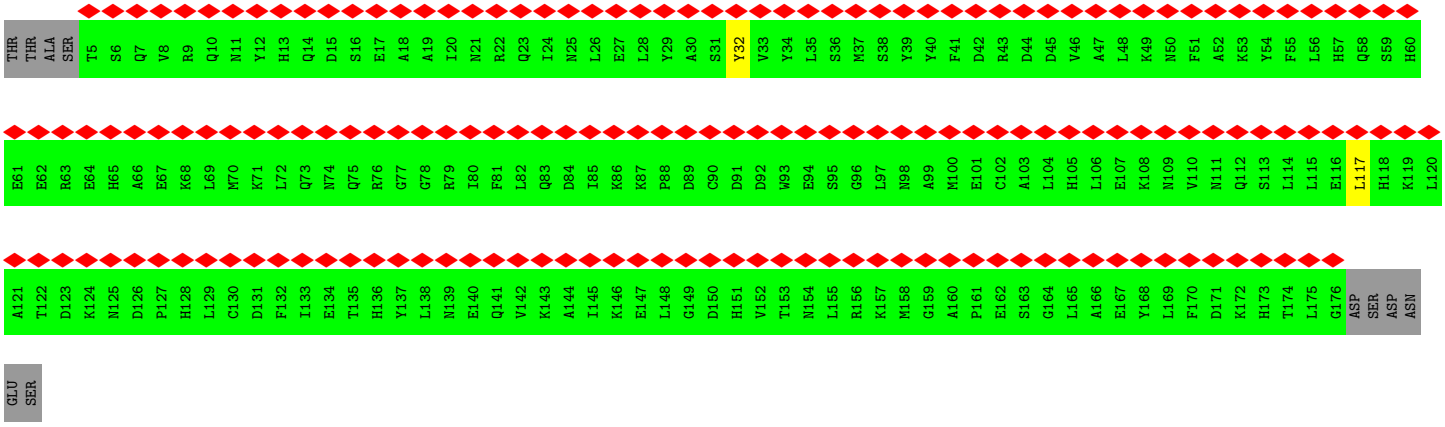




• Molecule 1: Ferritin heavy chain

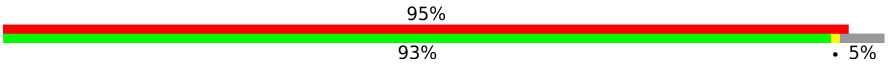
Chain An:

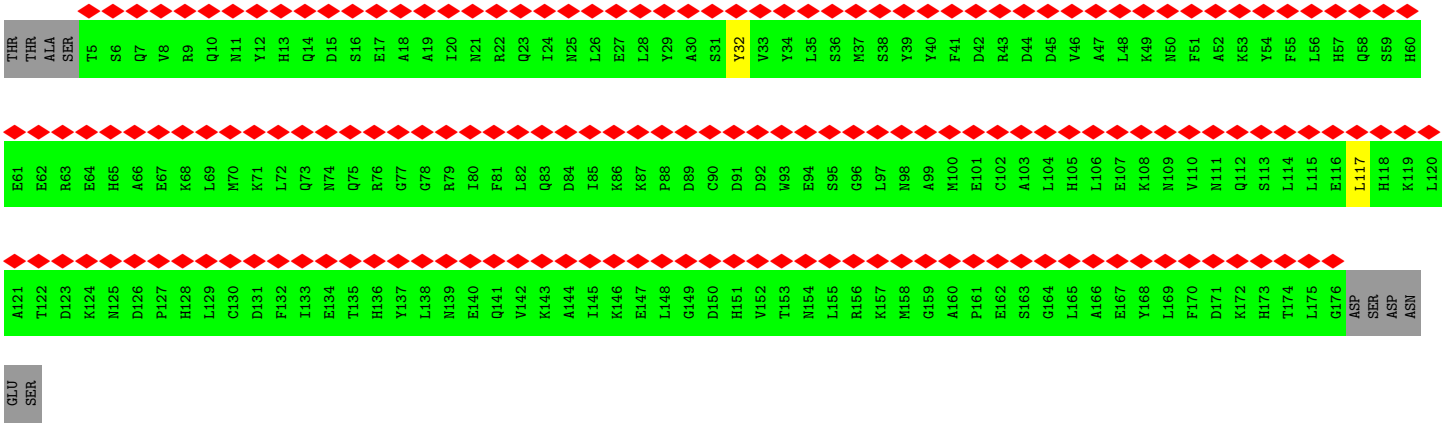




• Molecule 1: Ferritin heavy chain

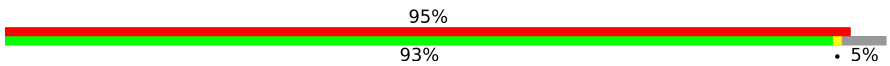
Chain Ao:

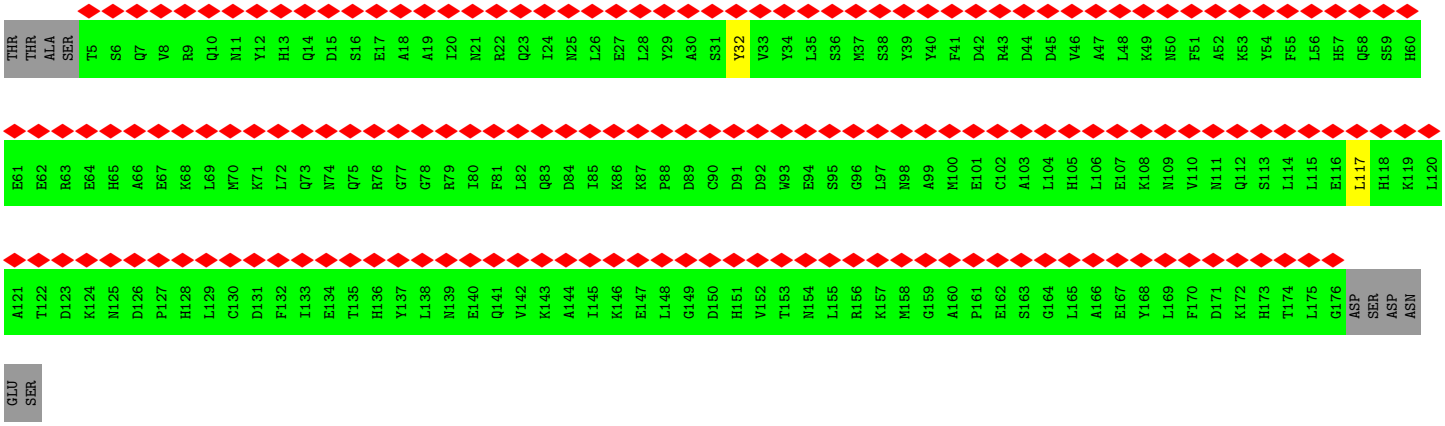




• Molecule 1: Ferritin heavy chain

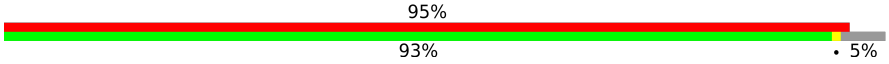
Chain Ap:

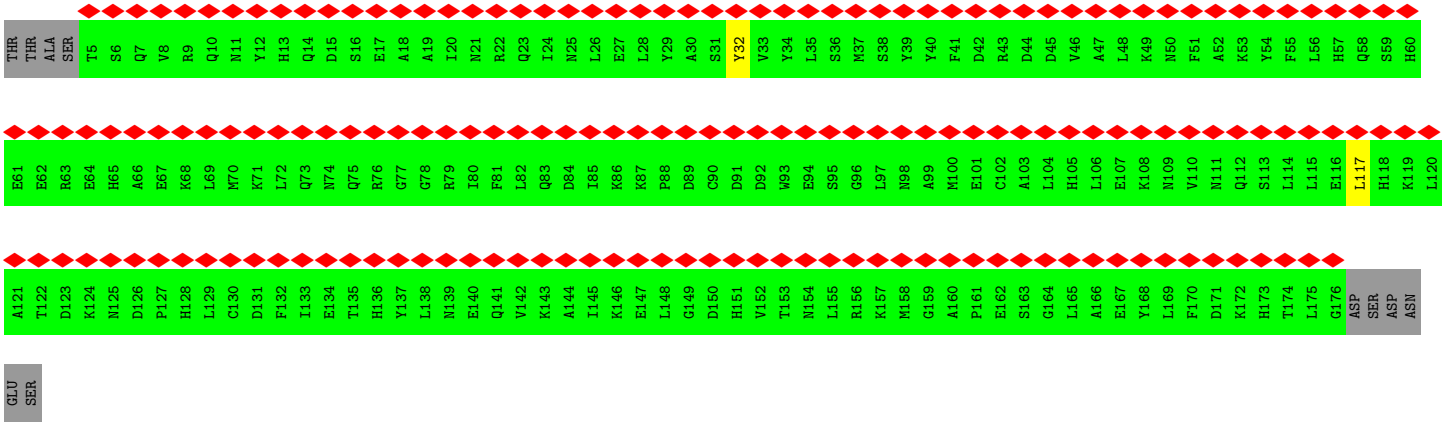




• Molecule 1: Ferritin heavy chain

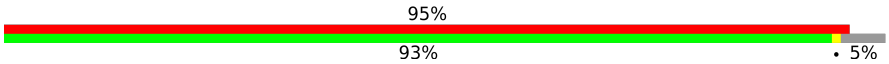
Chain Ar:

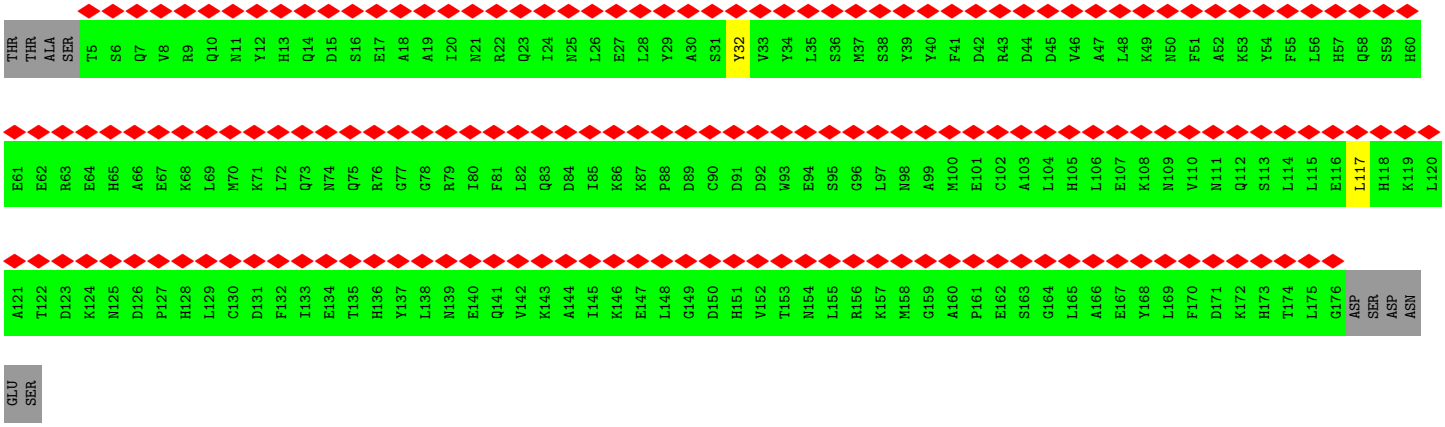




• Molecule 1: Ferritin heavy chain

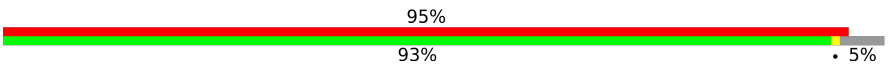
Chain As:

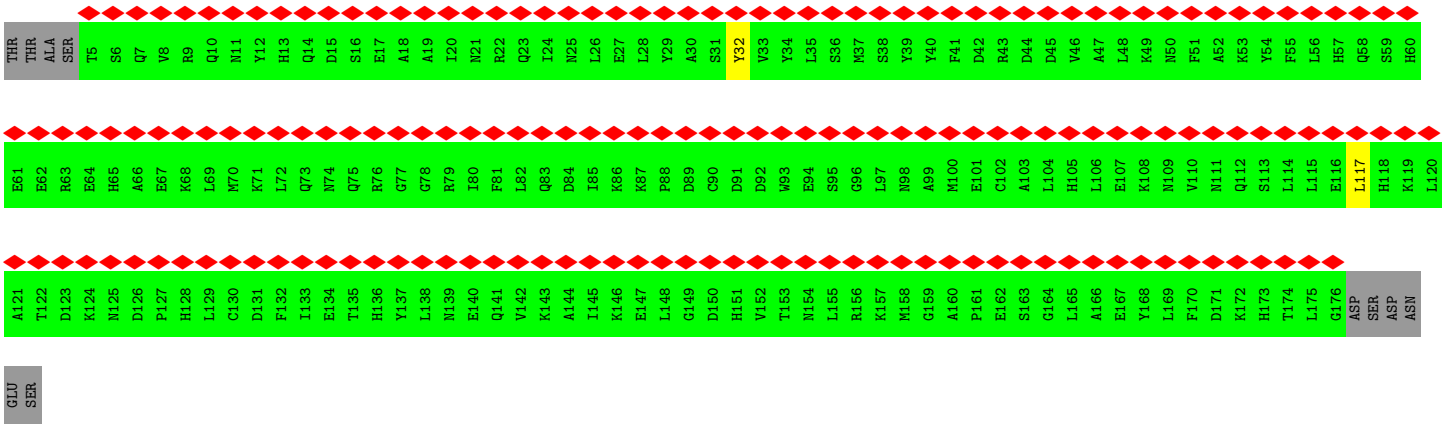




• Molecule 1: Ferritin heavy chain

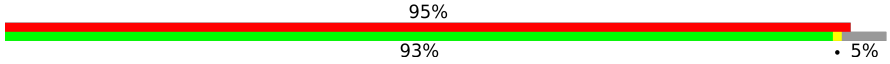
Chain At:

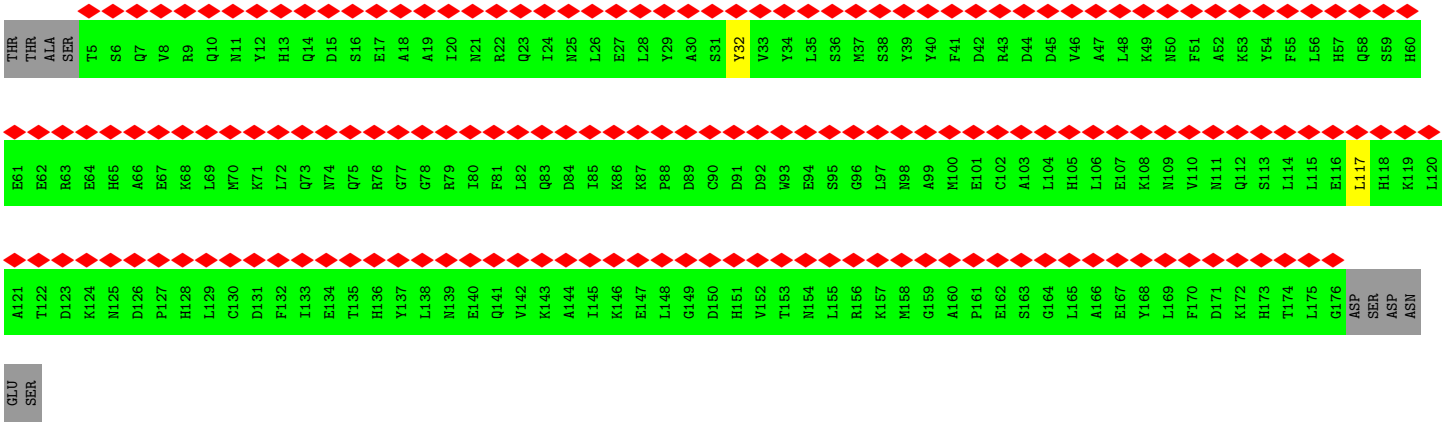




• Molecule 1: Ferritin heavy chain

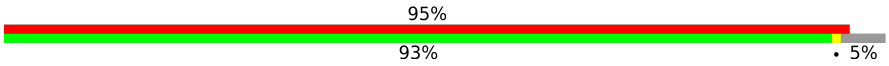
Chain Au:

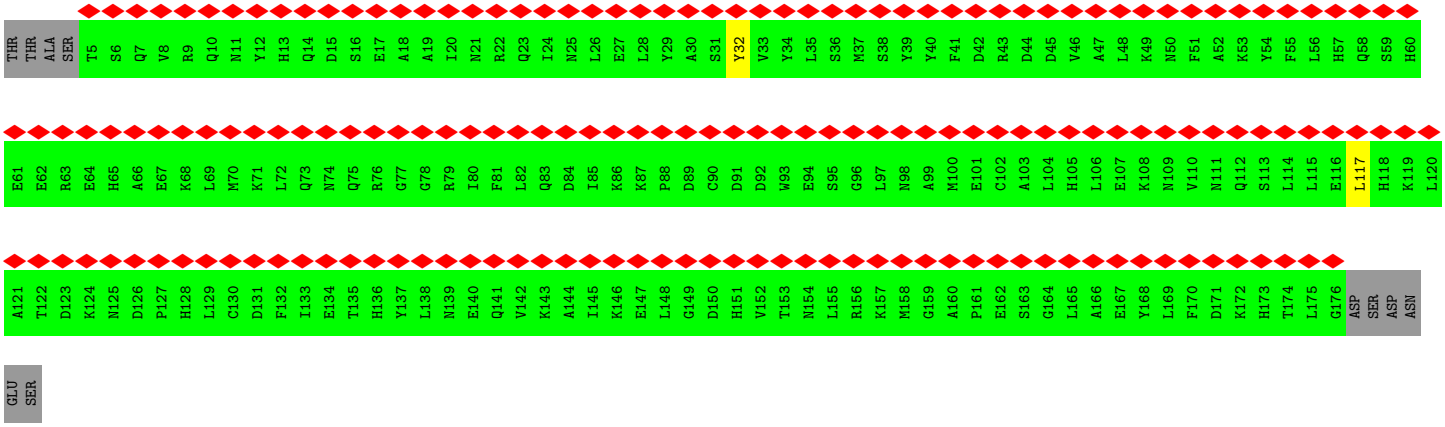




• Molecule 1: Ferritin heavy chain

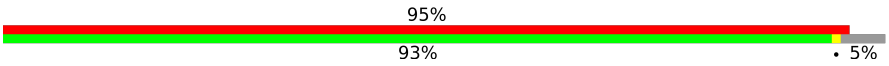
Chain Av:

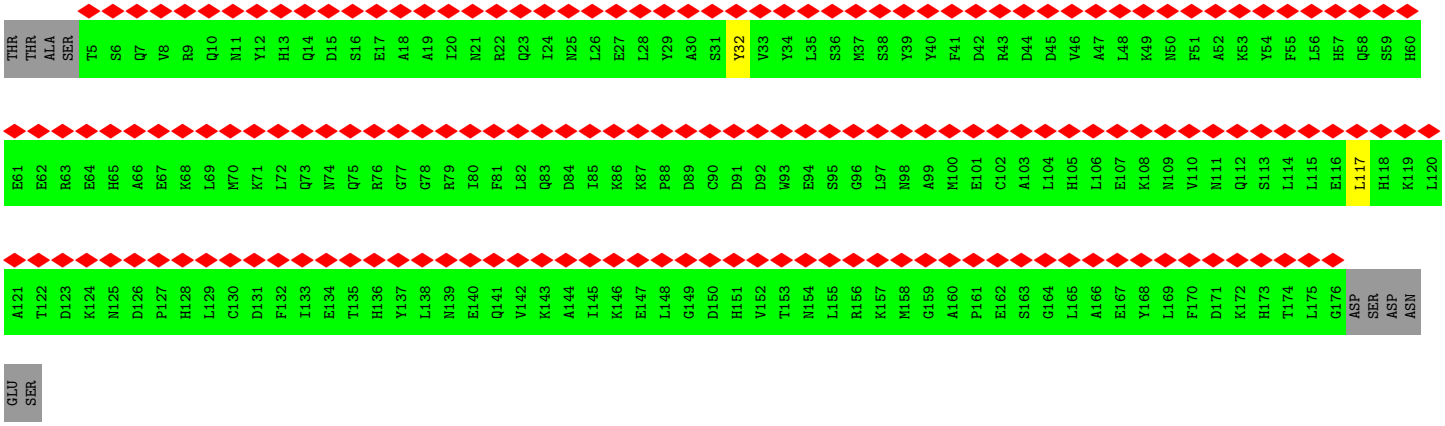




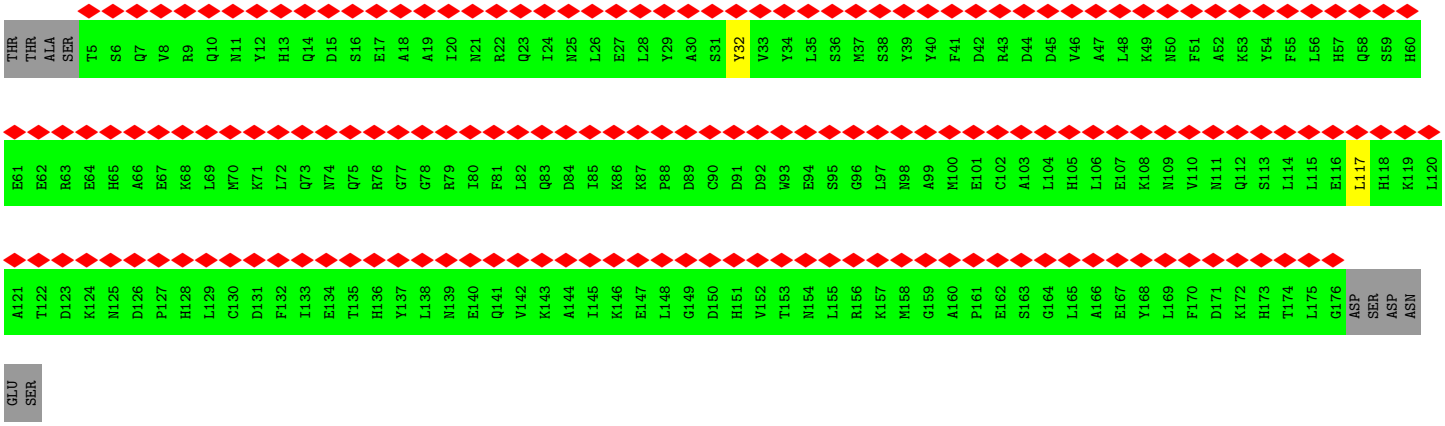
• Molecule 1: Ferritin heavy chain

Chain Aw:

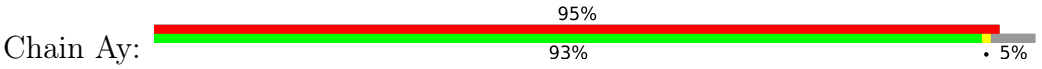




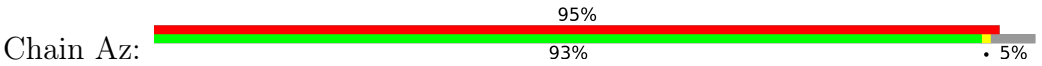
• Molecule 1: Ferritin heavy chain



• Molecule 1: Ferritin heavy chain



• Molecule 1: Ferritin heavy chain



THR THR ALA SER T5 S6 Q7 Y8 R9 Q10 N11 Y12 H13 Q14 D15 S16 E17 A18 A19 I20 N21 R22 Q23 I24 N25 L26 E27 L28 Y29 A30 S31 Y32 V33 Y34 L35 S36 M37 S38 Y39 Y40 F41 D42 R43 D44 D45 V46 A47 L48 K49 N50 F51 A52 K53 Y54 F55 L56 H57 Q58 S59 H60

E61 E62 R63 E64 H65 A66 E67 K68 L69 M70 K71 L72 Q73 N74 Q75 R76 G77 G78 R79 I80 F81 L82 Q83 D84 I85 K86 K87 P88 D89 C90 D91 D92 W93 E94 S95 G96 L97 N98 A99 M100 E101 C102 A103 L104 H105 L106 E107 K108 N109 V110 N111 Q112 S113 L114 L115 E116 L117 H118 K119 L120

A121 T122 D123 K124 N125 D126 P127 H128 L129 C130 D131 F132 I133 E134 T135 H136 Y137 L138 N139 E140 Q141 V142 K143 A144 I145 K146 E147 L148 G149 D150 H151 V152 T153 N154 L155 R156 K157 M158 G159 A160 P161 E162 S163 G164 L165 A166 E167 Y168 L169 F170 D171 K172 H173 T174 L175 G176 ASP SER ASP ASN

GLU SER

• Molecule 2: Transferrin receptor protein 1

Chain Ab: 99% 97%

R121 L122 Y123 W124 D125 D126 L127 K128 R129 K130 L131 S132 E133 K134 L135 D136 S137 T138 D139 F140 T141 S142 T143 I144 K145 L146 L147 N148 E149 N150 S151 Y152 V153 P154 R155 E156 A157 G158 S159 Q160 K161 D162 E163 N164 L165 A166 L167 Y168 V169 E170 N171 Q172 F173 R174 E175 F176 K177 L178 S179 K180

V181 W182 R183 D184 Q185 H186 F187 V188 K189 I190 Q191 V192 K193 D194 S195 A196 Q197 N198 S199 V200 I201 I202 V203 D204 K205 N206 G207 R208 L209 V210 Y211 L212 V213 E214 N215 P216 G217 G218 Y219 V220 A221 Y222 S223 K224 A225 A226 T227 V228 T229 G230 K231 L232 V233 H234 A235 N236 F237 G238 T239 K240

K241 D242 F243 E244 D245 L246 Y247 T248 P249 V250 N251 G252 S253 I254 V255 I256 V257 R258 A259 G260 K261 I262 T263 F264 A265 E266 K267 V268 A269 N270 A271 E272 S273 L274 N275 A276 I277 G278 V279 L280 I281 Y282 M283 D284 Q285 T286 K287 F288 P289 I290 V291 N292 A293 E294 L295 S296 F297 F298 G299 H300

A301 H302 L303 G304 T305 G306 D307 P308 Y309 T310 P311 G312 F313 P314 S315 PHE ASN HIS T319 Q320 F321 P322 P323 S324 R325 S326 S327 G328 L329 P330 N331 I332 P333 V334 Q335 T336 I337 S338 R339 A340 A341 A342 E343 K344 L345 F346 G347 N348 M349 E350 G351 D352 C353 P354 S355 D356 W357 K358 T359 D360

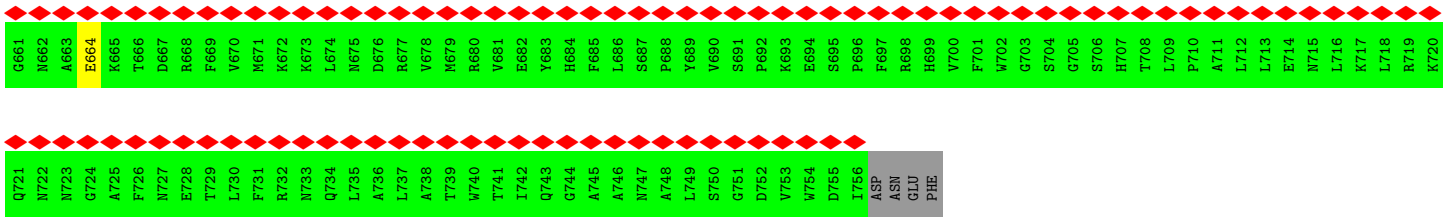
S361 T362 C363 R364 M365 V366 T367 S368 E369 S370 K371 N372 V373 K374 L375 T376 V377 S378 N379 V380 L381 K382 E383 I384 K385 I386 L387 N388 I389 F390 G391 V392 I393 K394 G395 F396 V397 E398 P399 D400 H401 Y402 V403 V404 V405 G406 A407 Q408 R409 D410 A411 W412 G413 P414 G415 A416 A417 K418 S419 G420

V421 G422 T423 A424 L425 L426 L427 K428 L429 A430 Q431 M432 F433 S434 D435 M436 V437 L438 K439 D440 G441 F442 Q443 P444 S445 R446 S447 I448 I449 F450 A451 S452 W453 S454 A455 G456 D457 F458 G459 S460 V461 G462 A463 T464 E465 W466 L467 E468 G469 Y470 L471 S472 S473 L474 H475 L476 K477 A478 F479 T480

Y481 I482 N483 L484 D485 K486 A487 V488 L489 G490 T491 S492 N493 F494 K495 V496 S497 A498 S499 P500 L501 L502 Y503 T504 L505 I506 E507 K508 T509 M510 Q511 N512 V513 K514 H515 P516 V517 T518 G519 Q520 F521 L522 Y523 Q524 D525 S526 N527 W528 A529 S530 K531 V532 E533 K534 L535 T536 L537 D538 N539 A540

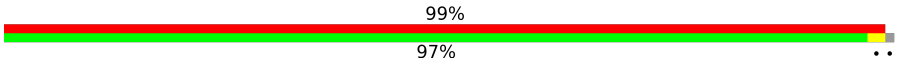
A541 F542 P543 F544 L545 A546 Y547 S548 G549 I550 P551 A552 V553 S554 F555 C556 F557 C558 E559 D560 T561 D562 Y563 P564 Y565 L566 G567 T568 T569 M570 D571 T572 Y573 K574 E575 L576 I577 E578 R579 I580 P581 E582 L583 N584 K585 V586 A587 R588 A589 A590 A591 E592 V593 A594 G595 Q596 F597 V598 I599 K600

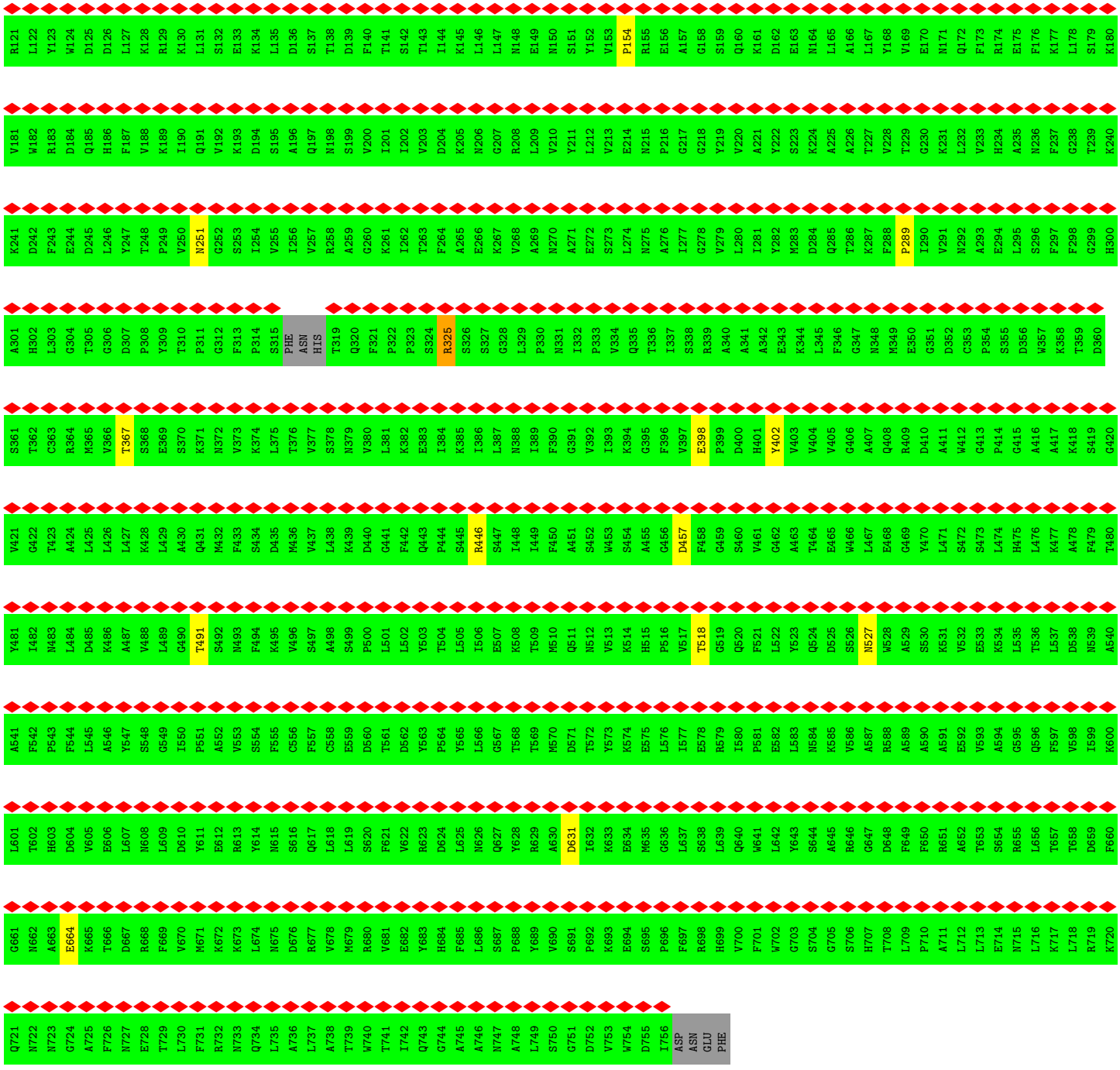
L601 T602 H603 D604 V605 E606 L607 N608 L609 D610 Y611 E612 R613 Y614 N615 S616 Q617 L618 L619 S620 F621 V622 R623 D624 L625 N626 Q627 Y628 R629 A630 D631 I632 K633 E634 M635 G636 L637 S638 L639 Q640 W641 L642 Y643 S644 A645 R646 G647 D648 F649 F650 R651 A652 T653 S654 R655 L656 T657 T658 D659 F660



• Molecule 2: Transferrin receptor protein 1

Chain Aq:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	25870	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.358	Depositor
Minimum map value	-0.090	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.128	Depositor
Map size (Å)	340.48, 340.48, 340.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	Aa	0.32	0/1530	0.50	0/2057
1	Ac	0.32	0/1530	0.50	0/2057
1	Ad	0.32	0/1530	0.50	0/2057
1	Ae	0.32	0/1530	0.50	0/2057
1	Af	0.32	0/1530	0.50	0/2057
1	Ag	0.32	0/1530	0.50	0/2057
1	Ah	0.32	0/1530	0.50	0/2057
1	Ai	0.32	0/1530	0.50	0/2057
1	Aj	0.32	0/1530	0.50	0/2057
1	Ak	0.32	0/1530	0.50	0/2057
1	Al	0.32	0/1530	0.50	0/2057
1	Am	0.32	0/1486	0.50	0/2004
1	An	0.32	0/1530	0.50	0/2057
1	Ao	0.32	0/1530	0.50	0/2057
1	Ap	0.32	0/1530	0.50	0/2057
1	Ar	0.32	0/1530	0.50	0/2057
1	As	0.32	0/1530	0.50	0/2057
1	At	0.32	0/1530	0.50	0/2057
1	Au	0.32	0/1530	0.50	0/2057
1	Av	0.32	0/1530	0.50	0/2057
1	Aw	0.32	0/1530	0.50	0/2057
1	Ax	0.32	0/1530	0.50	0/2057
1	Ay	0.32	0/1530	0.50	0/2057
1	Az	0.32	0/1530	0.50	0/2057
2	Ab	0.35	0/5110	0.51	0/6927
2	Aq	0.35	0/5121	0.51	0/6942
All	All	0.33	0/46907	0.50	0/63184

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Aa	1473	0	1447	0	0
1	Ac	1473	0	1447	0	0
1	Ad	1473	0	1447	0	0
1	Ae	1473	0	1447	0	0
1	Af	1473	0	1447	0	0
1	Ag	1473	0	1447	0	0
1	Ah	1473	0	1447	0	0
1	Ai	1473	0	1447	0	0
1	Aj	1473	0	1447	0	0
1	Ak	1473	0	1447	0	0
1	Al	1473	0	1447	0	0
1	Am	1431	0	1377	0	0
1	An	1473	0	1447	0	0
1	Ao	1473	0	1447	0	0
1	Ap	1473	0	1447	0	0
1	Ar	1473	0	1447	0	0
1	As	1473	0	1447	0	0
1	At	1473	0	1447	0	0
1	Au	1473	0	1447	0	0
1	Av	1473	0	1447	0	0
1	Aw	1473	0	1447	0	0
1	Ax	1473	0	1447	0	0
1	Ay	1473	0	1447	0	0
1	Az	1473	0	1447	0	0
2	Ab	4994	0	4937	0	0
2	Aq	5004	0	4957	0	0
All	All	45308	0	44552	0	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 6.

There are no clashes within the asymmetric unit.

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	Aa	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Ac	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Ad	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Ae	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Af	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Ag	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Ah	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Ai	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Aj	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Ak	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Al	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Am	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	An	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Ao	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Ap	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Ar	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	As	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	At	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Au	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Av	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Aw	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Ax	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Ay	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Az	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
2	Ab	629/640 (98%)	604 (96%)	22 (4%)	3 (0%)	29	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	Aq	629/640 (98%)	605 (96%)	21 (3%)	3 (0%)	29 69
All	All	5578/5648 (99%)	5457 (98%)	115 (2%)	6 (0%)	54 85

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Ab	325	ARG
2	Aq	325	ARG
2	Ab	154	PRO
2	Ab	289	PRO
2	Aq	154	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	Aa	163/162 (101%)	161 (99%)	2 (1%)	71 84
1	Ac	163/162 (101%)	161 (99%)	2 (1%)	71 84
1	Ad	163/162 (101%)	161 (99%)	2 (1%)	71 84
1	Ae	163/162 (101%)	161 (99%)	2 (1%)	71 84
1	Af	163/162 (101%)	161 (99%)	2 (1%)	71 84
1	Ag	163/162 (101%)	161 (99%)	2 (1%)	71 84
1	Ah	163/162 (101%)	161 (99%)	2 (1%)	71 84
1	Ai	163/162 (101%)	161 (99%)	2 (1%)	71 84
1	Aj	163/162 (101%)	161 (99%)	2 (1%)	71 84
1	Ak	163/162 (101%)	161 (99%)	2 (1%)	71 84
1	Al	163/162 (101%)	161 (99%)	2 (1%)	71 84
1	Am	155/162 (96%)	153 (99%)	2 (1%)	69 82
1	An	163/162 (101%)	161 (99%)	2 (1%)	71 84
1	Ao	163/162 (101%)	161 (99%)	2 (1%)	71 84
1	Ap	163/162 (101%)	161 (99%)	2 (1%)	71 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	Ar	163/162 (101%)	161 (99%)	2 (1%)	71 84
1	As	163/162 (101%)	161 (99%)	2 (1%)	71 84
1	At	163/162 (101%)	161 (99%)	2 (1%)	71 84
1	Au	163/162 (101%)	161 (99%)	2 (1%)	71 84
1	Av	163/162 (101%)	161 (99%)	2 (1%)	71 84
1	Aw	163/162 (101%)	161 (99%)	2 (1%)	71 84
1	Ax	163/162 (101%)	161 (99%)	2 (1%)	71 84
1	Ay	163/162 (101%)	161 (99%)	2 (1%)	71 84
1	Az	163/162 (101%)	161 (99%)	2 (1%)	71 84
2	Ab	540/549 (98%)	527 (98%)	13 (2%)	49 69
2	Aq	542/549 (99%)	530 (98%)	12 (2%)	52 71
All	All	4986/4986 (100%)	4913 (98%)	73 (2%)	66 80

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	As	32	TYR
1	Az	32	TYR
1	At	32	TYR
1	Aw	32	TYR
1	Ag	117	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	Au	112	GLN
1	Av	112	GLN
1	Ay	112	GLN
1	Ai	112	GLN
1	Ah	112	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

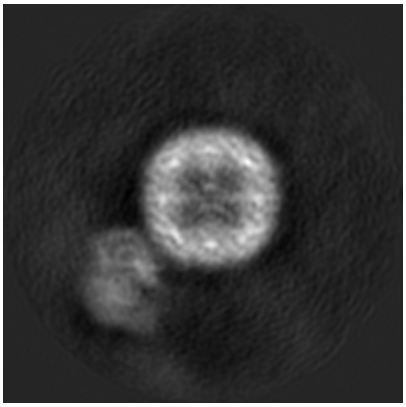
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0046. These allow visual inspection of the internal detail of the map and identification of artifacts.

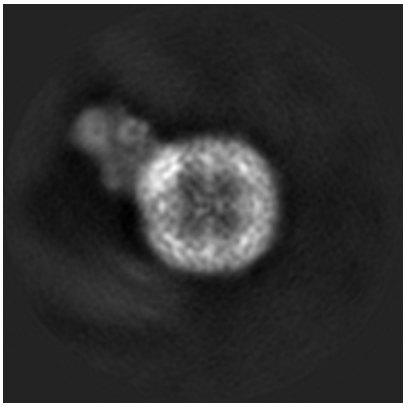
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

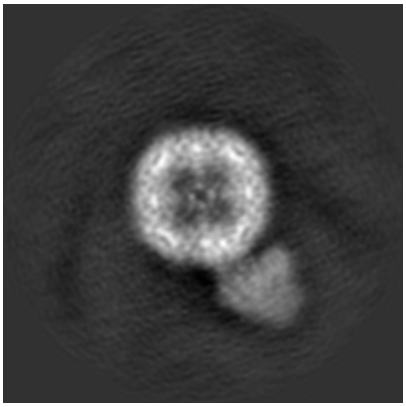
6.1.1 Primary map



X



Y

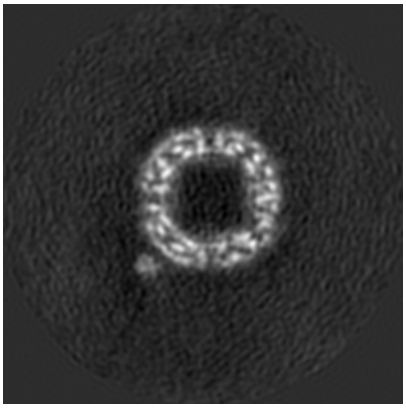


Z

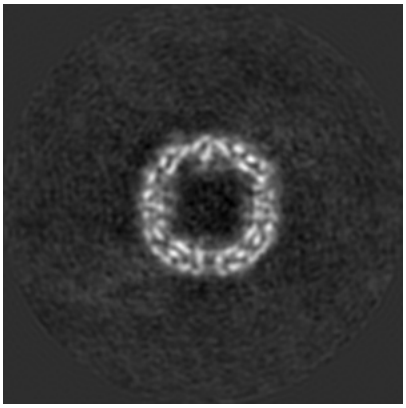
The images above show the map projected in three orthogonal directions.

6.2 Central slices

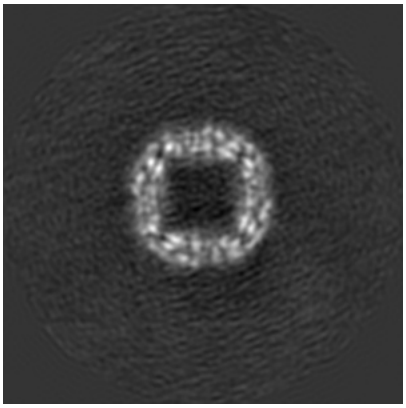
6.2.1 Primary map



X Index: 128



Y Index: 128

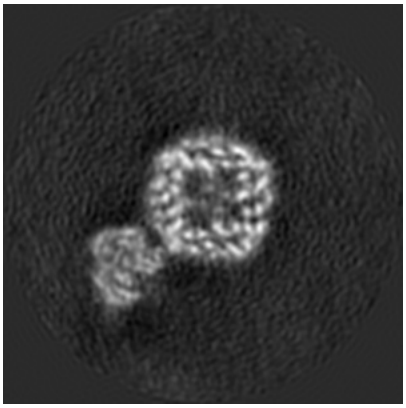


Z Index: 128

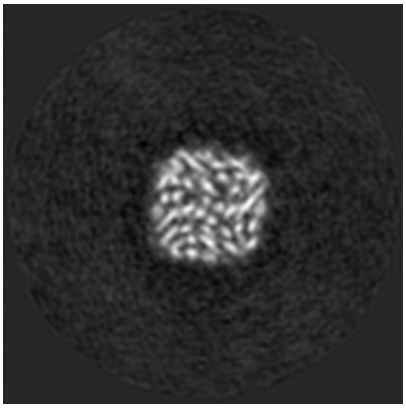
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

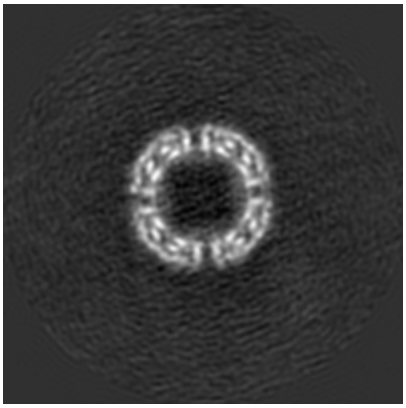
6.3.1 Primary map



X Index: 151



Y Index: 162

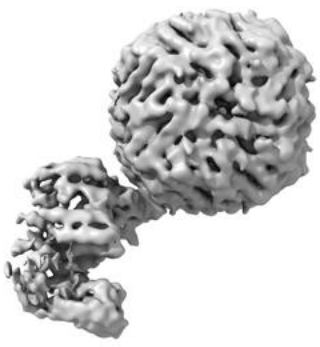


Z Index: 131

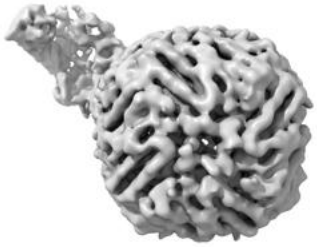
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

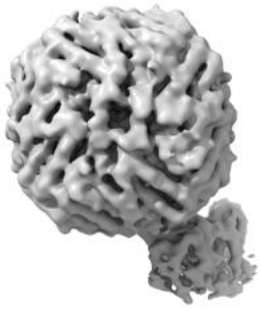
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.128. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

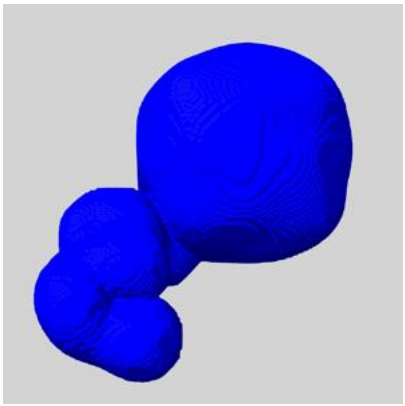
6.5 Mask visualisation (i)

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

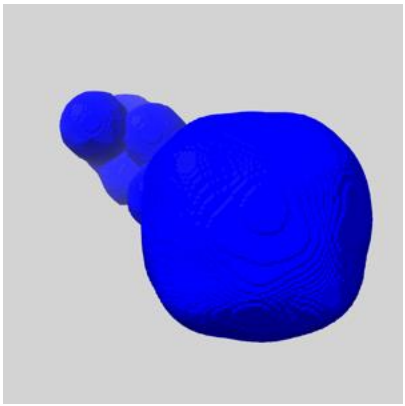
A mask typically either:

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

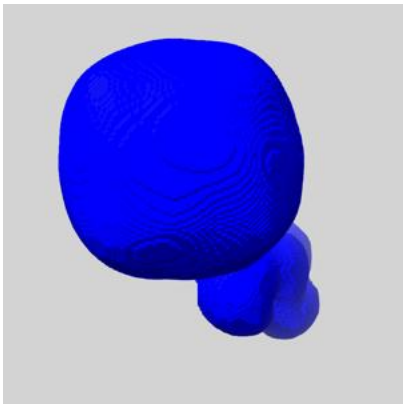
6.5.1 emd_0046_msk_1.map (i)



X



Y

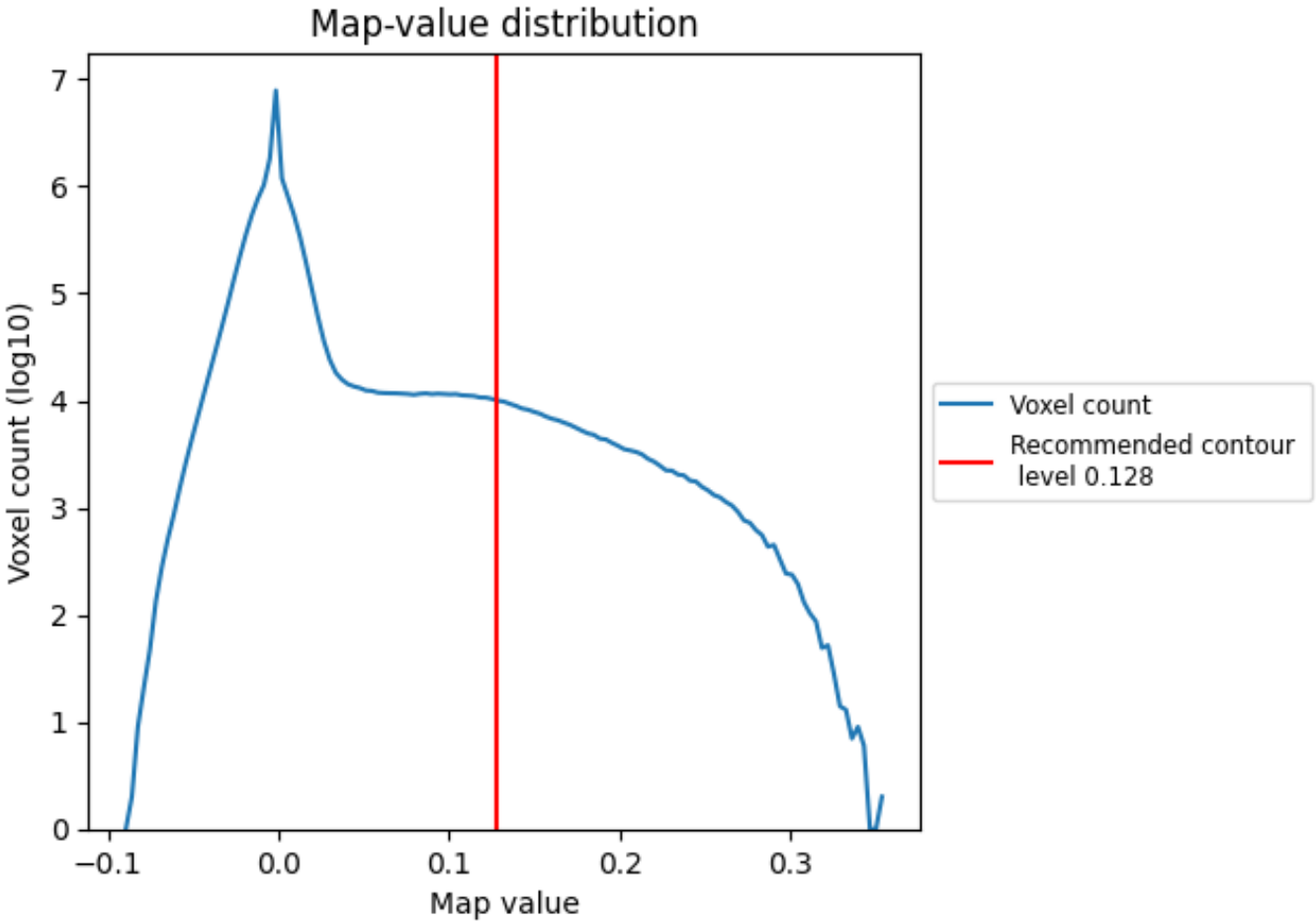


Z

7 Map analysis

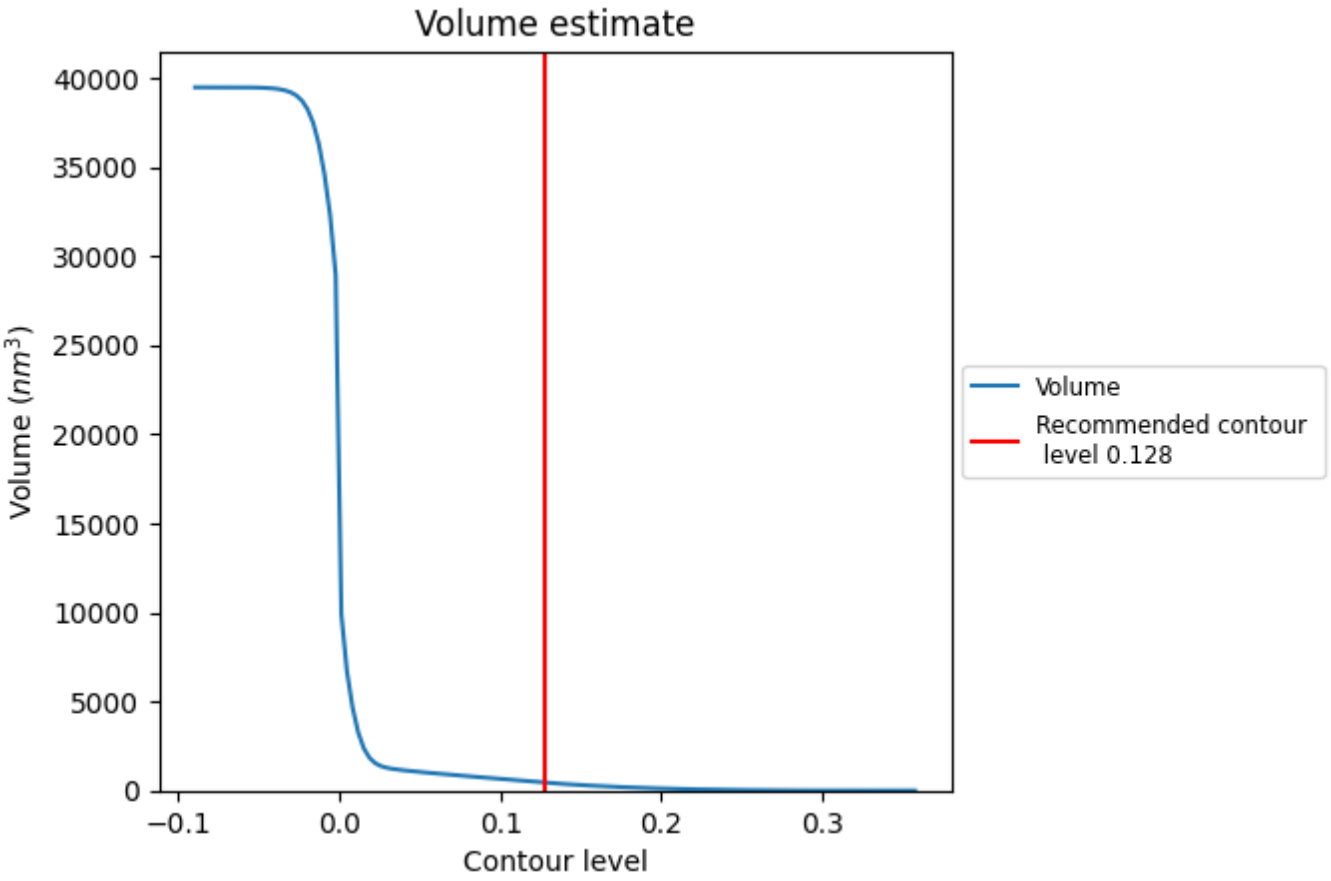
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

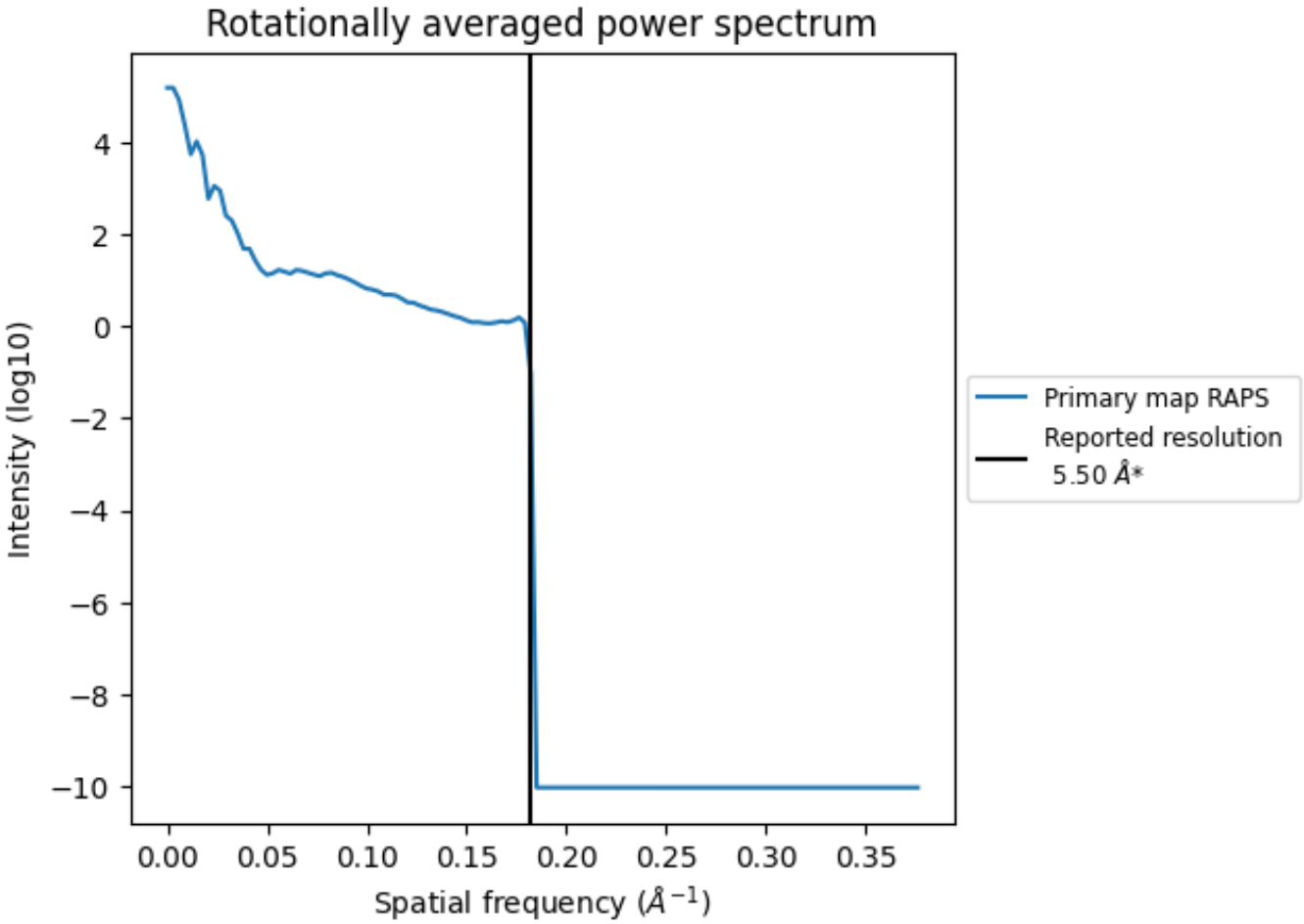
7.2 Volume estimate (i)



The volume at the recommended contour level is 444 nm^3; this corresponds to an approximate mass of 401 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)

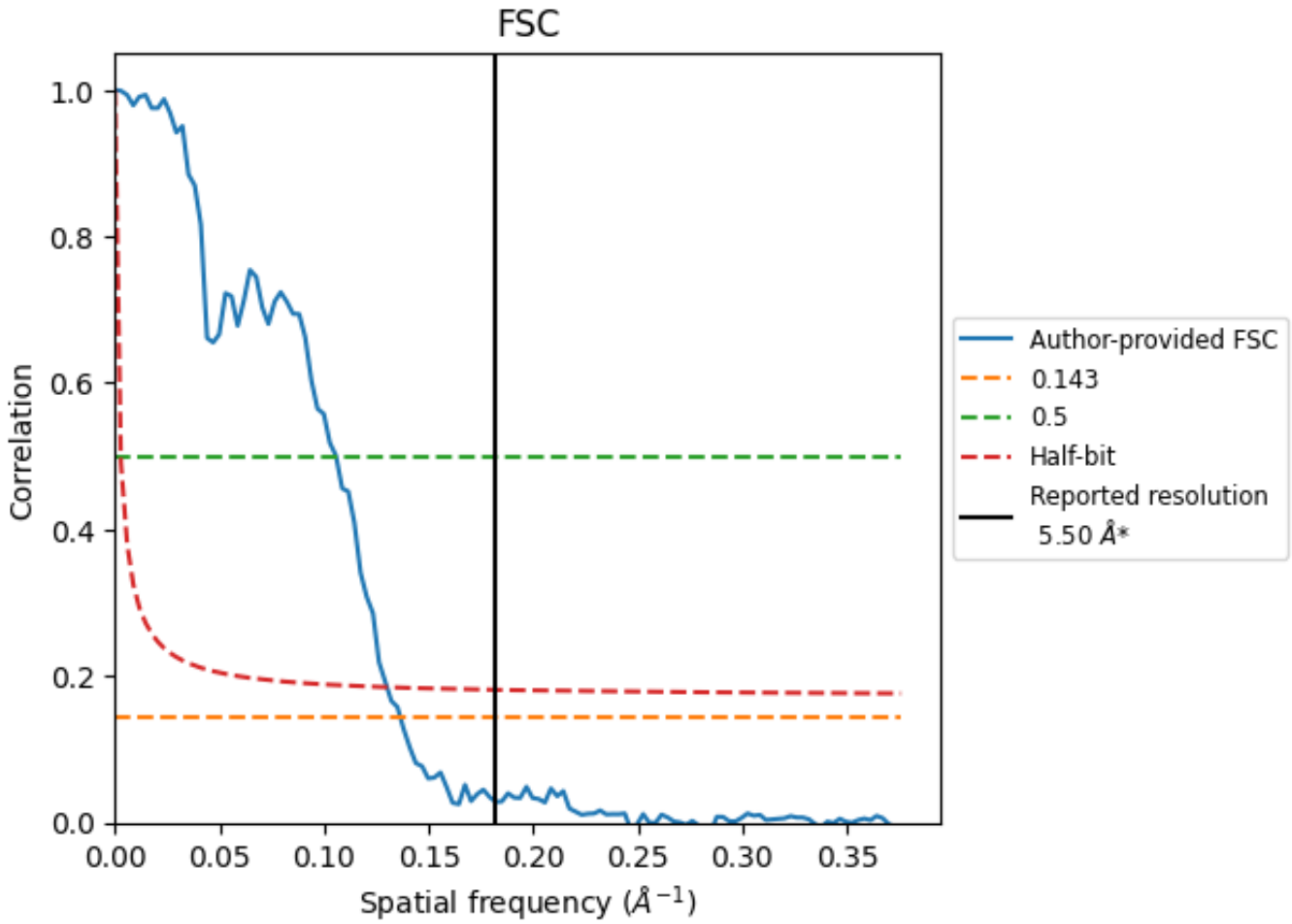


*Reported resolution corresponds to spatial frequency of 0.182 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.182 Å^{-1}

8.2 Resolution estimates (i)

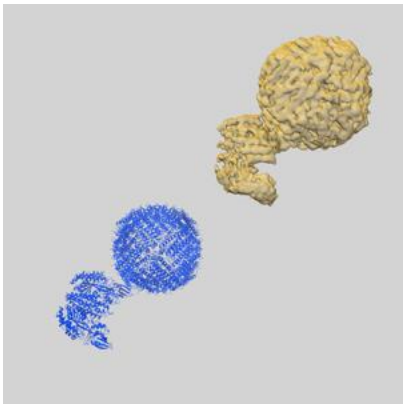
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.50	-	-
Author-provided FSC curve	7.33	9.45	7.69
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 7.33 differs from the reported value 5.5 by more than 10 %

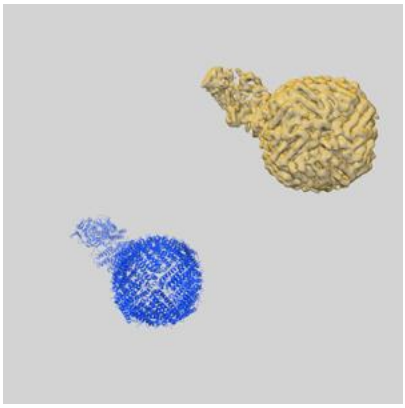
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0046 and PDB model 6GSR. Per-residue inclusion information can be found in section 3 on page 6.

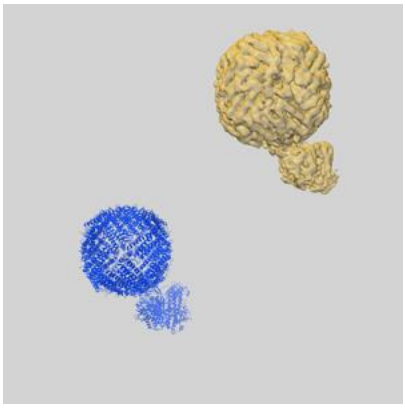
9.1 Map-model overlay



X



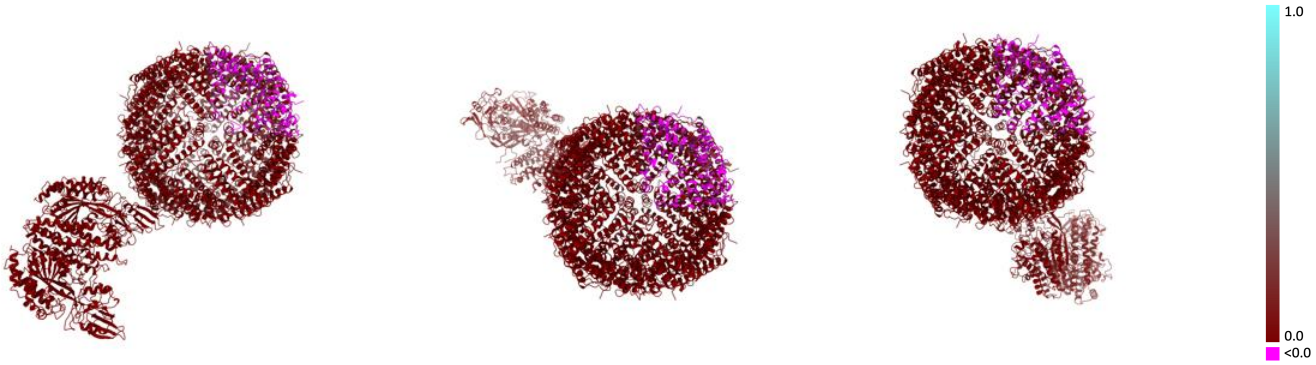
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.128 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

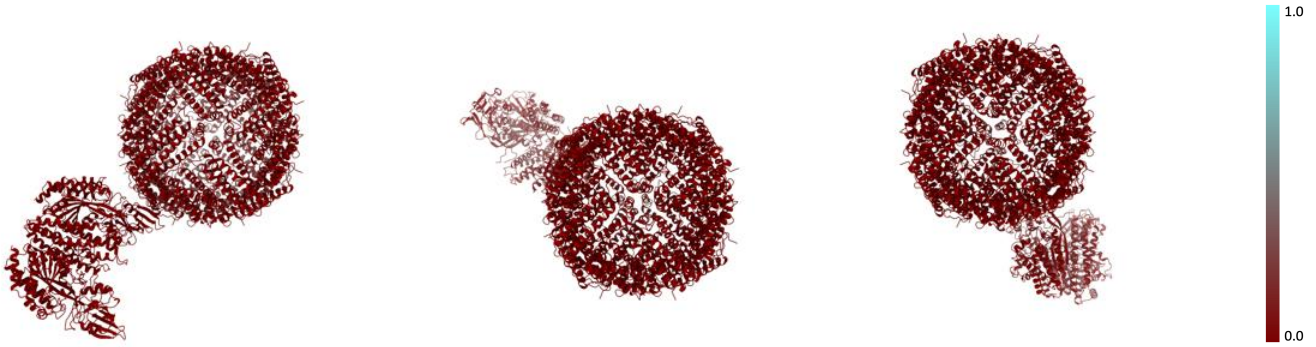
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

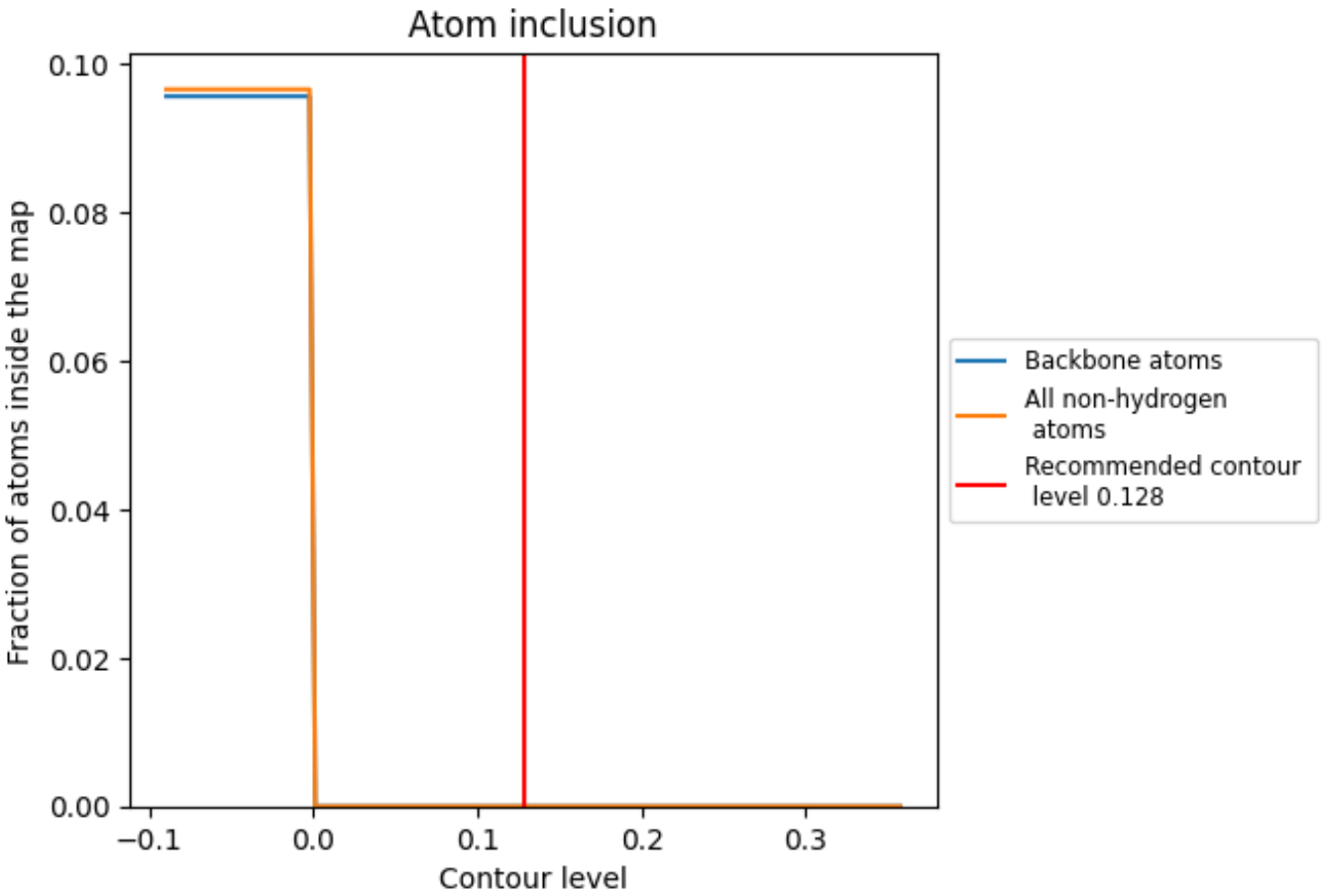
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.128).

9.4 Atom inclusion (i)



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

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.128) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0000	0.0010
Aa	0.0000	0.0020
Ab	0.0000	0.0000
Ac	0.0000	0.0000
Ad	0.0000	0.0030
Ae	0.0000	0.0060
Af	0.0000	0.0000
Ag	0.0000	0.0000
Ah	0.0000	0.0000
Ai	0.0000	0.0000
Aj	0.0000	0.0000
Ak	0.0000	0.0100
Al	0.0000	0.0010
Am	0.0000	0.0000
An	0.0000	0.0000
Ao	0.0000	0.0000
Ap	0.0000	-0.0020
Aq	0.0000	0.0000
Ar	0.0000	0.0000
As	0.0000	0.0000
At	0.0000	0.0000
Au	0.0000	0.0000
Av	0.0000	0.0010
Aw	0.0000	0.0000
Ax	0.0000	0.0090
Ay	0.0000	0.0000
Az	0.0000	0.0000