wwPDB EM Validation Summary Report (i)

Dec 18, 2022 – 03:08 am GMT

PDB ID	:	6ZXL
EMDB ID	:	EMD-11524
Title	:	Fully-loaded anthrax lethal toxin in its heptameric pre-pore state and PA7LF(2+1A) arrangement
Authors	:	Quentin, D.; Antoni, C.; Gatsogiannis, C.; Raunser, S.
Deposited on	:	2020-07-29
Resolution	:	4.20 Å(reported)
Based on initial model	:	6ZXK

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:

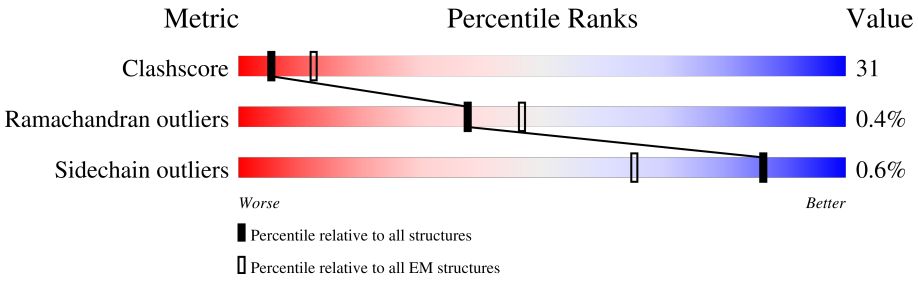
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 4.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	759	6% 36% 33% • 30%
1	B	759	• 36% 32% • 30%
1	C	759	• 33% 35% • 30%
1	D	759	• 35% 33% • 30%
1	E	759	5% 36% 32% • 30%
1	F	759	• 38% 31% • 30%
1	G	759	• 38% 31% 30%
2	H	809	8% 44% 40% • 14%

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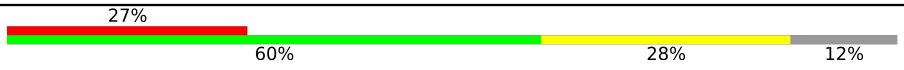
Mol	Chain	Length	Quality of chain
2	I	809	
2	J	809	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 42172 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 Protective antigen.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	529	Total	C	N	O	S	0	0
			3961	2477	691	789	4		
1	B	529	Total	C	N	O	S	0	0
			3977	2488	692	793	4		
1	C	529	Total	C	N	O	S	0	0
			3977	2488	692	793	4		
1	D	528	Total	C	N	O	S	0	0
			3970	2483	691	792	4		
1	E	529	Total	C	N	O	S	0	0
			3977	2488	692	793	4		
1	F	529	Total	C	N	O	S	0	0
			3977	2488	692	793	4		
1	G	529	Total	C	N	O	S	0	0
			3977	2488	692	793	4		

There are 161 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP Q68GS1
A	-22	GLY	-	expression tag	UNP Q68GS1
A	-21	HIS	-	expression tag	UNP Q68GS1
A	-20	HIS	-	expression tag	UNP Q68GS1
A	-19	HIS	-	expression tag	UNP Q68GS1
A	-18	HIS	-	expression tag	UNP Q68GS1
A	-17	HIS	-	expression tag	UNP Q68GS1
A	-16	HIS	-	expression tag	UNP Q68GS1
A	-15	HIS	-	expression tag	UNP Q68GS1
A	-14	HIS	-	expression tag	UNP Q68GS1
A	-13	HIS	-	expression tag	UNP Q68GS1
A	-12	HIS	-	expression tag	UNP Q68GS1
A	-11	SER	-	expression tag	UNP Q68GS1
A	-10	SER	-	expression tag	UNP Q68GS1
A	-9	GLY	-	expression tag	UNP Q68GS1
A	-8	HIS	-	expression tag	UNP Q68GS1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ILE	-	expression tag	UNP Q68GS1
A	-6	ASP	-	expression tag	UNP Q68GS1
A	-5	ASP	-	expression tag	UNP Q68GS1
A	-4	ASP	-	expression tag	UNP Q68GS1
A	-3	ASP	-	expression tag	UNP Q68GS1
A	-2	LYS	-	expression tag	UNP Q68GS1
A	-1	HIS	-	expression tag	UNP Q68GS1
B	-23	MET	-	initiating methionine	UNP Q68GS1
B	-22	GLY	-	expression tag	UNP Q68GS1
B	-21	HIS	-	expression tag	UNP Q68GS1
B	-20	HIS	-	expression tag	UNP Q68GS1
B	-19	HIS	-	expression tag	UNP Q68GS1
B	-18	HIS	-	expression tag	UNP Q68GS1
B	-17	HIS	-	expression tag	UNP Q68GS1
B	-16	HIS	-	expression tag	UNP Q68GS1
B	-15	HIS	-	expression tag	UNP Q68GS1
B	-14	HIS	-	expression tag	UNP Q68GS1
B	-13	HIS	-	expression tag	UNP Q68GS1
B	-12	HIS	-	expression tag	UNP Q68GS1
B	-11	SER	-	expression tag	UNP Q68GS1
B	-10	SER	-	expression tag	UNP Q68GS1
B	-9	GLY	-	expression tag	UNP Q68GS1
B	-8	HIS	-	expression tag	UNP Q68GS1
B	-7	ILE	-	expression tag	UNP Q68GS1
B	-6	ASP	-	expression tag	UNP Q68GS1
B	-5	ASP	-	expression tag	UNP Q68GS1
B	-4	ASP	-	expression tag	UNP Q68GS1
B	-3	ASP	-	expression tag	UNP Q68GS1
B	-2	LYS	-	expression tag	UNP Q68GS1
B	-1	HIS	-	expression tag	UNP Q68GS1
C	-23	MET	-	initiating methionine	UNP Q68GS1
C	-22	GLY	-	expression tag	UNP Q68GS1
C	-21	HIS	-	expression tag	UNP Q68GS1
C	-20	HIS	-	expression tag	UNP Q68GS1
C	-19	HIS	-	expression tag	UNP Q68GS1
C	-18	HIS	-	expression tag	UNP Q68GS1
C	-17	HIS	-	expression tag	UNP Q68GS1
C	-16	HIS	-	expression tag	UNP Q68GS1
C	-15	HIS	-	expression tag	UNP Q68GS1
C	-14	HIS	-	expression tag	UNP Q68GS1
C	-13	HIS	-	expression tag	UNP Q68GS1
C	-12	HIS	-	expression tag	UNP Q68GS1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	SER	-	expression tag	UNP Q68GS1
C	-10	SER	-	expression tag	UNP Q68GS1
C	-9	GLY	-	expression tag	UNP Q68GS1
C	-8	HIS	-	expression tag	UNP Q68GS1
C	-7	ILE	-	expression tag	UNP Q68GS1
C	-6	ASP	-	expression tag	UNP Q68GS1
C	-5	ASP	-	expression tag	UNP Q68GS1
C	-4	ASP	-	expression tag	UNP Q68GS1
C	-3	ASP	-	expression tag	UNP Q68GS1
C	-2	LYS	-	expression tag	UNP Q68GS1
C	-1	HIS	-	expression tag	UNP Q68GS1
D	-23	MET	-	initiating methionine	UNP Q68GS1
D	-22	GLY	-	expression tag	UNP Q68GS1
D	-21	HIS	-	expression tag	UNP Q68GS1
D	-20	HIS	-	expression tag	UNP Q68GS1
D	-19	HIS	-	expression tag	UNP Q68GS1
D	-18	HIS	-	expression tag	UNP Q68GS1
D	-17	HIS	-	expression tag	UNP Q68GS1
D	-16	HIS	-	expression tag	UNP Q68GS1
D	-15	HIS	-	expression tag	UNP Q68GS1
D	-14	HIS	-	expression tag	UNP Q68GS1
D	-13	HIS	-	expression tag	UNP Q68GS1
D	-12	HIS	-	expression tag	UNP Q68GS1
D	-11	SER	-	expression tag	UNP Q68GS1
D	-10	SER	-	expression tag	UNP Q68GS1
D	-9	GLY	-	expression tag	UNP Q68GS1
D	-8	HIS	-	expression tag	UNP Q68GS1
D	-7	ILE	-	expression tag	UNP Q68GS1
D	-6	ASP	-	expression tag	UNP Q68GS1
D	-5	ASP	-	expression tag	UNP Q68GS1
D	-4	ASP	-	expression tag	UNP Q68GS1
D	-3	ASP	-	expression tag	UNP Q68GS1
D	-2	LYS	-	expression tag	UNP Q68GS1
D	-1	HIS	-	expression tag	UNP Q68GS1
E	-23	MET	-	initiating methionine	UNP Q68GS1
E	-22	GLY	-	expression tag	UNP Q68GS1
E	-21	HIS	-	expression tag	UNP Q68GS1
E	-20	HIS	-	expression tag	UNP Q68GS1
E	-19	HIS	-	expression tag	UNP Q68GS1
E	-18	HIS	-	expression tag	UNP Q68GS1
E	-17	HIS	-	expression tag	UNP Q68GS1
E	-16	HIS	-	expression tag	UNP Q68GS1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-15	HIS	-	expression tag	UNP Q68GS1
E	-14	HIS	-	expression tag	UNP Q68GS1
E	-13	HIS	-	expression tag	UNP Q68GS1
E	-12	HIS	-	expression tag	UNP Q68GS1
E	-11	SER	-	expression tag	UNP Q68GS1
E	-10	SER	-	expression tag	UNP Q68GS1
E	-9	GLY	-	expression tag	UNP Q68GS1
E	-8	HIS	-	expression tag	UNP Q68GS1
E	-7	ILE	-	expression tag	UNP Q68GS1
E	-6	ASP	-	expression tag	UNP Q68GS1
E	-5	ASP	-	expression tag	UNP Q68GS1
E	-4	ASP	-	expression tag	UNP Q68GS1
E	-3	ASP	-	expression tag	UNP Q68GS1
E	-2	LYS	-	expression tag	UNP Q68GS1
E	-1	HIS	-	expression tag	UNP Q68GS1
F	-23	MET	-	initiating methionine	UNP Q68GS1
F	-22	GLY	-	expression tag	UNP Q68GS1
F	-21	HIS	-	expression tag	UNP Q68GS1
F	-20	HIS	-	expression tag	UNP Q68GS1
F	-19	HIS	-	expression tag	UNP Q68GS1
F	-18	HIS	-	expression tag	UNP Q68GS1
F	-17	HIS	-	expression tag	UNP Q68GS1
F	-16	HIS	-	expression tag	UNP Q68GS1
F	-15	HIS	-	expression tag	UNP Q68GS1
F	-14	HIS	-	expression tag	UNP Q68GS1
F	-13	HIS	-	expression tag	UNP Q68GS1
F	-12	HIS	-	expression tag	UNP Q68GS1
F	-11	SER	-	expression tag	UNP Q68GS1
F	-10	SER	-	expression tag	UNP Q68GS1
F	-9	GLY	-	expression tag	UNP Q68GS1
F	-8	HIS	-	expression tag	UNP Q68GS1
F	-7	ILE	-	expression tag	UNP Q68GS1
F	-6	ASP	-	expression tag	UNP Q68GS1
F	-5	ASP	-	expression tag	UNP Q68GS1
F	-4	ASP	-	expression tag	UNP Q68GS1
F	-3	ASP	-	expression tag	UNP Q68GS1
F	-2	LYS	-	expression tag	UNP Q68GS1
F	-1	HIS	-	expression tag	UNP Q68GS1
G	-23	MET	-	initiating methionine	UNP Q68GS1
G	-22	GLY	-	expression tag	UNP Q68GS1
G	-21	HIS	-	expression tag	UNP Q68GS1
G	-20	HIS	-	expression tag	UNP Q68GS1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-19	HIS	-	expression tag	UNP Q68GS1
G	-18	HIS	-	expression tag	UNP Q68GS1
G	-17	HIS	-	expression tag	UNP Q68GS1
G	-16	HIS	-	expression tag	UNP Q68GS1
G	-15	HIS	-	expression tag	UNP Q68GS1
G	-14	HIS	-	expression tag	UNP Q68GS1
G	-13	HIS	-	expression tag	UNP Q68GS1
G	-12	HIS	-	expression tag	UNP Q68GS1
G	-11	SER	-	expression tag	UNP Q68GS1
G	-10	SER	-	expression tag	UNP Q68GS1
G	-9	GLY	-	expression tag	UNP Q68GS1
G	-8	HIS	-	expression tag	UNP Q68GS1
G	-7	ILE	-	expression tag	UNP Q68GS1
G	-6	ASP	-	expression tag	UNP Q68GS1
G	-5	ASP	-	expression tag	UNP Q68GS1
G	-4	ASP	-	expression tag	UNP Q68GS1
G	-3	ASP	-	expression tag	UNP Q68GS1
G	-2	LYS	-	expression tag	UNP Q68GS1
G	-1	HIS	-	expression tag	UNP Q68GS1

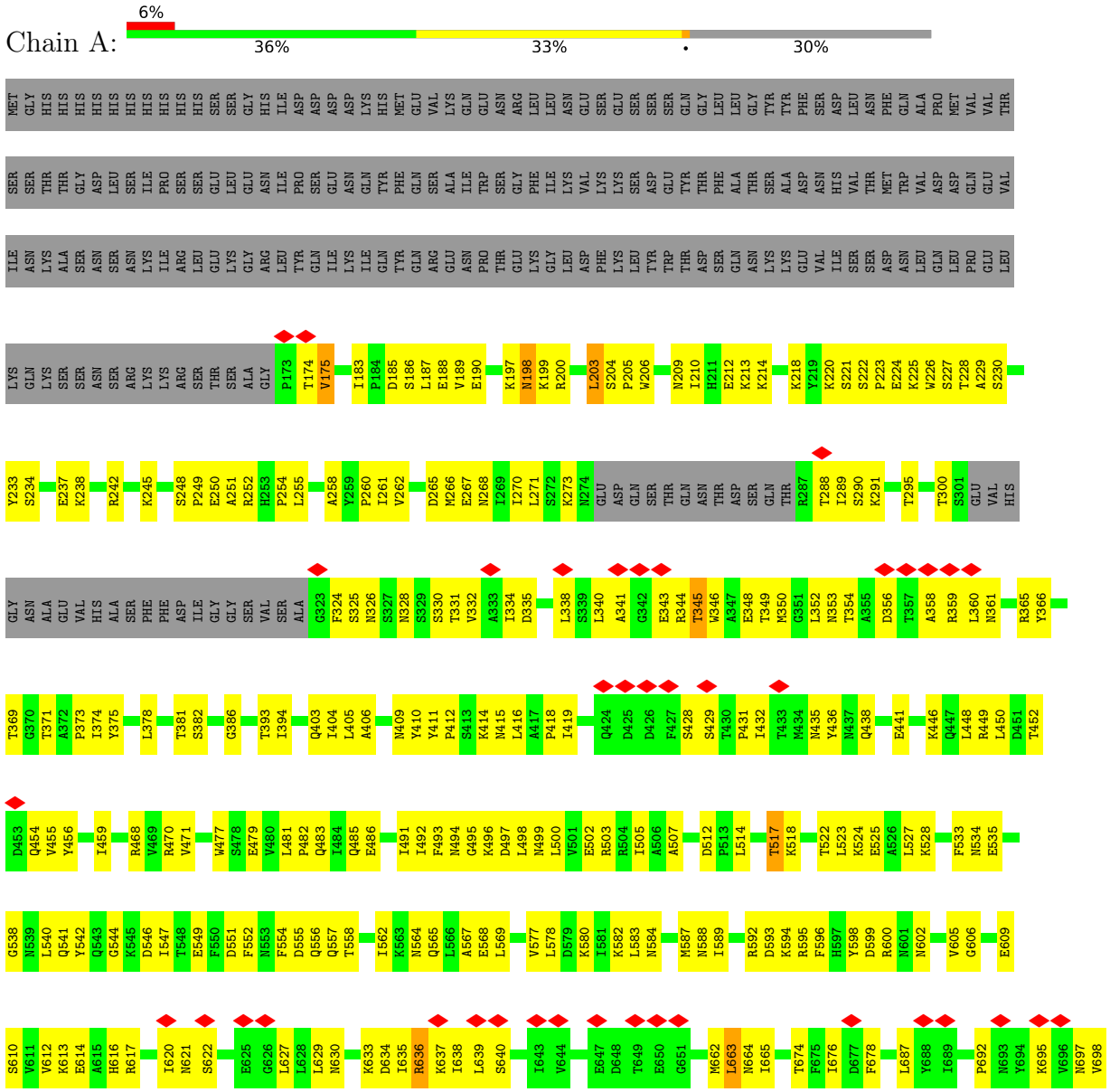
- Molecule 2 is a protein called Lethal factor.

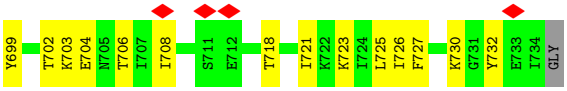
Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	699	Total	C	N	O	S	0	0
			5378	3404	913	1055	6		
2	I	710	Total	C	N	O	S	0	0
			4739	2982	841	912	4		
2	J	661	Total	C	N	O	S	0	0
			4239	2655	752	830	2		

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.

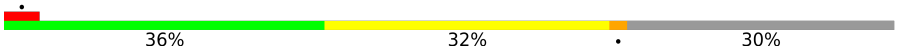
- Molecule 1: Protective antigen

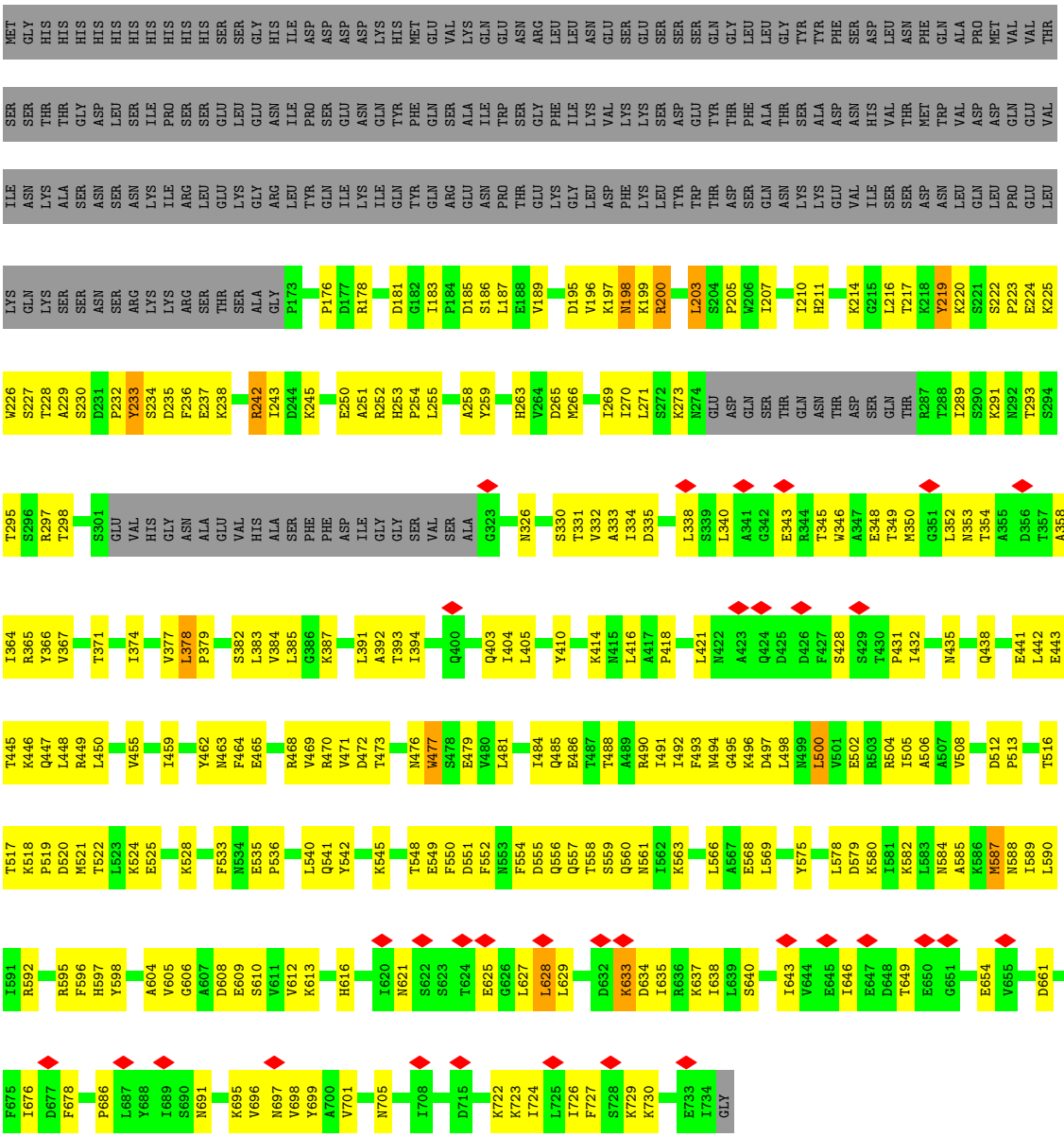




• Molecule 1: Protective antigen

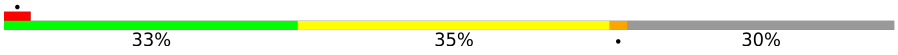
Chain B:

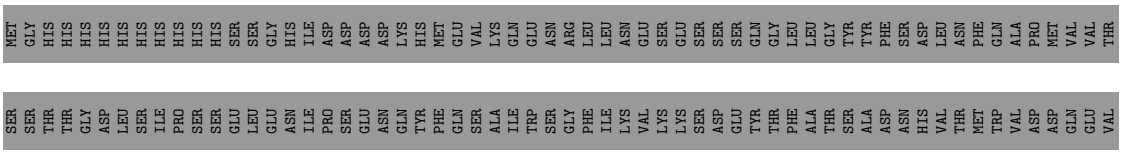


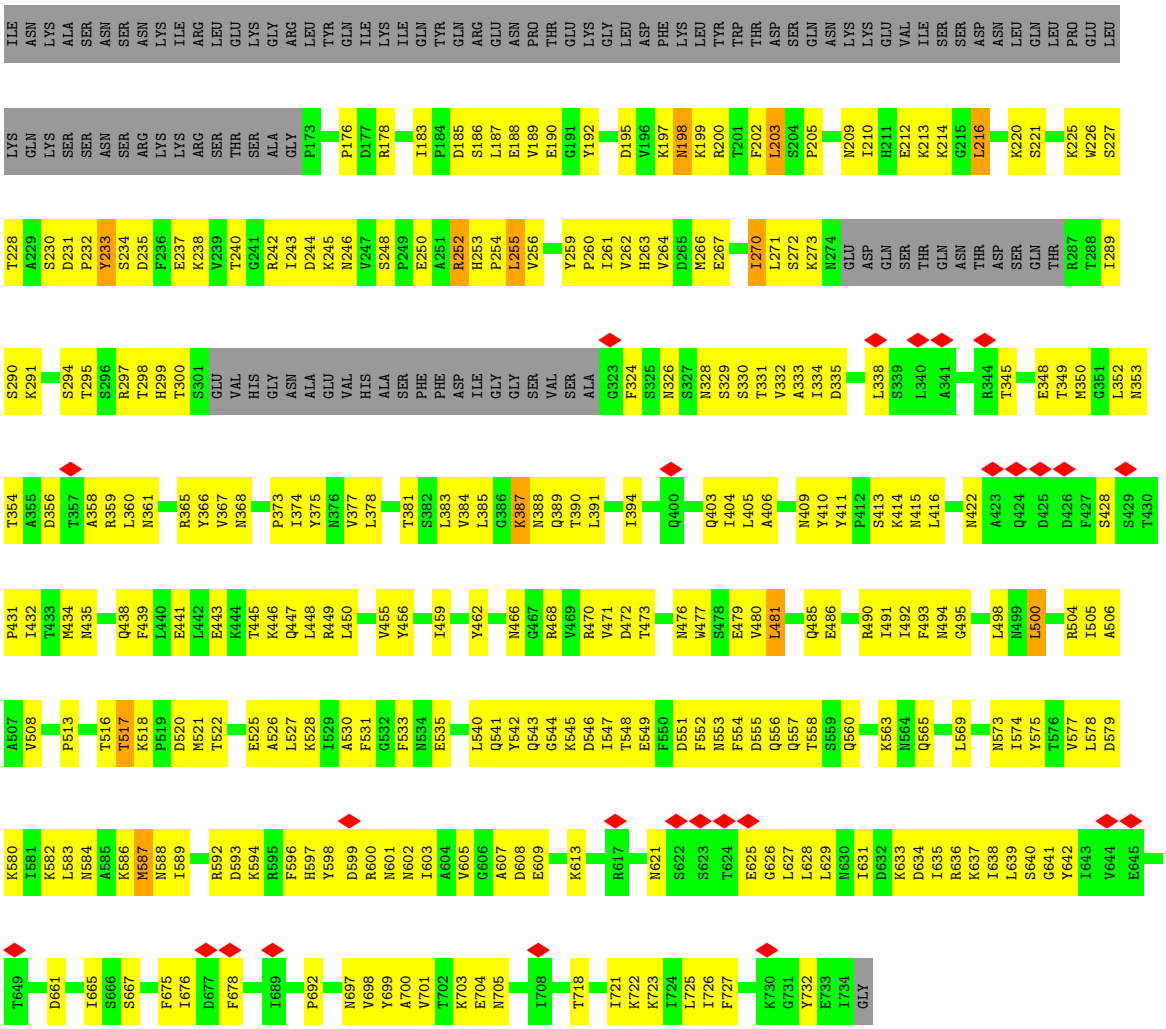


• Molecule 1: Protective antigen

Chain C:

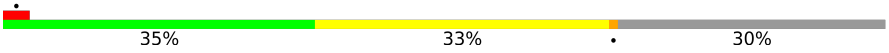


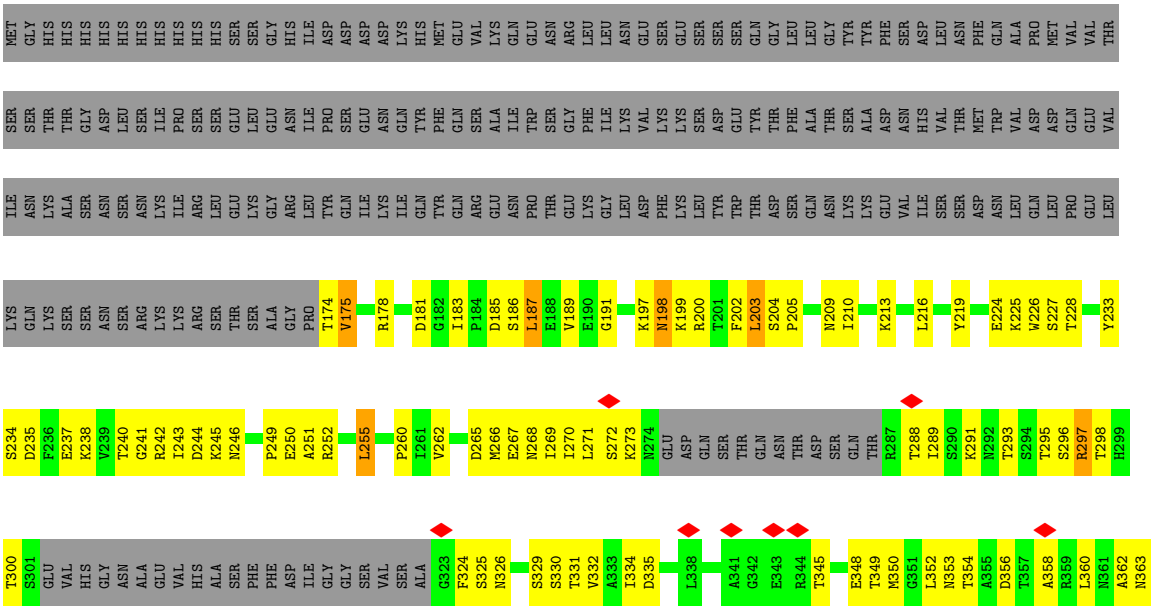


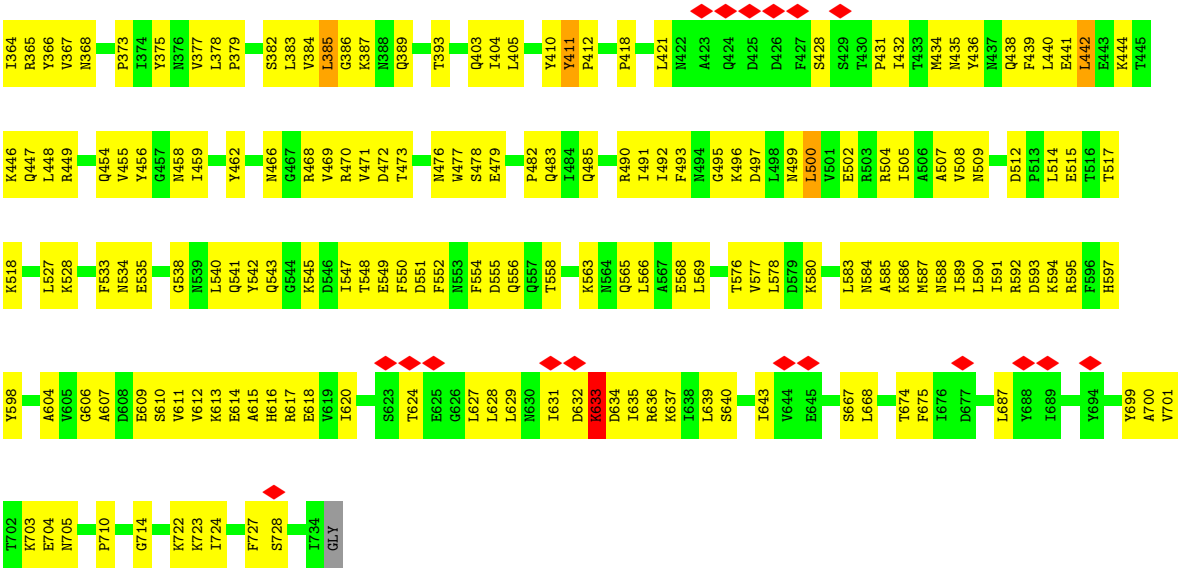


• Molecule 1: Protective antigen

Chain D:

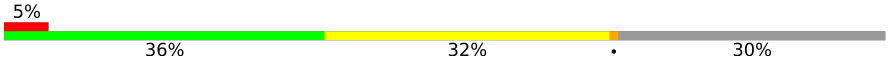


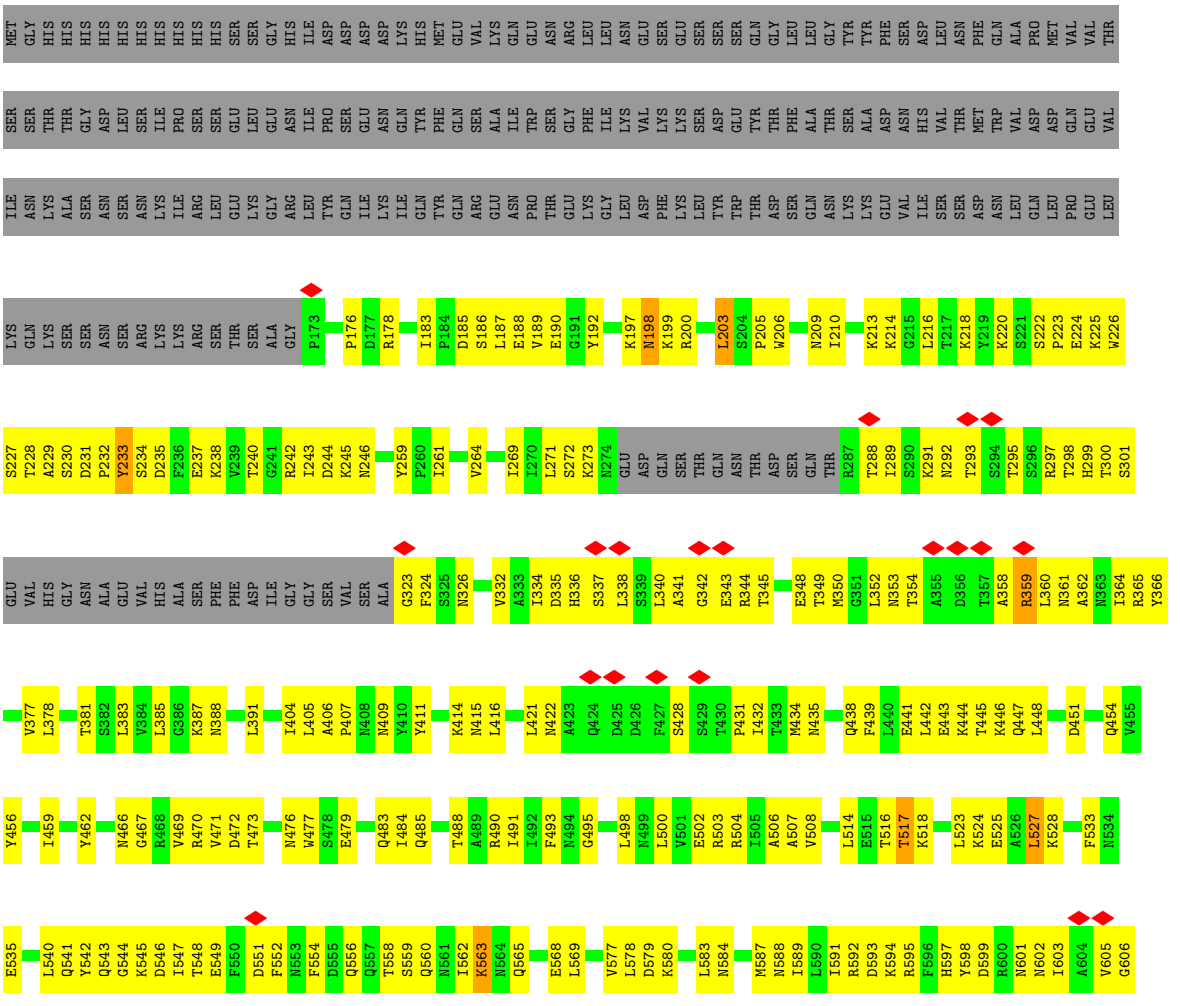


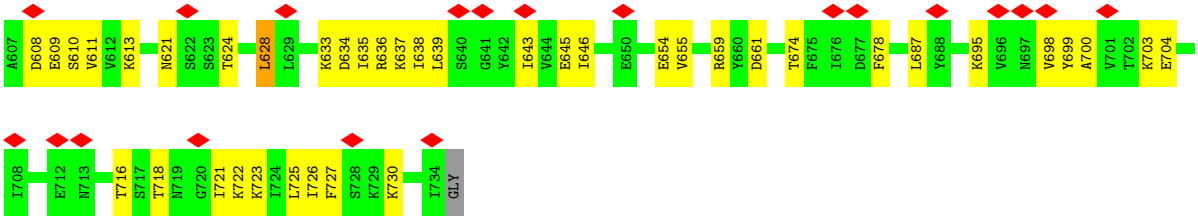


• Molecule 1: Protective antigen

Chain E:

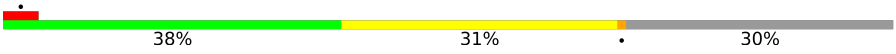


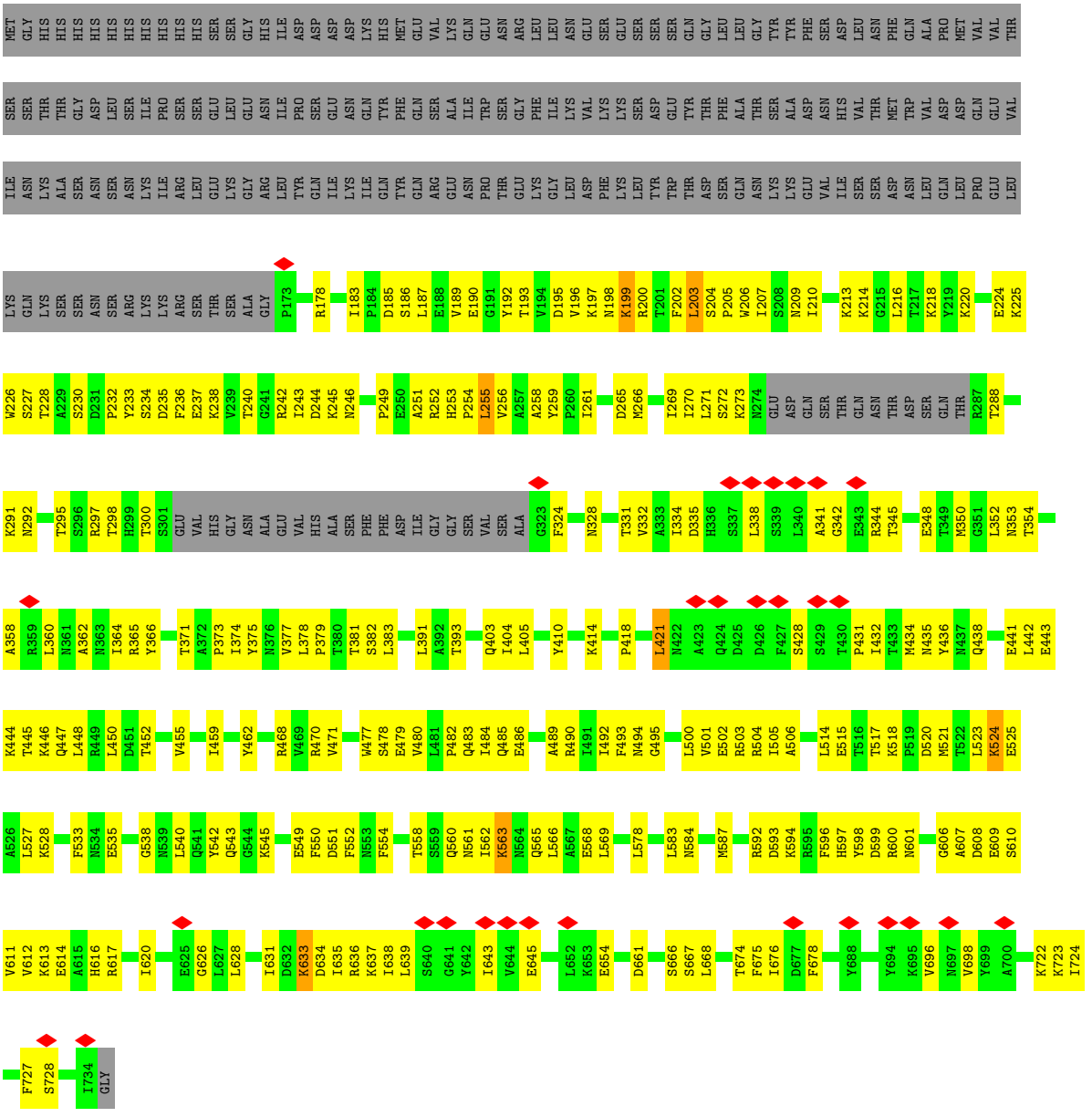




• Molecule 1: Protective antigen

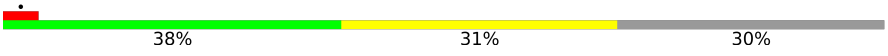
Chain F:

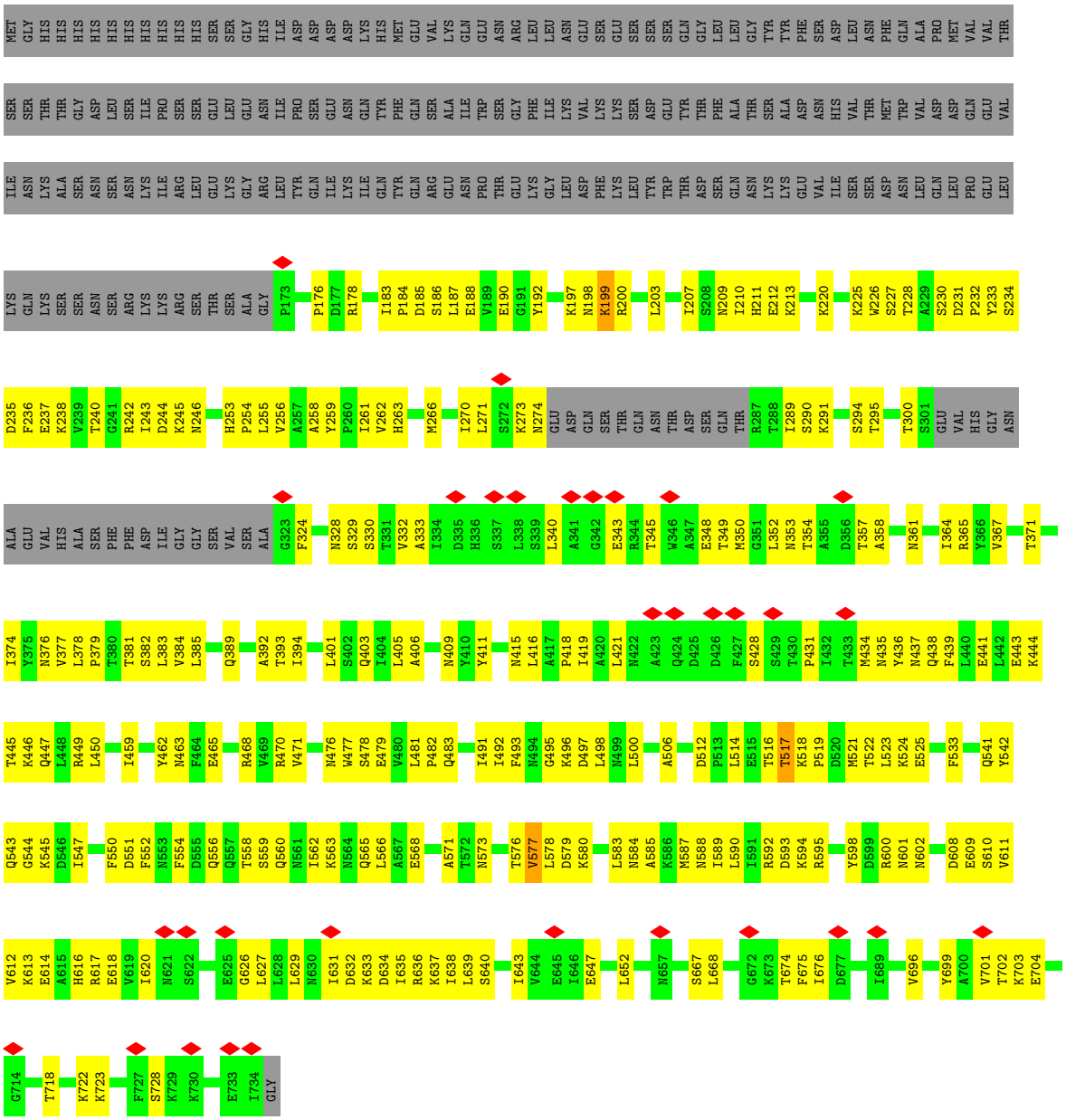




• Molecule 1: Protective antigen

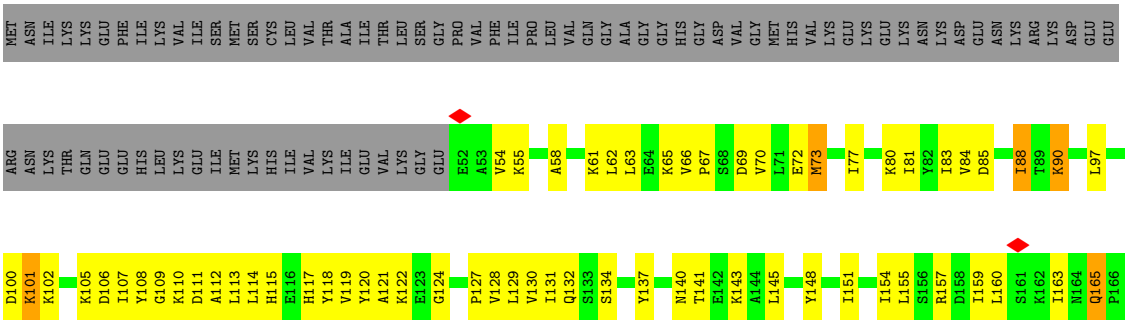
Chain G:





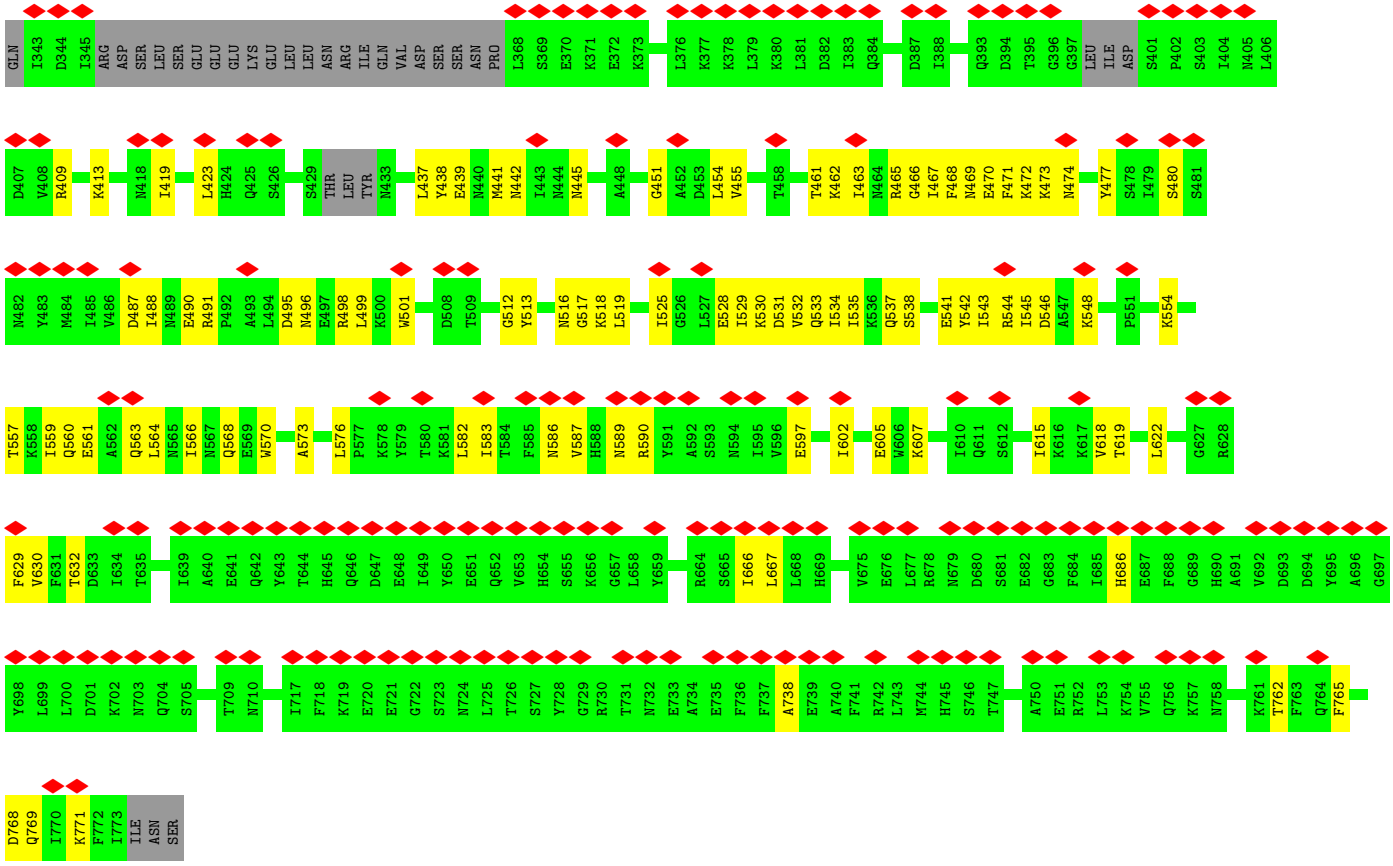
• Molecule 2: Lethal factor

Chain H:



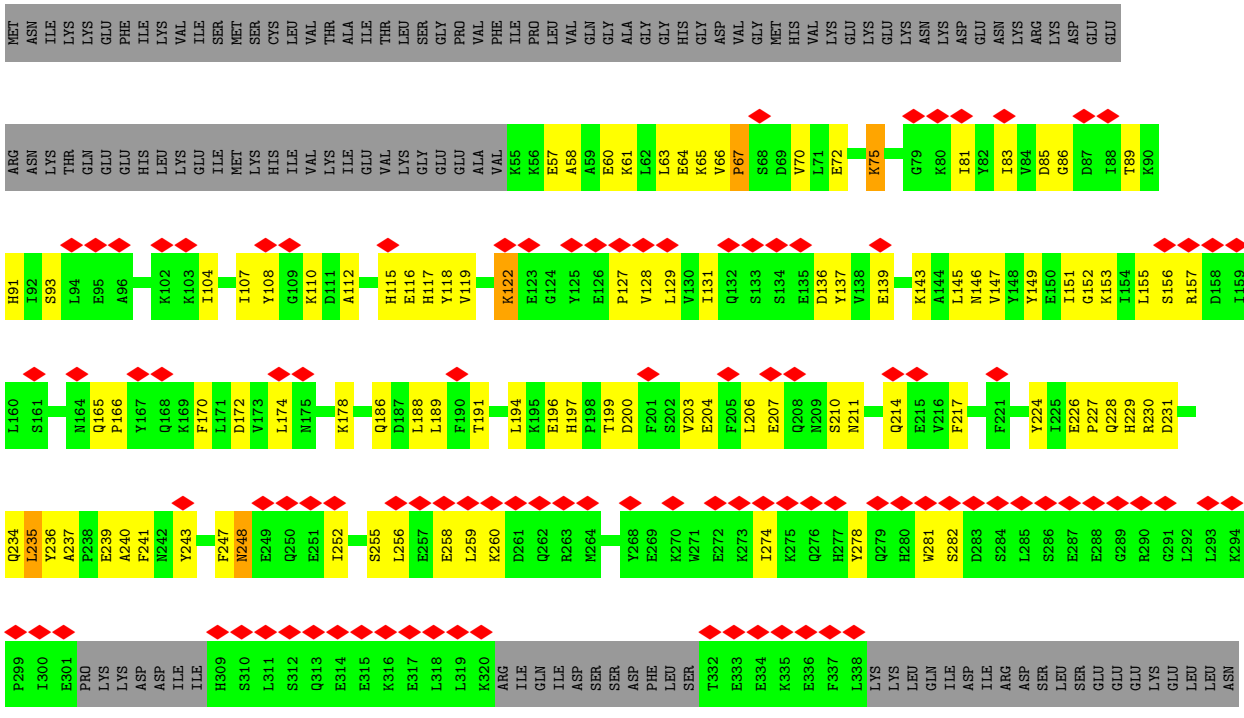
• Molecule 2: Lethal factor

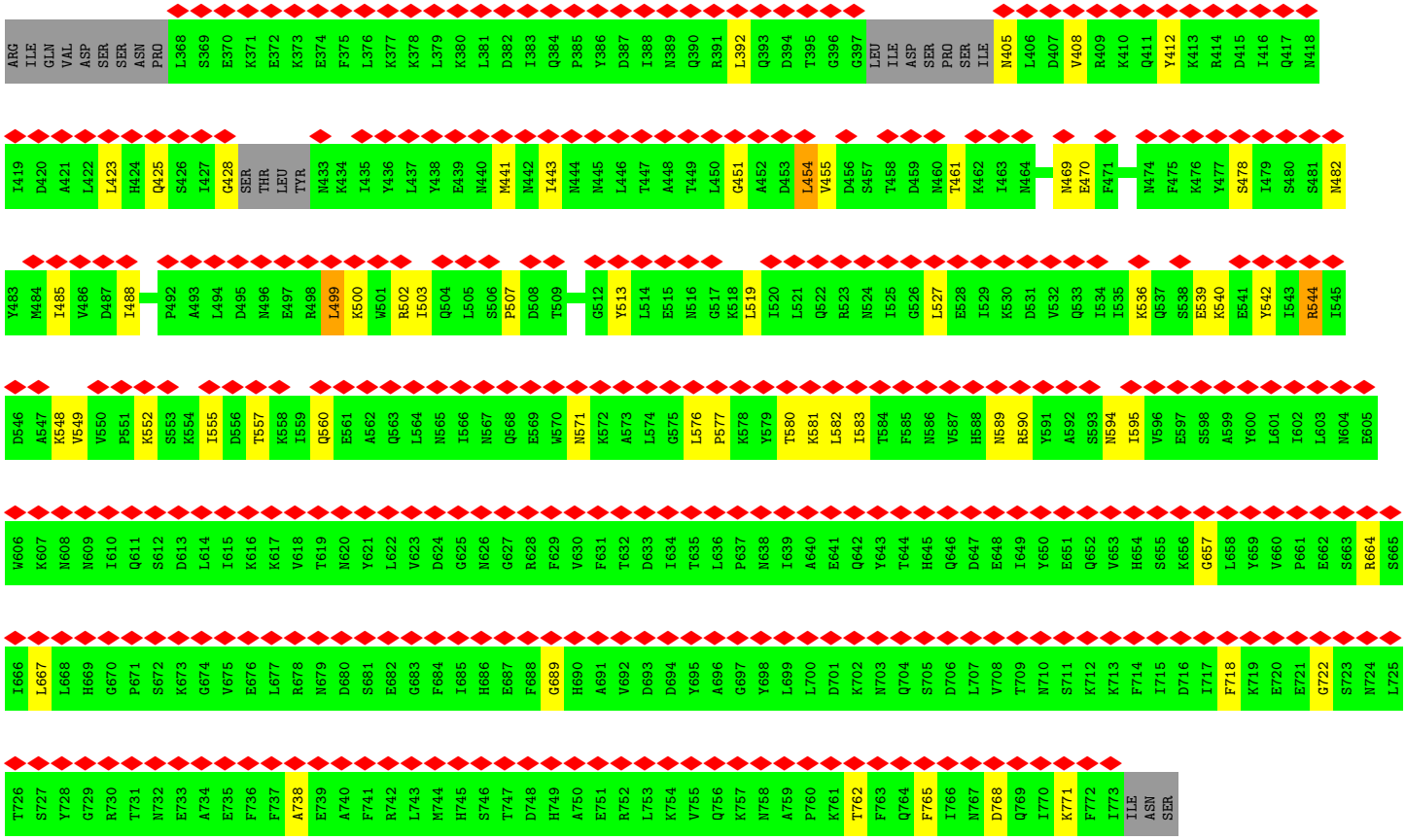
Chain I:



• Molecule 2: Lethal factor

Chain J:




ARG ILE GLN VAL ASP SER SER ASN PRO L368 S369 E370 K371 E372 K373 E374 F375 L376 K377 K378 L379 K380 L381 D382 I383 Q384 P385 Y386 D387 I388 N389 Q390 R391 L392 Q393 D394 T395 G396 G397 LEU ILE ASP SER PRO SER ILE N405 L406 D407 V408 R409 K410 Q411 Y412 K413 R414 D415 I416 Q417 N418
I419 D420 A421 L422 L423 H424 Q425 S426 I427 G428 SER THR LEU TYR N433 K434 I435 Y436 L437 Y438 E439 N440 M441 N442 I443 N444 N445 L446 T447 A448 T449 L450 G451 A452 D453 L454 V455 D456 S457 T458 D459 N460 T461 K462 I463 N464 N469 E470 F471 N474 F475 K476 Y477 S478 I479 S480 S481 N482
Y483 M484 I485 V486 D487 I488 P492 A493 L494 D495 N496 E497 R498 L499 K500 W501 R502 I503 Q504 L505 S506 P507 D508 T509 G512 Y513 L514 E515 N516 G517 K518 L519 I520 L521 Q522 R523 N524 I525 G526 L527 E528 I529 K530 D531 V532 Q533 I534 I535 K536 Q537 S538 E539 K540 E541 Y542 I543 R544 I545
D546 A547 K548 V549 V550 P551 K552 S553 K554 I555 D556 T557 K558 I559 Q560 E561 A562 Q563 L564 N565 I566 N567 Q568 E569 W570 N571 K572 A573 L574 G575 L576 P577 K578 Y579 T580 K581 L582 I583 T584 F585 N586 V587 H588 N589 R590 Y591 A592 S593 N594 I595 V596 E597 S598 A599 Y600 L601 I602 L603 N604 E605
W606 K607 N608 N609 I610 Q611 S612 D613 L614 I615 K616 K617 V618 T619 N620 Y621 L622 V623 D624 G625 N626 G627 R628 F629 V630 F631 T632 D633 I634 T635 L636 P637 N638 I639 A640 E641 Q642 Y643 T644 H645 Q646 D647 E648 I649 Y650 E651 Q652 V653 H654 S655 K656 G657 L658 Y659 V660 P661 E662 S663 R664 S665
I666 L667 L668 H669 G670 P671 S672 K673 G674 V675 E676 L677 R678 N679 D680 S681 E682 G683 F684 I685 H686 E687 F688 G689 H690 A691 V692 D693 D694 Y695 A696 G697 Y698 L699 L700 D701 K702 N703 Q704 S705 D706 L707 V708 T709 N710 S711 K712 K713 F714 I715 D716 I717 F718 K719 E720 E721 G722 S723 N724 L725
T726 S727 Y728 G729 R730 T731 N732 E733 A734 E735 F736 F737 A738 E739 A740 F741 R742 L743 M744 H745 S746 T747 D748 H749 A750 E751 R752 L753 K754 V755 Q756 K757 N758 A759 P760 K761 T762 F763 Q764 F765 I766 N767 D768 Q769 I770 K771 F772 I773 ILE ASN SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	44000	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 ($e^-/Å^2$)	74.4	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.098	Depositor
Minimum map value	-0.772	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	359.52002, 359.52002, 359.52002	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.67	1/4029 (0.0%)	0.73	3/5491 (0.1%)
1	B	0.73	3/4045 (0.1%)	0.77	5/5511 (0.1%)
1	C	0.75	2/4045 (0.0%)	0.78	8/5511 (0.1%)
1	D	0.74	1/4037 (0.0%)	0.82	10/5500 (0.2%)
1	E	0.69	1/4045 (0.0%)	0.78	6/5511 (0.1%)
1	F	0.70	1/4045 (0.0%)	0.75	3/5511 (0.1%)
1	G	0.68	1/4045 (0.0%)	0.71	0/5511
2	H	0.50	0/5476	0.71	5/7434 (0.1%)
2	I	0.47	0/4804	0.64	4/6565 (0.1%)
2	J	0.32	0/4294	0.58	8/5903 (0.1%)
All	All	0.63	10/42865 (0.0%)	0.73	52/58448 (0.1%)

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	H	0	1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	517	THR	C-N	-10.63	1.09	1.34
1	G	517	THR	C-N	-10.43	1.10	1.34
1	B	517	THR	C-N	-9.98	1.11	1.34
1	F	517	THR	C-N	-8.53	1.14	1.34
1	A	517	THR	C-N	-7.07	1.17	1.34

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	582	LEU	CA-CB-CG	10.52	139.48	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	88	ILE	C-N-CA	8.96	144.10	121.70
1	D	297	ARG	NE-CZ-NH1	-8.65	115.98	120.30
1	A	203	LEU	CA-CB-CG	-8.57	95.59	115.30
1	A	450	LEU	CA-CB-CG	-7.98	96.95	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	165	GLN	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	A	3961	0	3728	237	0
1	B	3977	0	3760	302	0
1	C	3977	0	3760	311	0
1	D	3970	0	3753	283	0
1	E	3977	0	3761	266	0
1	F	3977	0	3760	242	0
1	G	3977	0	3760	239	0
2	H	5378	0	5004	353	0
2	I	4739	0	3782	223	0
2	J	4239	0	3182	123	0
All	All	42172	0	38250	2526	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 31.

The worst 5 of 2526 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)
2:I:89:THR:CG2	2:I:115:HIS:HA	1.55	1.35
1:C:233:TYR:CD1	1:C:243:ILE:HD11	1.74	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:117:HIS:NE2	2:H:119:VAL:HG23	1.56	1.21
2:I:89:THR:HG21	2:I:115:HIS:CB	1.72	1.19
2:H:578:LYS:HD3	2:H:579:TYR:HE1	1.04	1.16

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	523/759 (69%)	480 (92%)	39 (8%)	4 (1%)	19	60
1	B	523/759 (69%)	480 (92%)	42 (8%)	1 (0%)	47	80
1	C	523/759 (69%)	478 (91%)	44 (8%)	1 (0%)	47	80
1	D	522/759 (69%)	474 (91%)	45 (9%)	3 (1%)	25	64
1	E	523/759 (69%)	473 (90%)	49 (9%)	1 (0%)	47	80
1	F	523/759 (69%)	471 (90%)	50 (10%)	2 (0%)	34	72
1	G	523/759 (69%)	479 (92%)	42 (8%)	2 (0%)	34	72
2	H	695/809 (86%)	638 (92%)	52 (8%)	5 (1%)	22	62
2	I	700/809 (86%)	649 (93%)	51 (7%)	0	100	100
2	J	649/809 (80%)	604 (93%)	44 (7%)	1 (0%)	47	80
All	All	5704/7740 (74%)	5226 (92%)	458 (8%)	20 (0%)	38	72

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ASN
1	B	198	ASN
1	C	198	ASN
1	D	198	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	198	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	410/683 (60%)	409 (100%)	1 (0%)	93 96
1	B	415/683 (61%)	411 (99%)	4 (1%)	76 86
1	C	415/683 (61%)	413 (100%)	2 (0%)	88 93
1	D	414/683 (61%)	412 (100%)	2 (0%)	88 93
1	E	415/683 (61%)	410 (99%)	5 (1%)	71 83
1	F	415/683 (61%)	413 (100%)	2 (0%)	88 93
1	G	415/683 (61%)	415 (100%)	0	100 100
2	H	544/739 (74%)	539 (99%)	5 (1%)	78 87
2	I	338/739 (46%)	336 (99%)	2 (1%)	86 92
2	J	274/739 (37%)	271 (99%)	3 (1%)	73 84
All	All	4055/6998 (58%)	4029 (99%)	26 (1%)	86 92

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	524	LYS
2	H	434	LYS
2	J	122	LYS
2	H	413	LYS
2	H	579	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	563	GLN
2	I	469	ASN

Continued on next page...

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Mol	Chain	Res	Type
2	J	228	GLN
2	I	594	ASN
1	D	447	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	1
1	A	1
1	F	1
1	B	1
1	G	1
1	C	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	517:THR	C	518:LYS	N	1.18
1	A	517:THR	C	518:LYS	N	1.17
1	F	517:THR	C	518:LYS	N	1.14
1	B	517:THR	C	518:LYS	N	1.11
1	G	517:THR	C	518:LYS	N	1.10

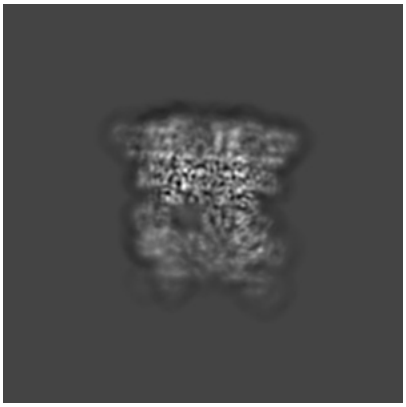
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11524. These allow visual inspection of the internal detail of the map and identification of artifacts.

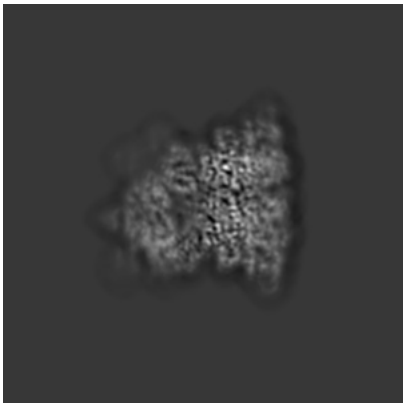
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

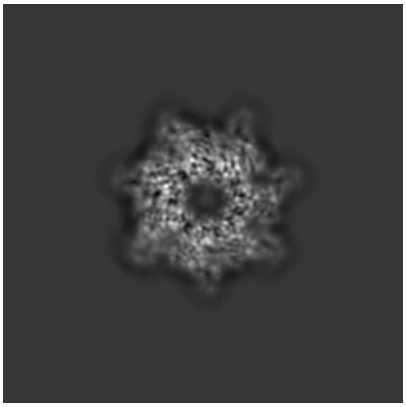
6.1.1 Primary map



X



Y

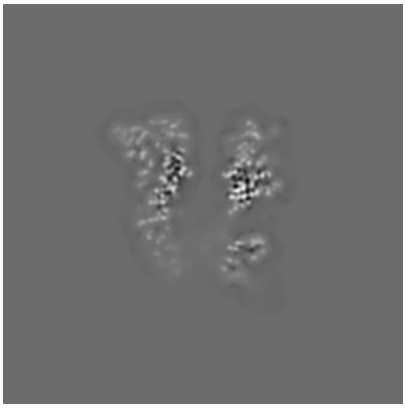


Z

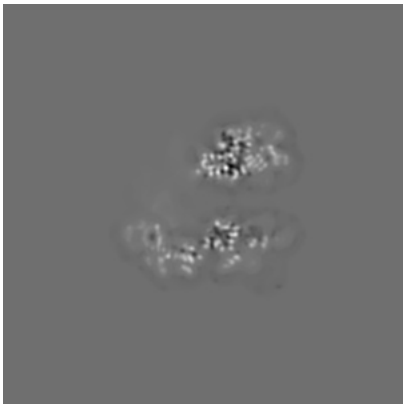
The images above show the map projected in three orthogonal directions.

6.2 Central slices

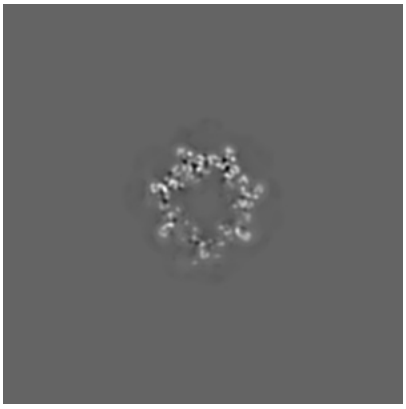
6.2.1 Primary map



X Index: 168



Y Index: 168

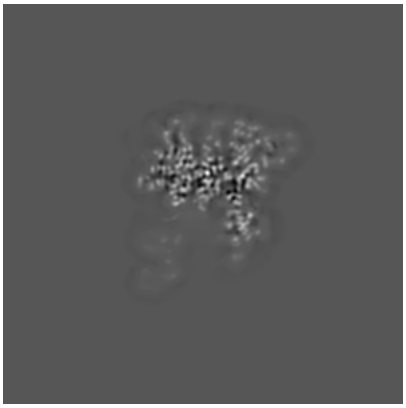


Z Index: 168

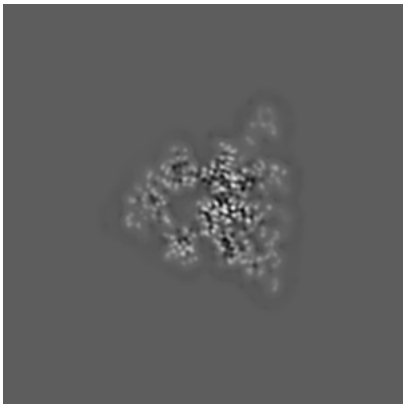
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

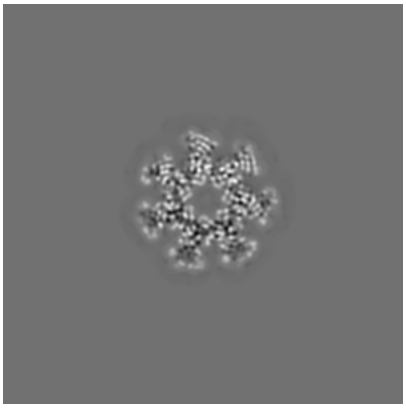
6.3.1 Primary map



X Index: 196



Y Index: 196

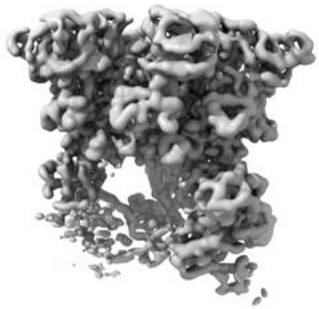


Z Index: 192

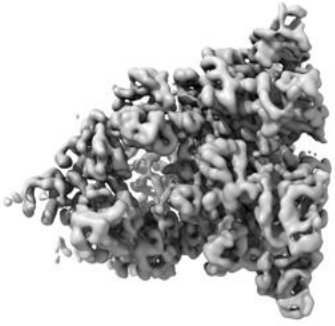
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

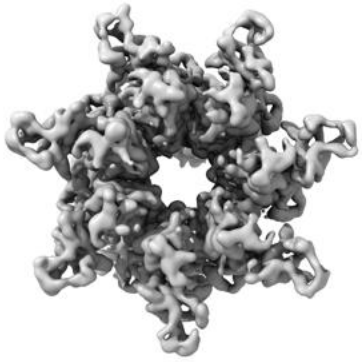
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

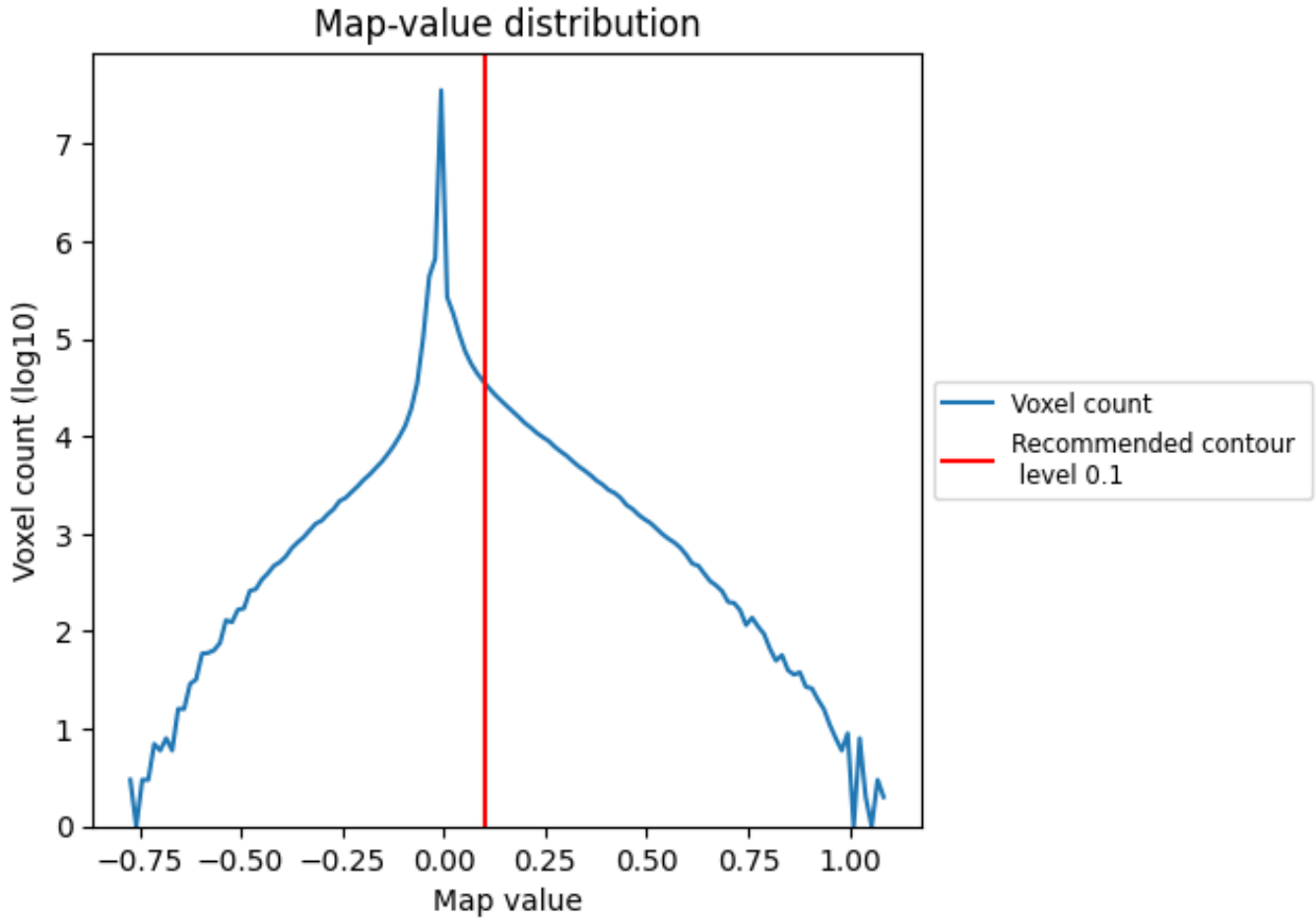
6.5 Mask visualisation (i)

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

7 Map analysis

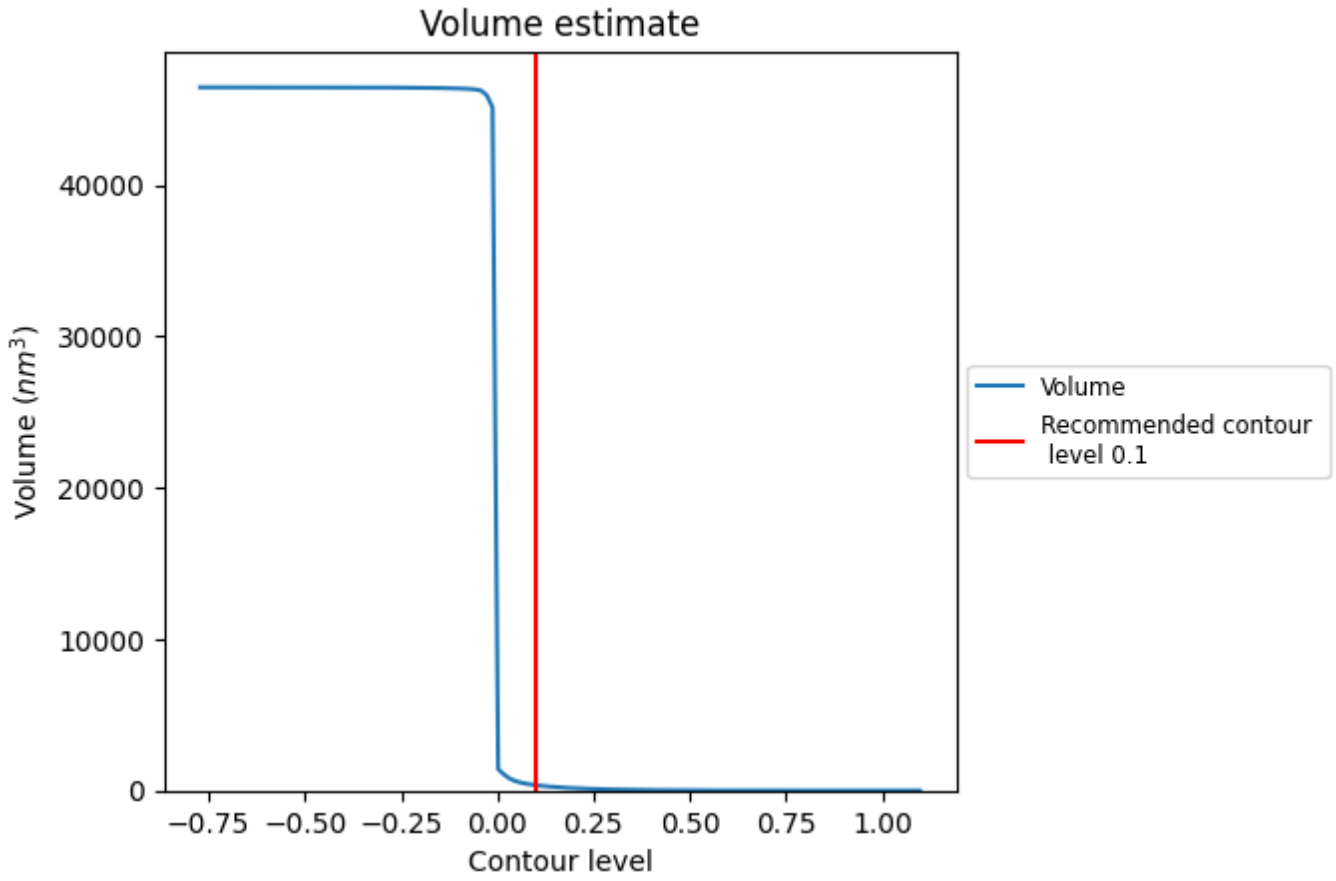
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

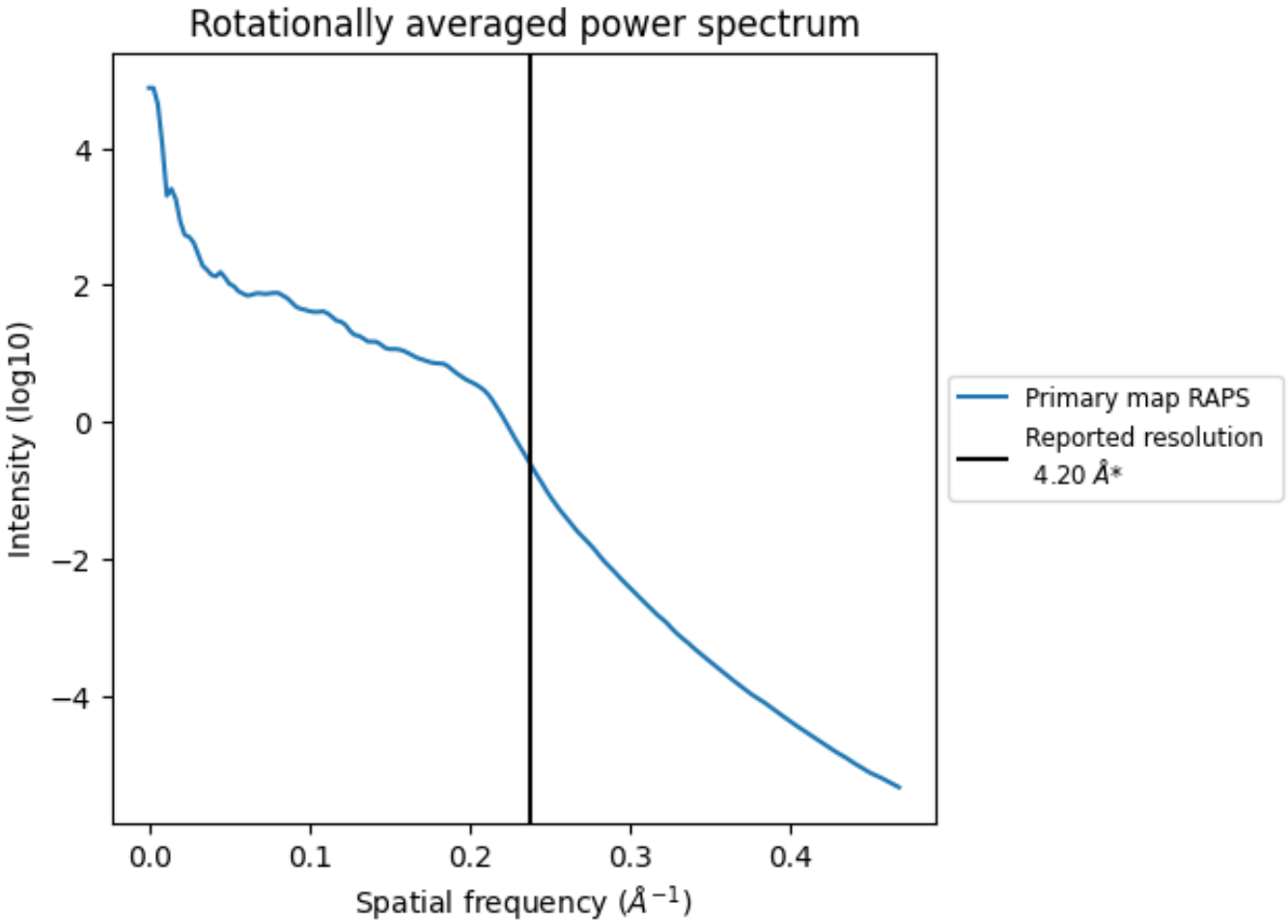
7.2 Volume estimate (i)



The volume at the recommended contour level is 357 nm^3; this corresponds to an approximate mass of 322 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 0.238 Å^{-1}

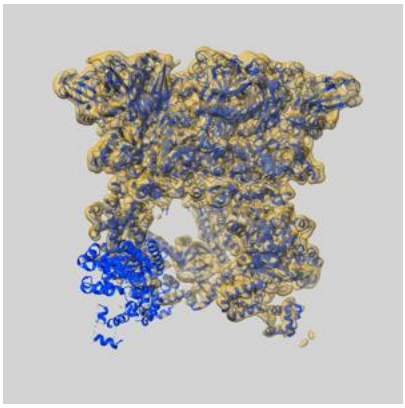
8 Fourier-Shell correlation (i)

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

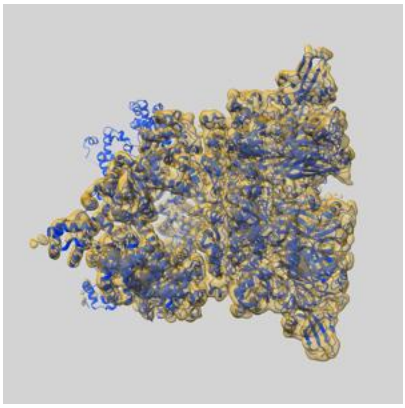
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11524 and PDB model 6ZXL. Per-residue inclusion information can be found in section 3 on page 9.

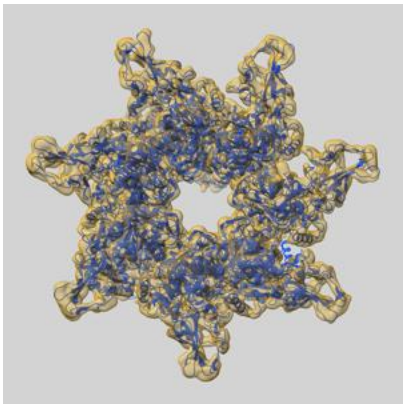
9.1 Map-model overlay



X



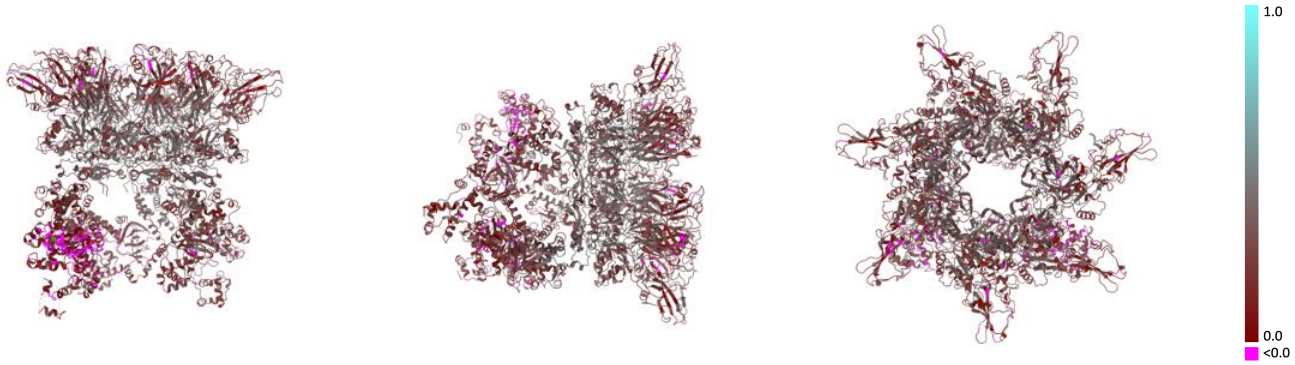
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

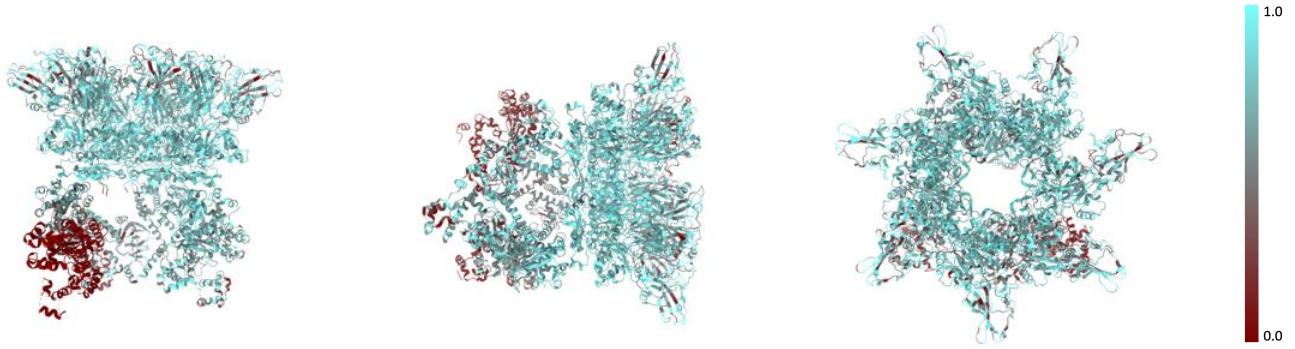
9.2 Q-score mapped to coordinate model (i)



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.

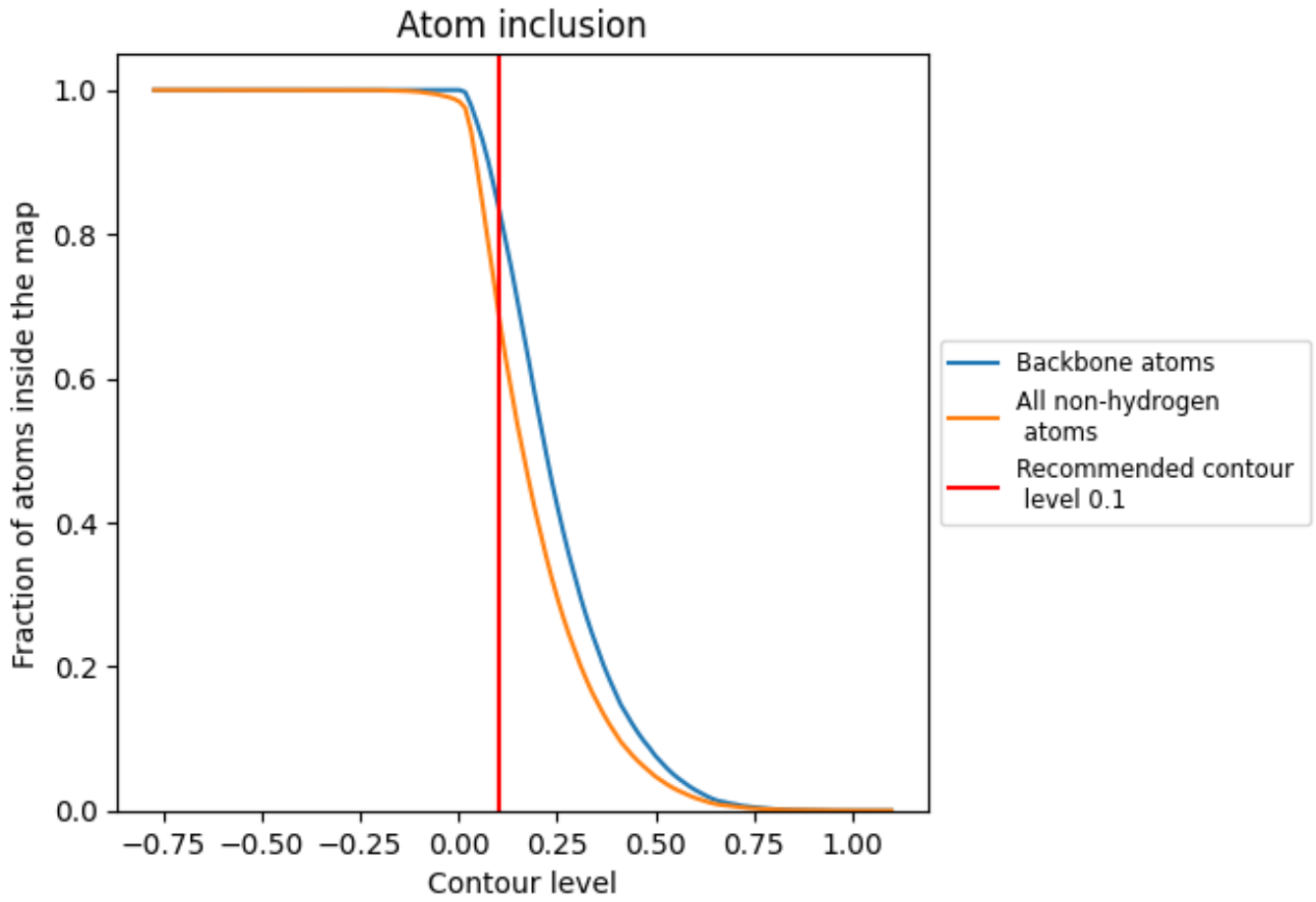
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 70% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6953	0.2870
A	0.7667	0.3190
B	0.7815	0.3230
C	0.7853	0.3270
D	0.7852	0.3280
E	0.7728	0.3160
F	0.7848	0.3240
G	0.7697	0.3130
H	0.7001	0.2540
I	0.5939	0.2320
J	0.2631	0.1620