wwPDB EM Validation Summary Report

Apr 16, 2022 – 12:28 am BST

PDB ID	:	7PK6
EMDB ID	:	EMD-13466
Title	:	Providencia stuartii Arginine decarboxylase (Adc), stack structure
Authors	:	Jessop, M.; Desfosses, A.; Bacia-Verloop, M.; Gutsche, I.
Deposited on	:	2021-08-25
Resolution	:	2.15 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 ⓘ symbol.

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

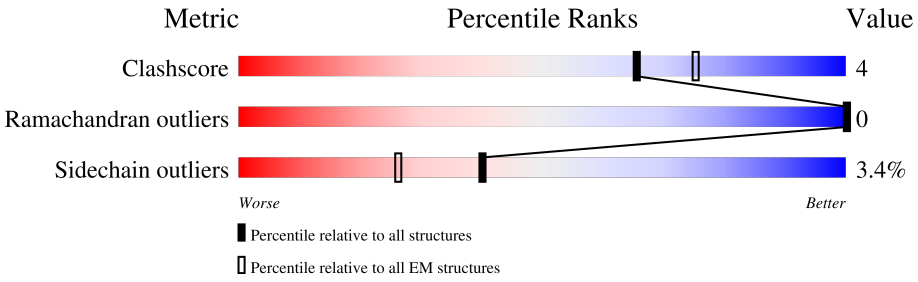
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.15 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	758	86% 12%
1	B	758	85% 13%
1	C	758	73% 87% 12%
1	D	758	73% 87% 12%
1	E	758	73% 87% 11%
1	F	758	26% 87% 12%
1	G	758	26% 86% 12%
1	H	758	26% 87% 11%

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Mol	Chain	Length	Quality of chain
1	I	758	27% 87% 12%
1	J	758	73% 87% 12%
1	K	758	86% 13%
1	L	758	86% 12%
1	M	758	87% 11%
1	N	758	87% 12%
1	O	758	73% 87% 12%
1	P	758	86% 12%
1	Q	758	87% 11%
1	R	758	88% 11%
1	S	758	86% 12%
1	T	758	26% 86% 12%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 120580 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 Biodegradative arginine decarboxylase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	755	Total	C	N	O	P	S	0	0
			6029	3816	1038	1138	1	36		
1	B	755	Total	C	N	O	P	S	0	0
			6029	3816	1038	1138	1	36		
1	K	755	Total	C	N	O	P	S	0	0
			6029	3816	1038	1138	1	36		
1	P	755	Total	C	N	O	P	S	0	0
			6029	3816	1038	1138	1	36		
1	L	755	Total	C	N	O	P	S	0	0
			6029	3816	1038	1138	1	36		
1	Q	755	Total	C	N	O	P	S	0	0
			6029	3816	1038	1138	1	36		
1	M	755	Total	C	N	O	P	S	0	0
			6029	3816	1038	1138	1	36		
1	R	755	Total	C	N	O	P	S	0	0
			6029	3816	1038	1138	1	36		
1	N	755	Total	C	N	O	P	S	0	0
			6029	3816	1038	1138	1	36		
1	S	755	Total	C	N	O	P	S	0	0
			6029	3816	1038	1138	1	36		
1	O	755	Total	C	N	O	P	S	0	0
			6029	3816	1038	1138	1	36		
1	T	755	Total	C	N	O	P	S	0	0
			6029	3816	1038	1138	1	36		
1	C	755	Total	C	N	O	P	S	0	0
			6029	3816	1038	1138	1	36		
1	G	755	Total	C	N	O	P	S	0	0
			6029	3816	1038	1138	1	36		
1	D	755	Total	C	N	O	P	S	0	0
			6029	3816	1038	1138	1	36		
1	H	755	Total	C	N	O	P	S	0	0
			6029	3816	1038	1138	1	36		
1	E	755	Total	C	N	O	P	S	0	0
			6029	3816	1038	1138	1	36		

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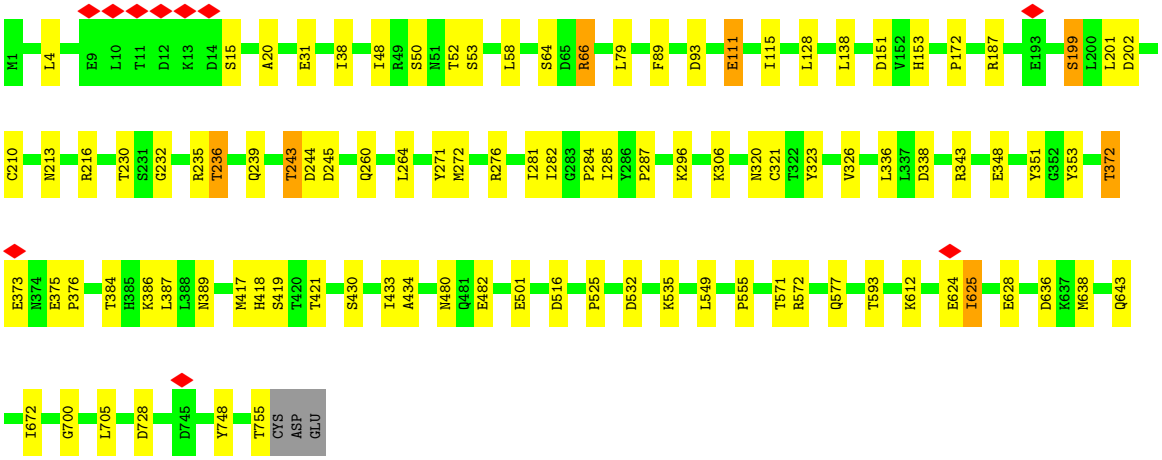
Mol	Chain	Residues	Atoms						AltConf	Trace
1	I	755	Total	C	N	O	P	S	0	0
			6029	3816	1038	1138	1	36		
1	F	755	Total	C	N	O	P	S	0	0
			6029	3816	1038	1138	1	36		
1	J	755	Total	C	N	O	P	S	0	0
			6029	3816	1038	1138	1	36		

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.

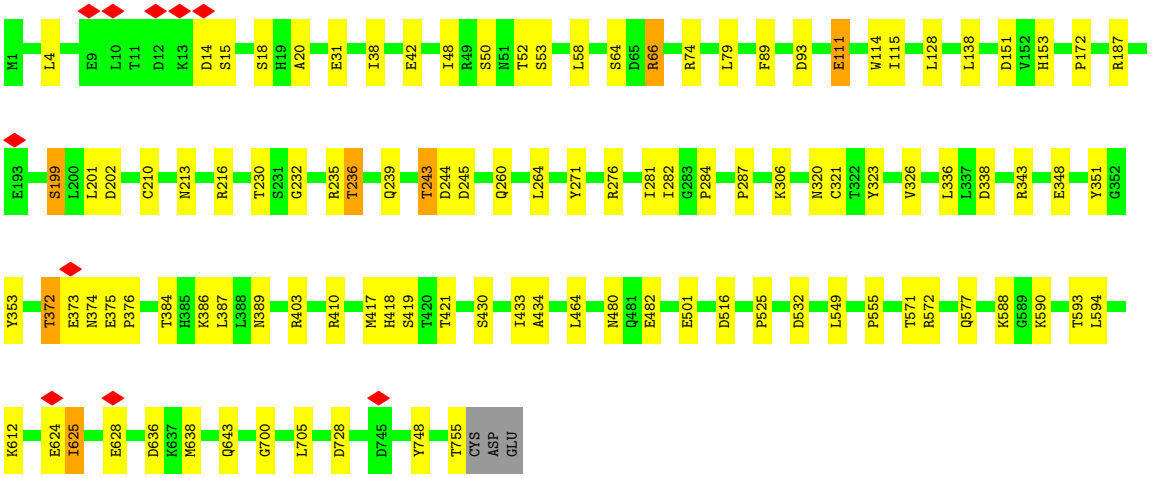
• Molecule 1: Biodegradative arginine decarboxylase

Chain A:



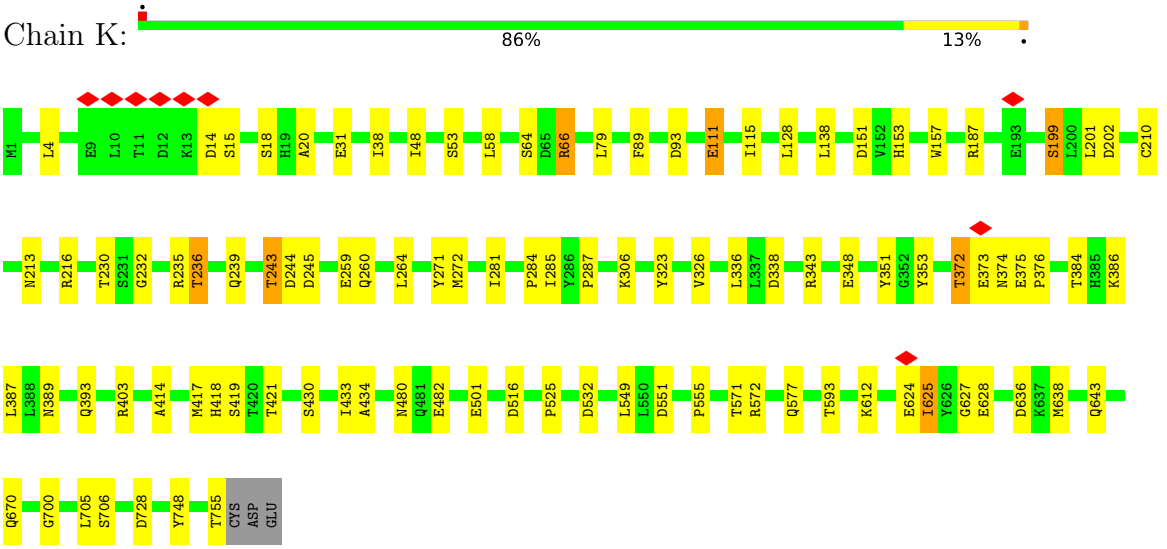
• Molecule 1: Biodegradative arginine decarboxylase

Chain B:



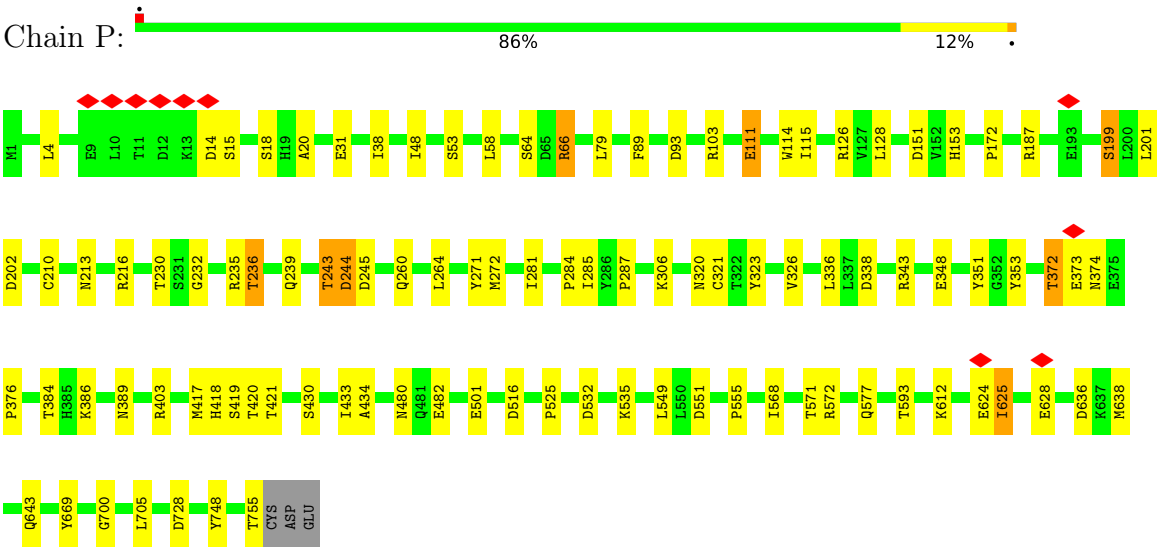
• Molecule 1: Biodegradative arginine decarboxylase

Chain K:



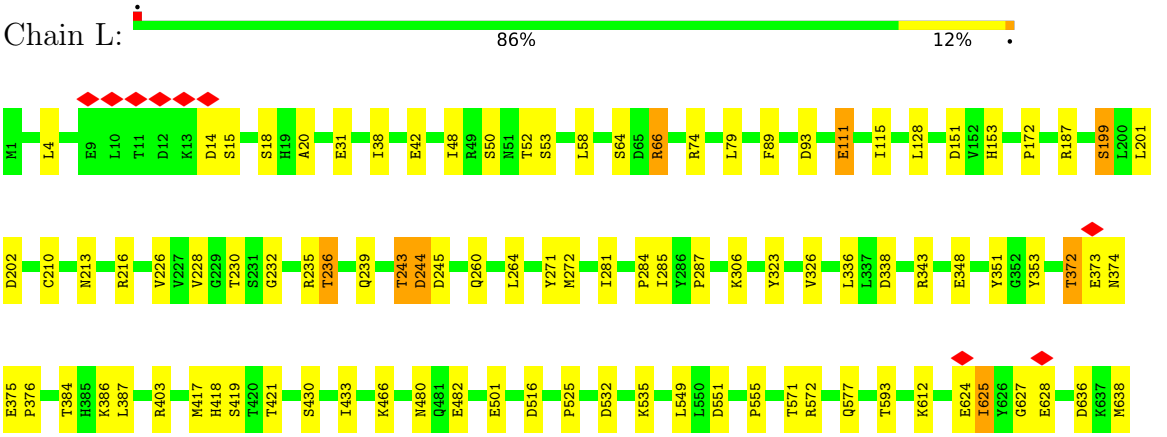
• Molecule 1: Biodegradative arginine decarboxylase

Chain P:



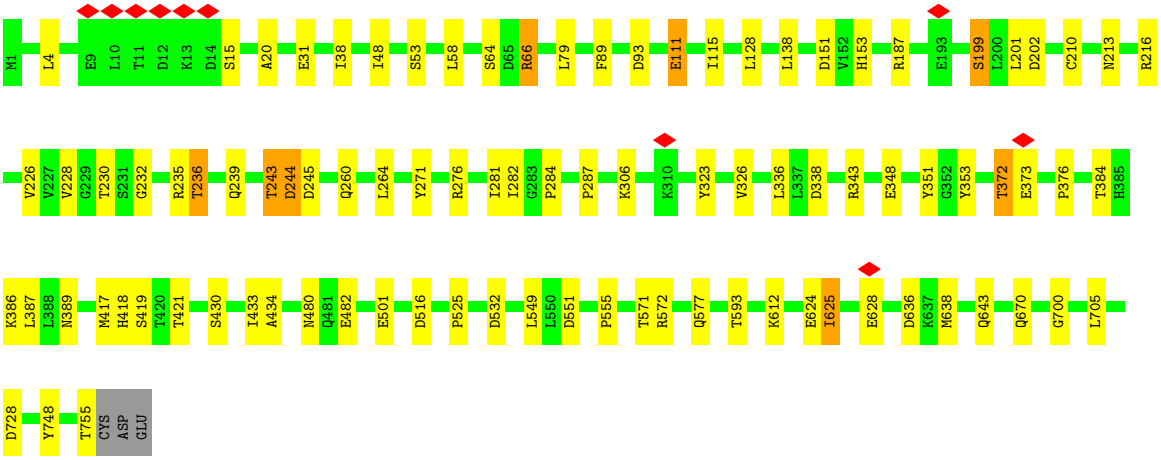
• Molecule 1: Biodegradative arginine decarboxylase

Chain L:



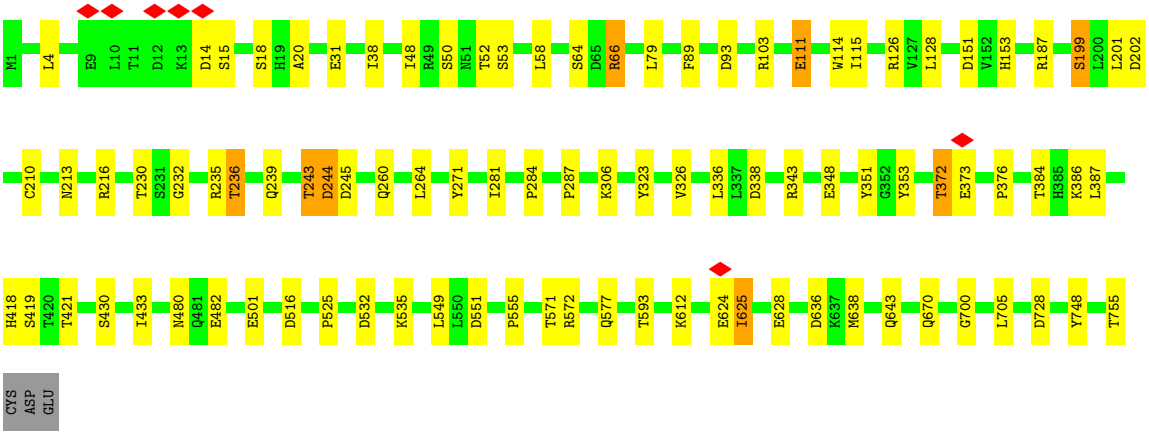
• Molecule 1: Biodegradative arginine decarboxylase

Chain Q:



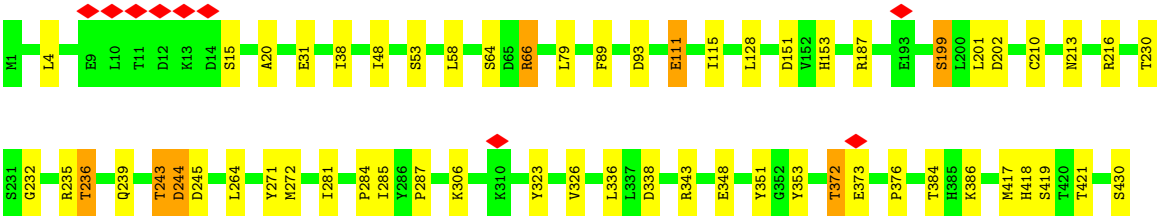
• Molecule 1: Biodegradative arginine decarboxylase

Chain M:



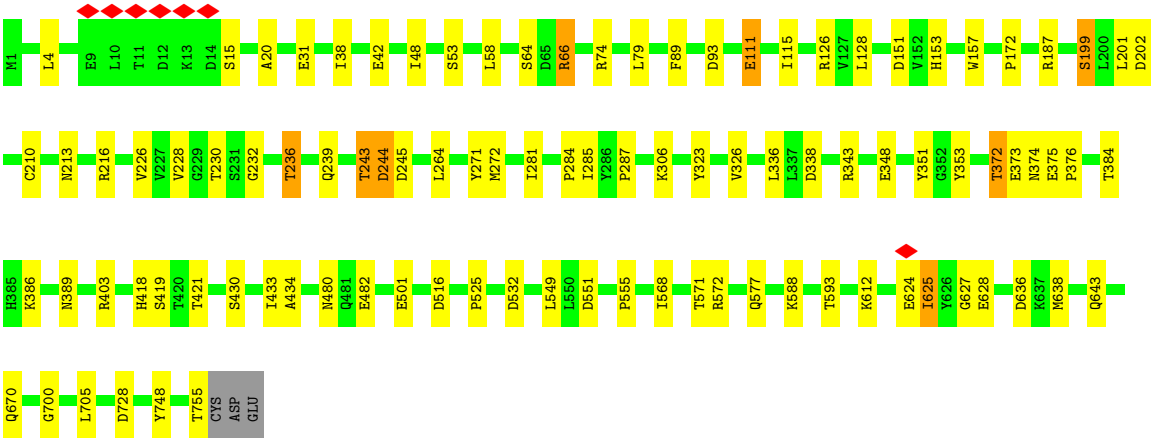
• Molecule 1: Biodegradative arginine decarboxylase

Chain R:



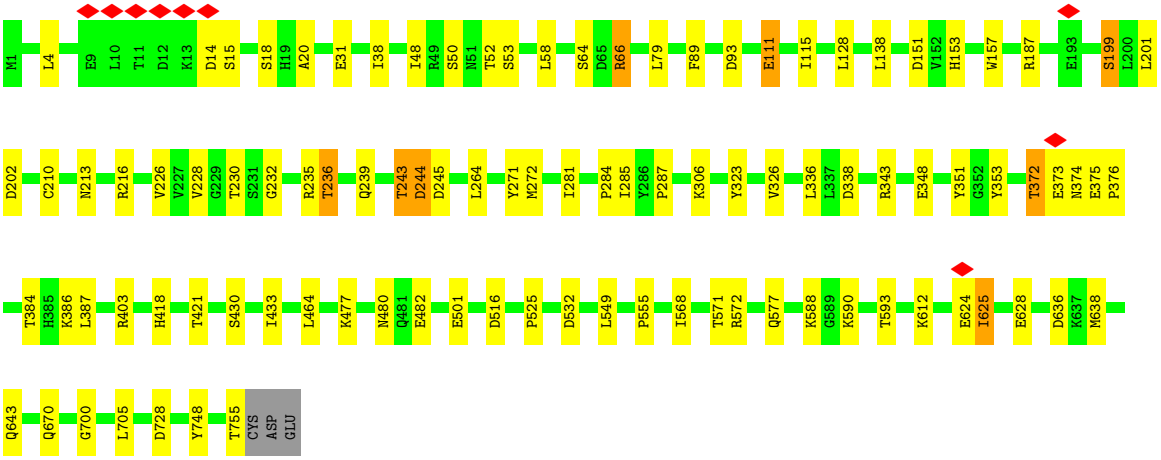
• Molecule 1: Biodegradative arginine decarboxylase

Chain N:



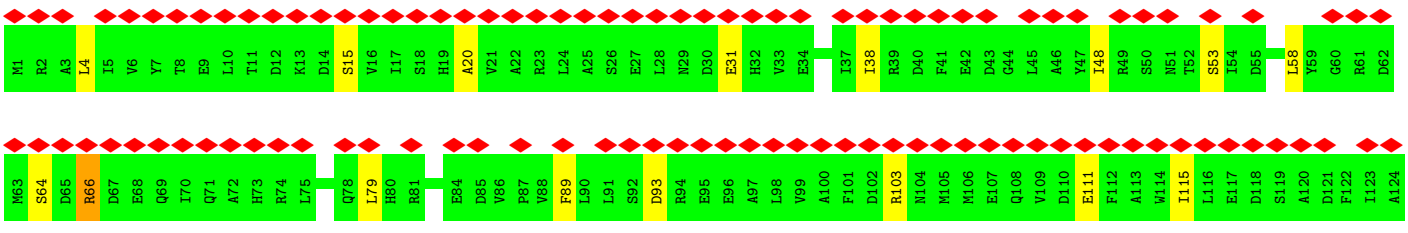
• Molecule 1: Biodegradative arginine decarboxylase

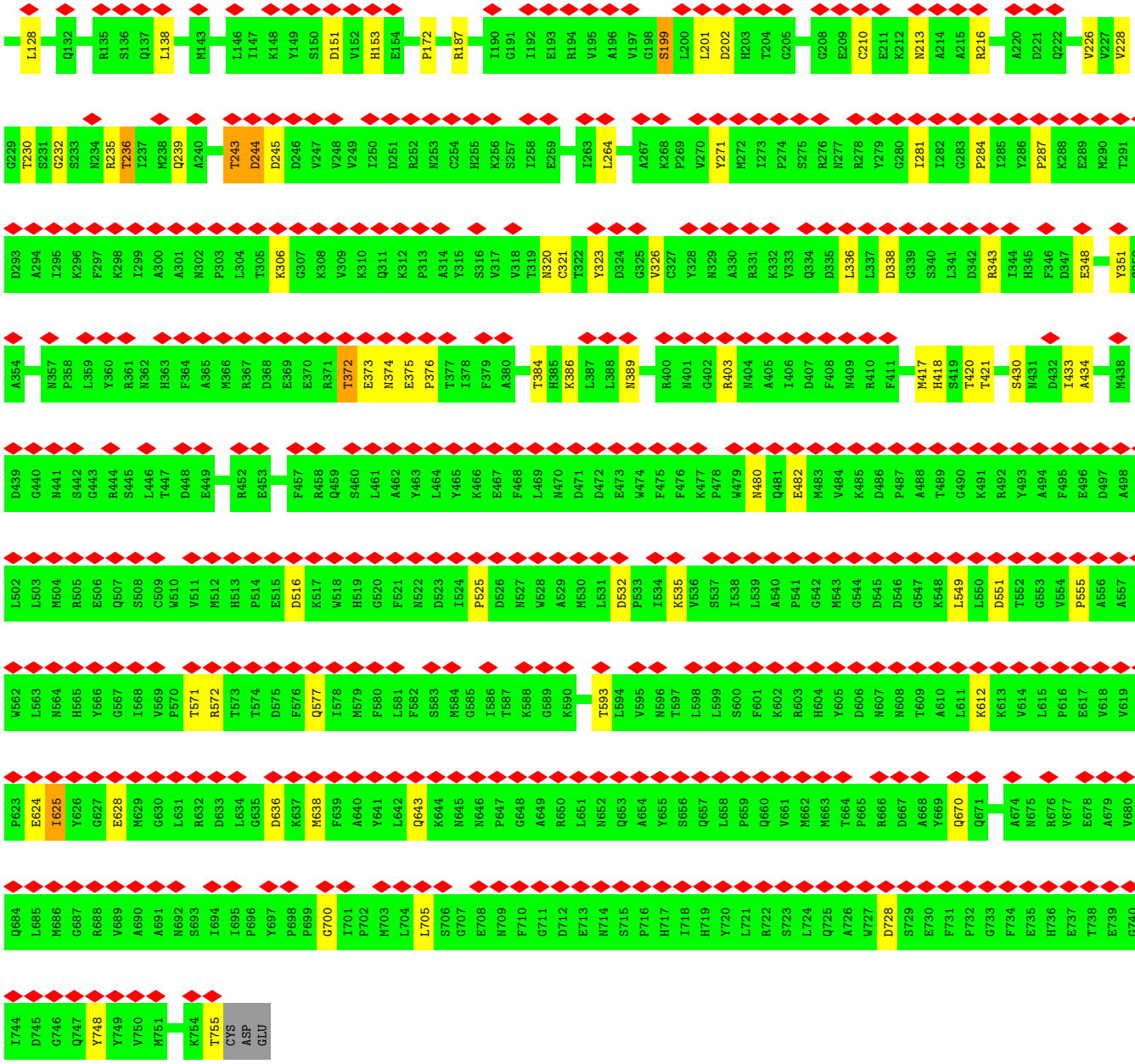
Chain S:



• Molecule 1: Biodegradative arginine decarboxylase

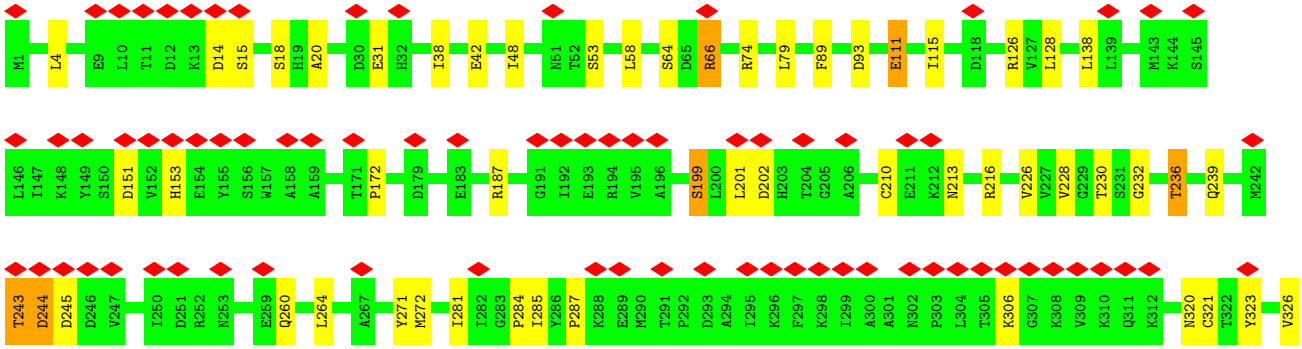
Chain O:

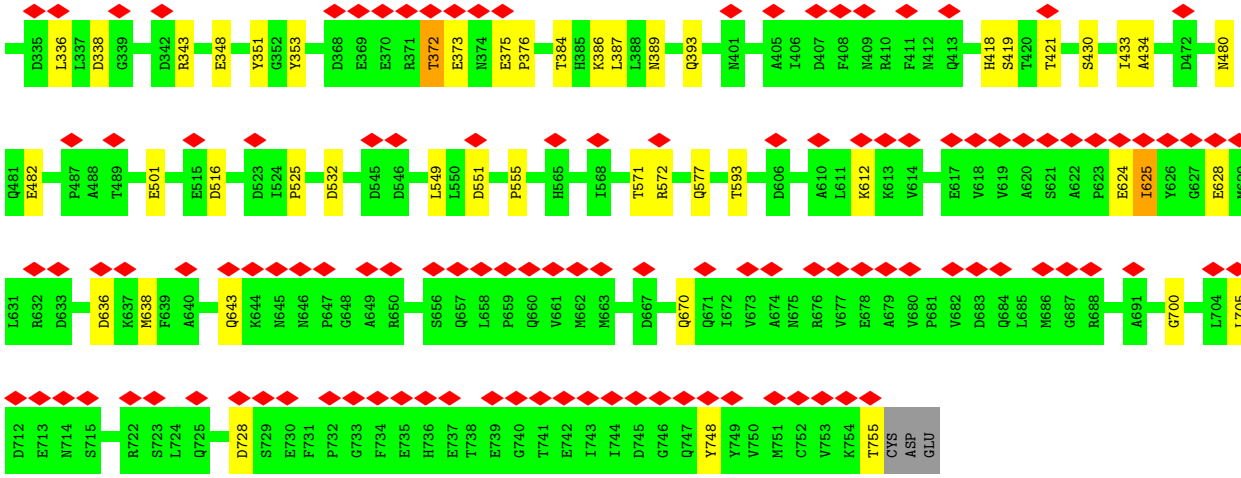




• Molecule 1: Biodegradative arginine decarboxylase

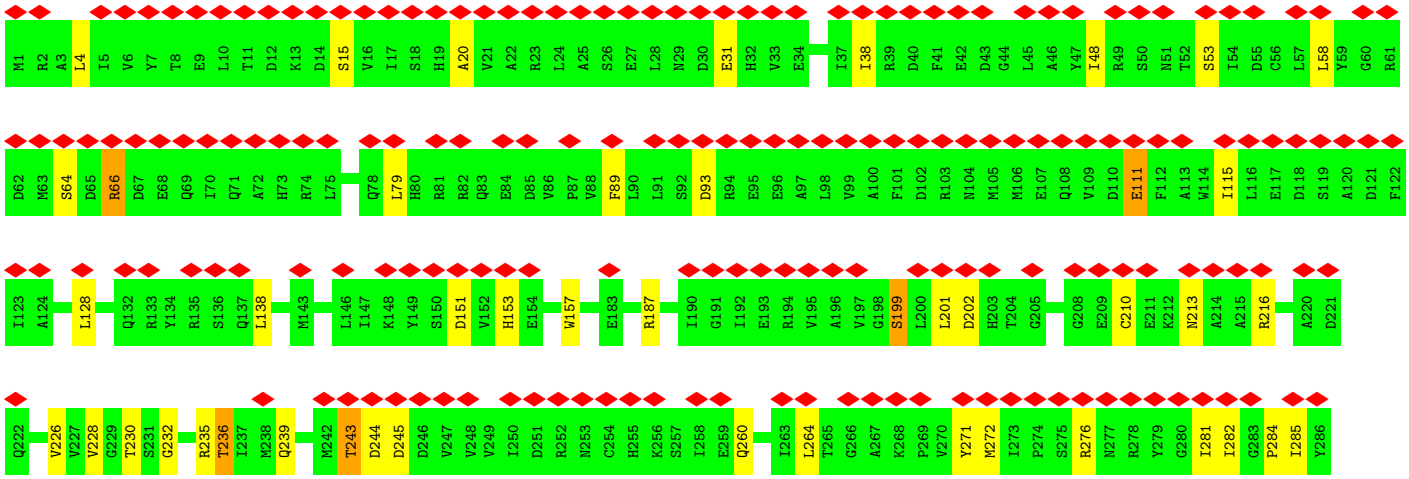
Chain T:

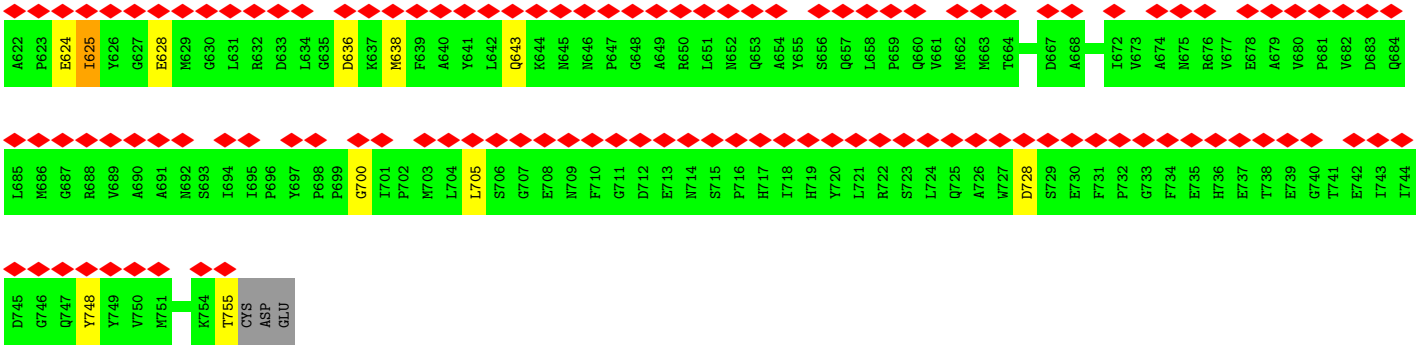




• Molecule 1: Biodegradative arginine decarboxylase

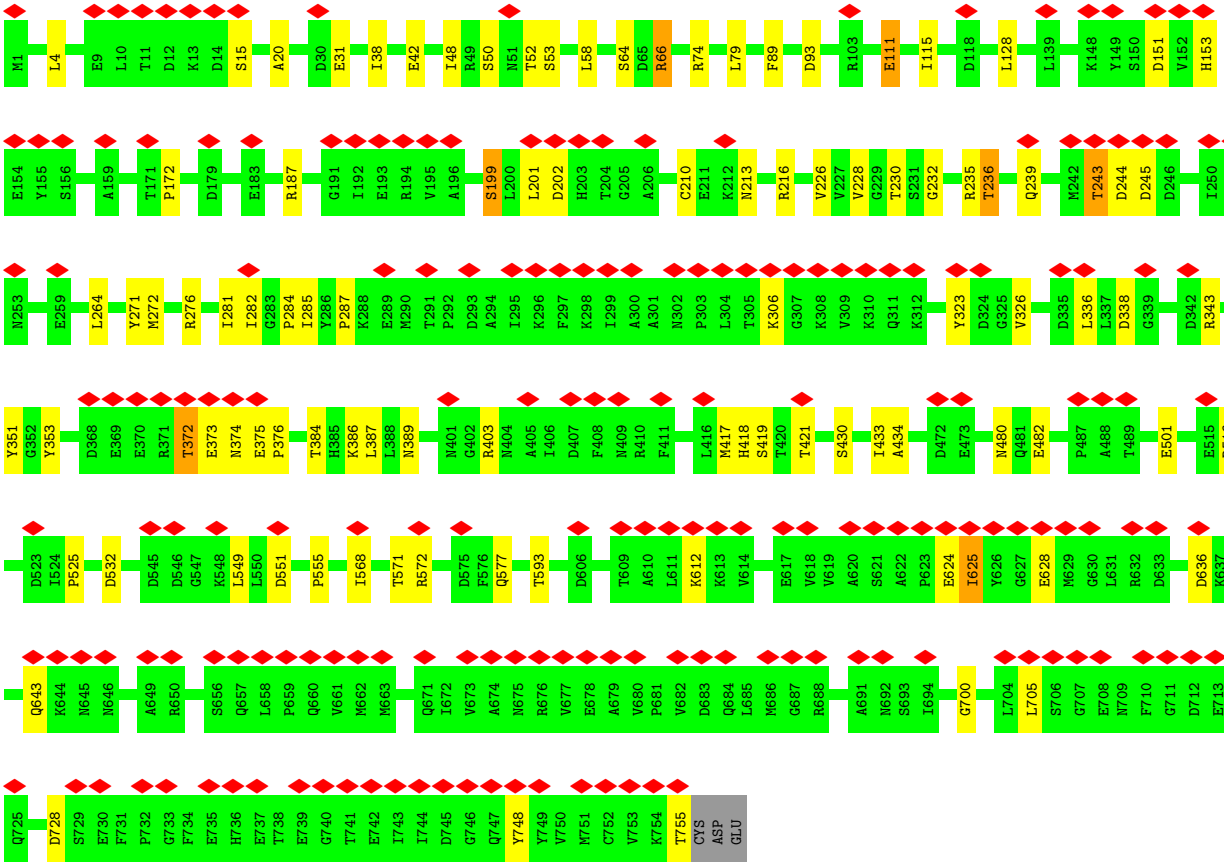
Chain C:





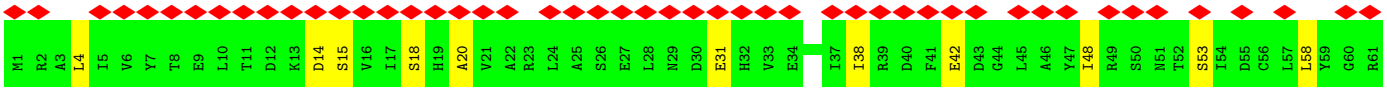
• Molecule 1: Biodegradative arginine decarboxylase

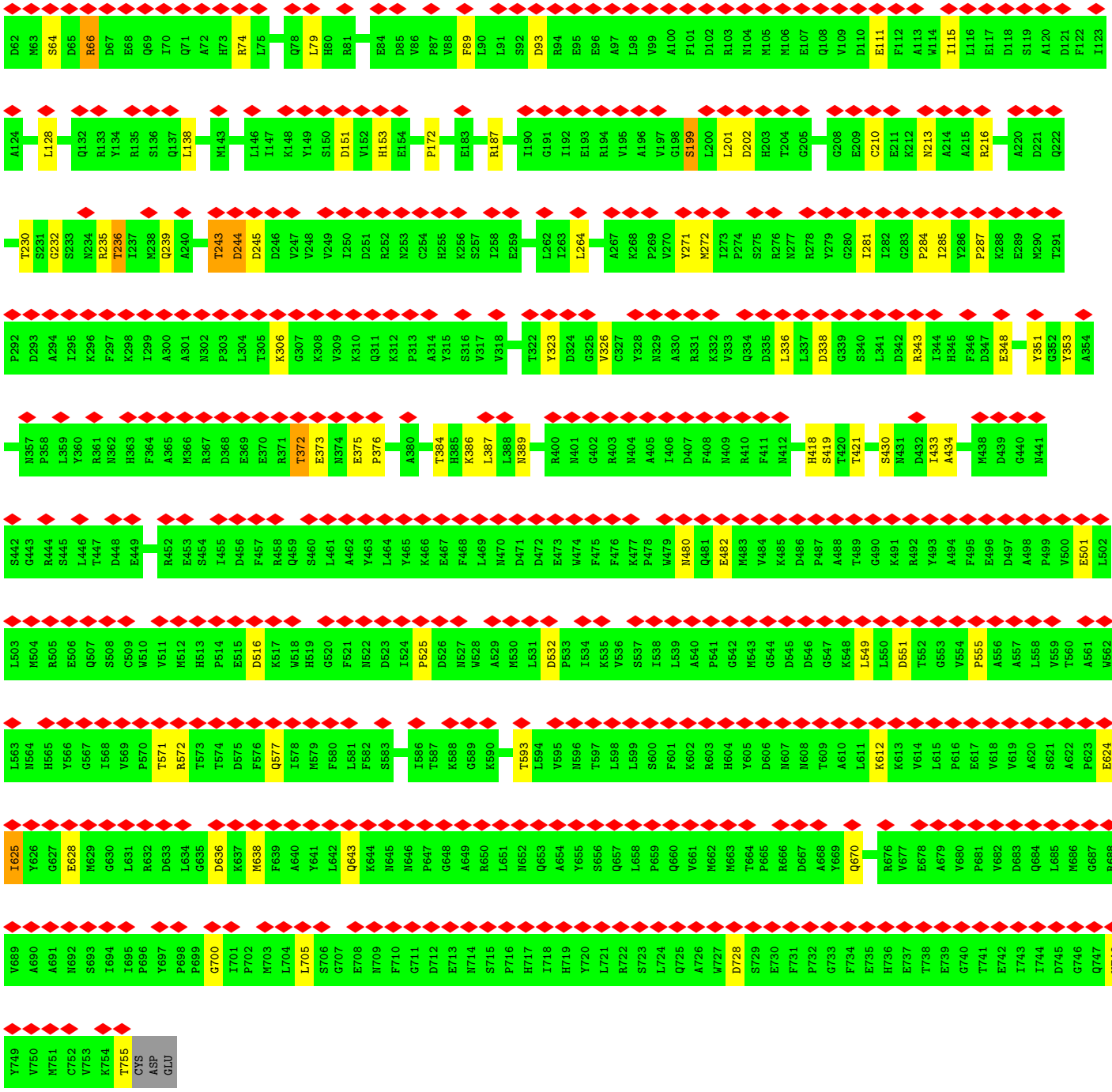
Chain G:



• Molecule 1: Biodegradative arginine decarboxylase

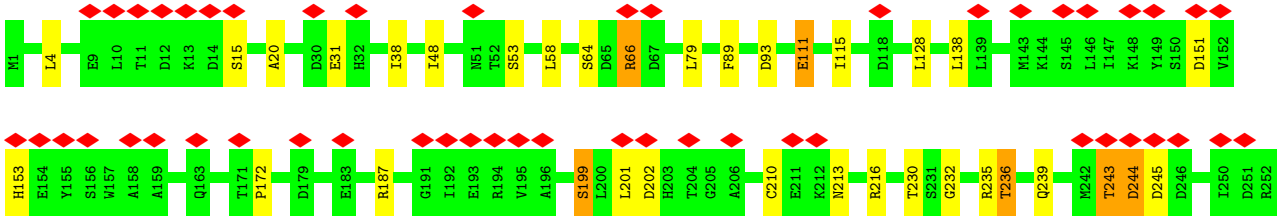
Chain D:

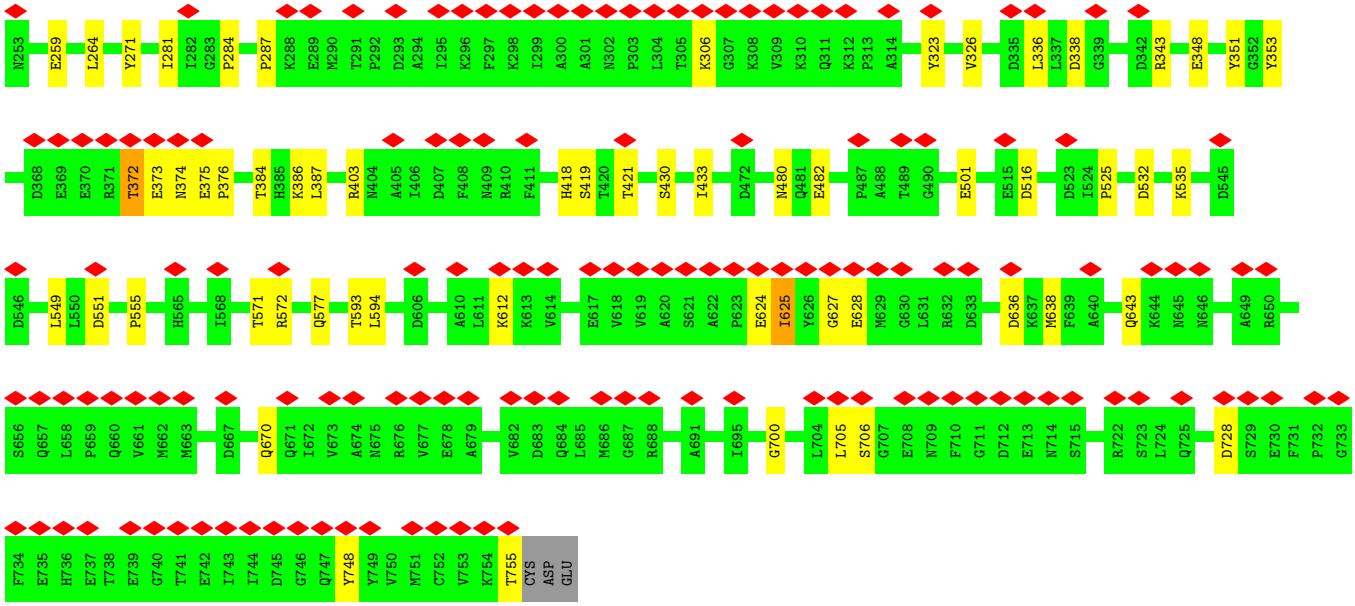




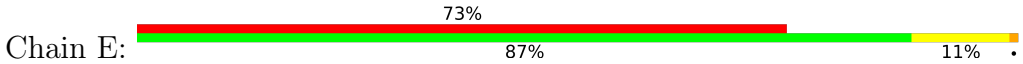
• Molecule 1: Biodegradative arginine decarboxylase

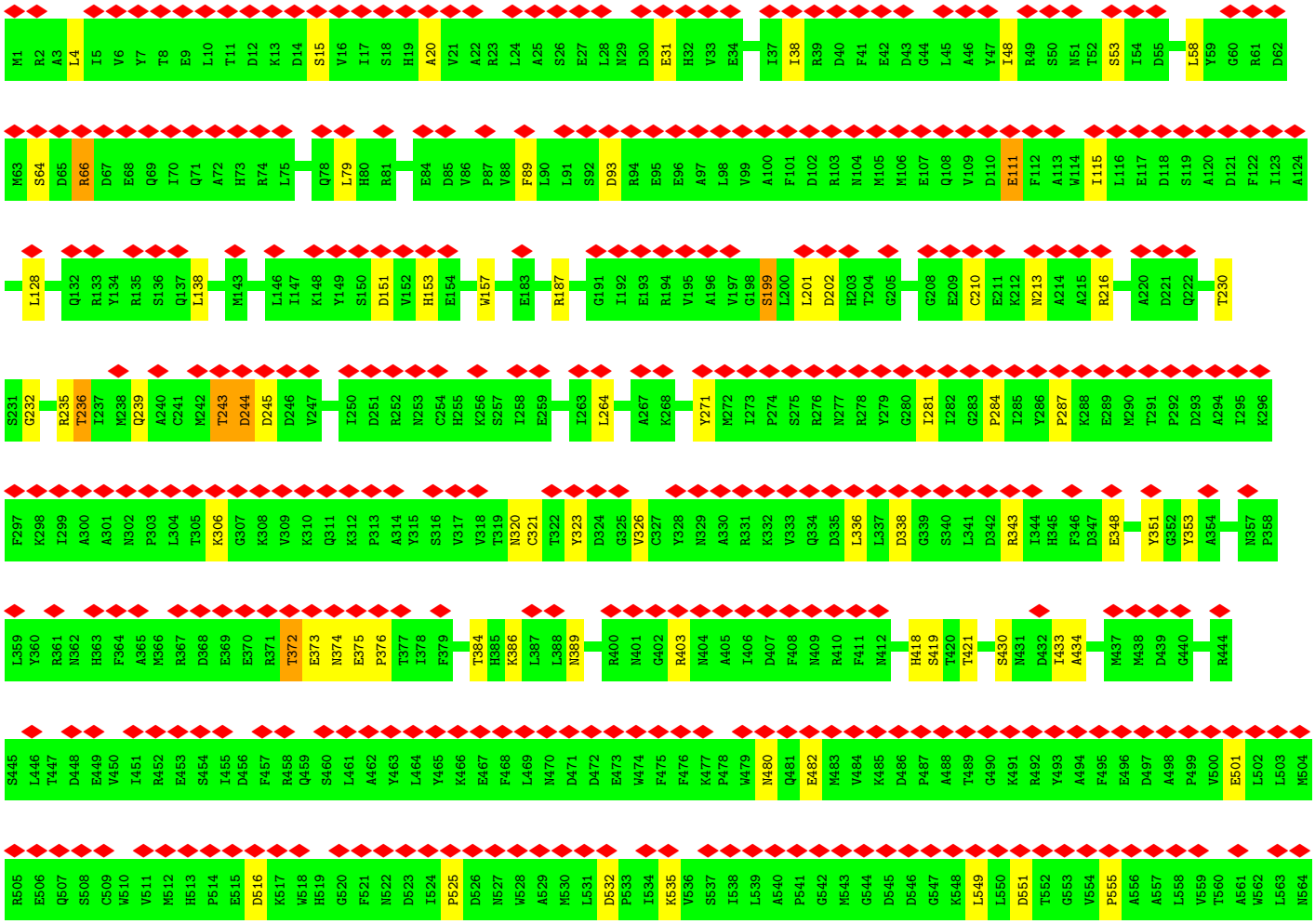
Chain H:

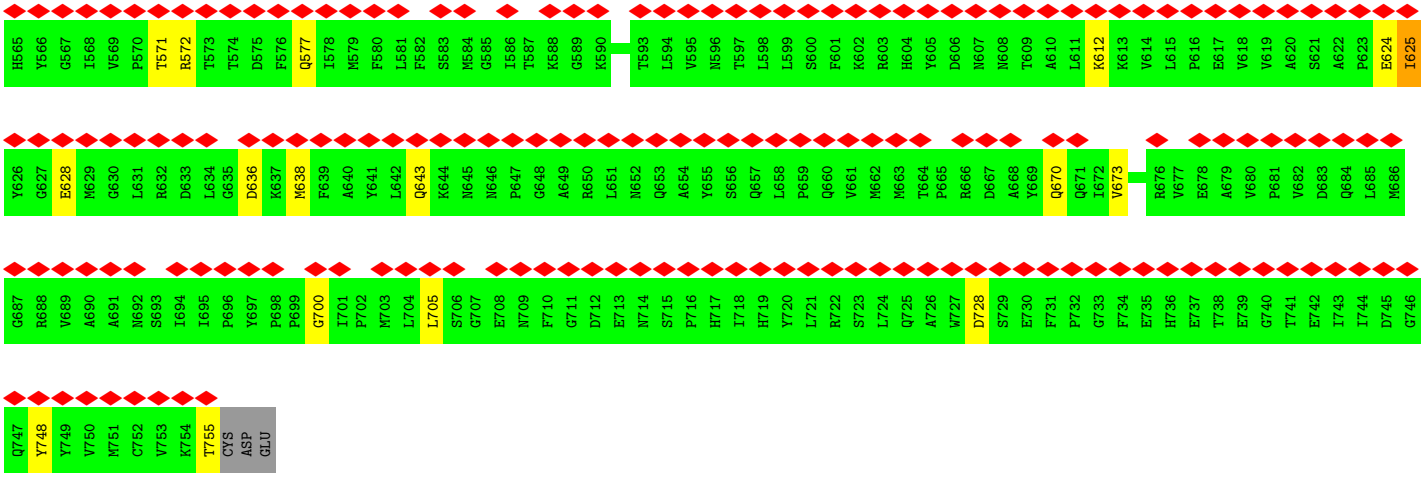




• Molecule 1: Biodegradative arginine decarboxylase

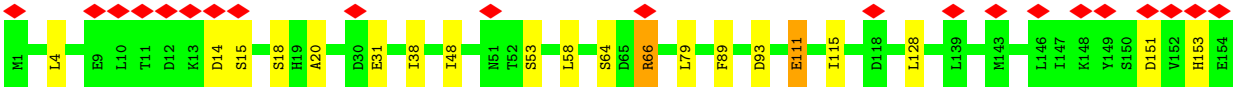






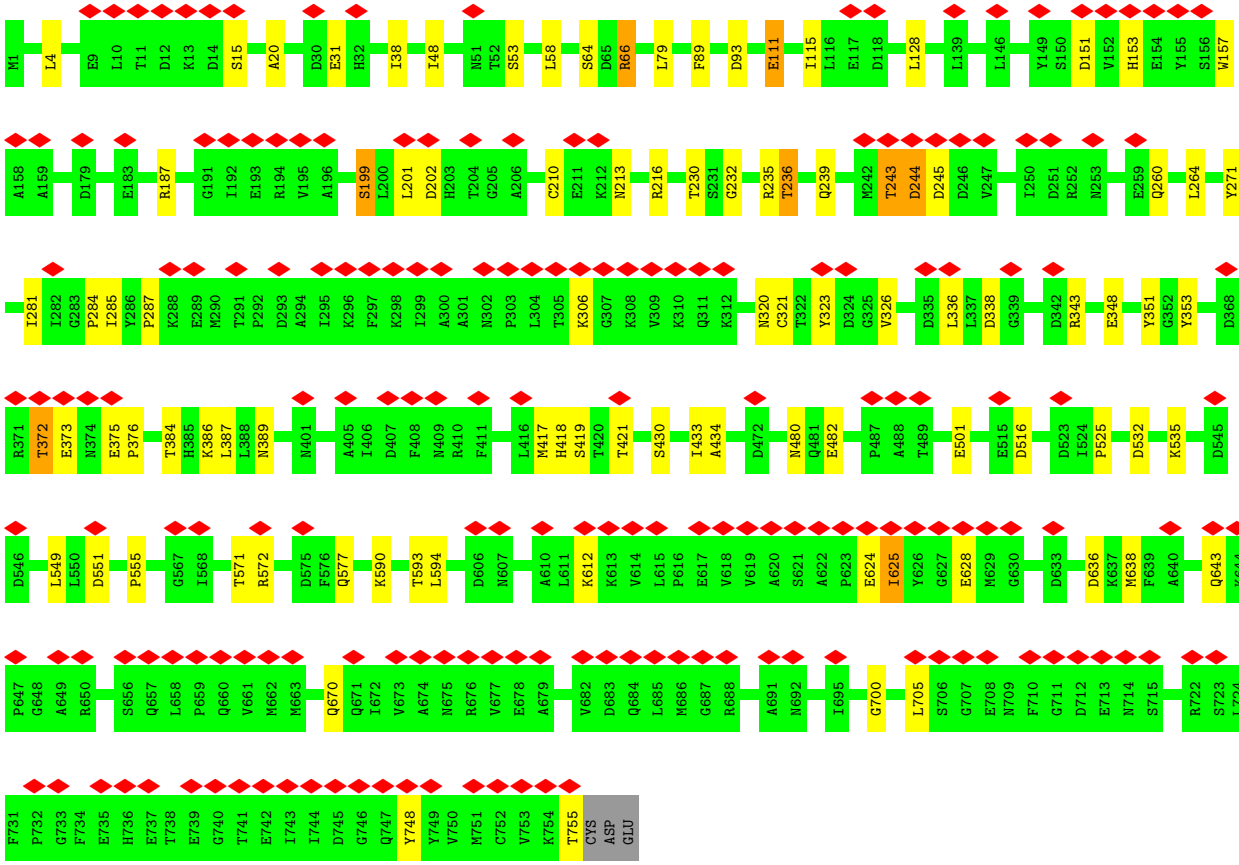
• Molecule 1: Biodegradative arginine decarboxylase

Chain I:



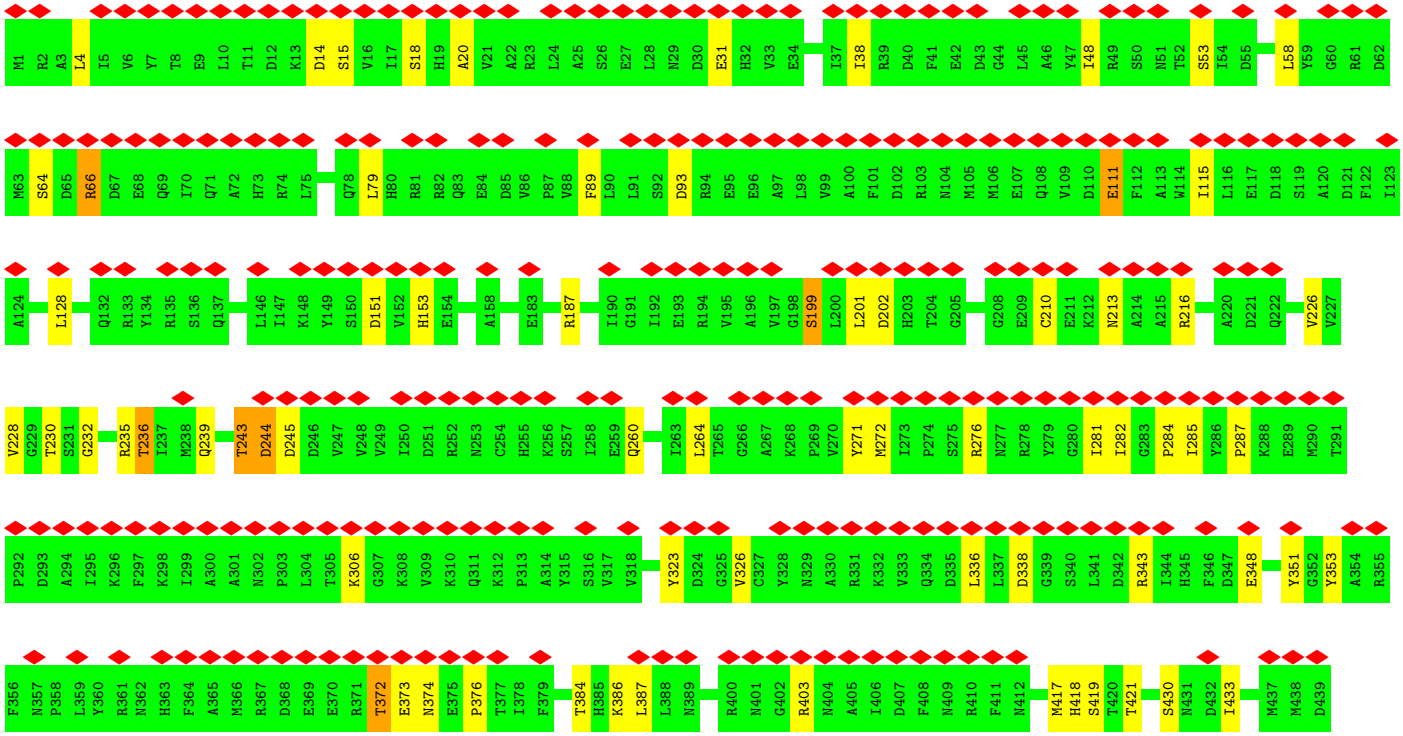
• Molecule 1: Biodegradative arginine decarboxylase

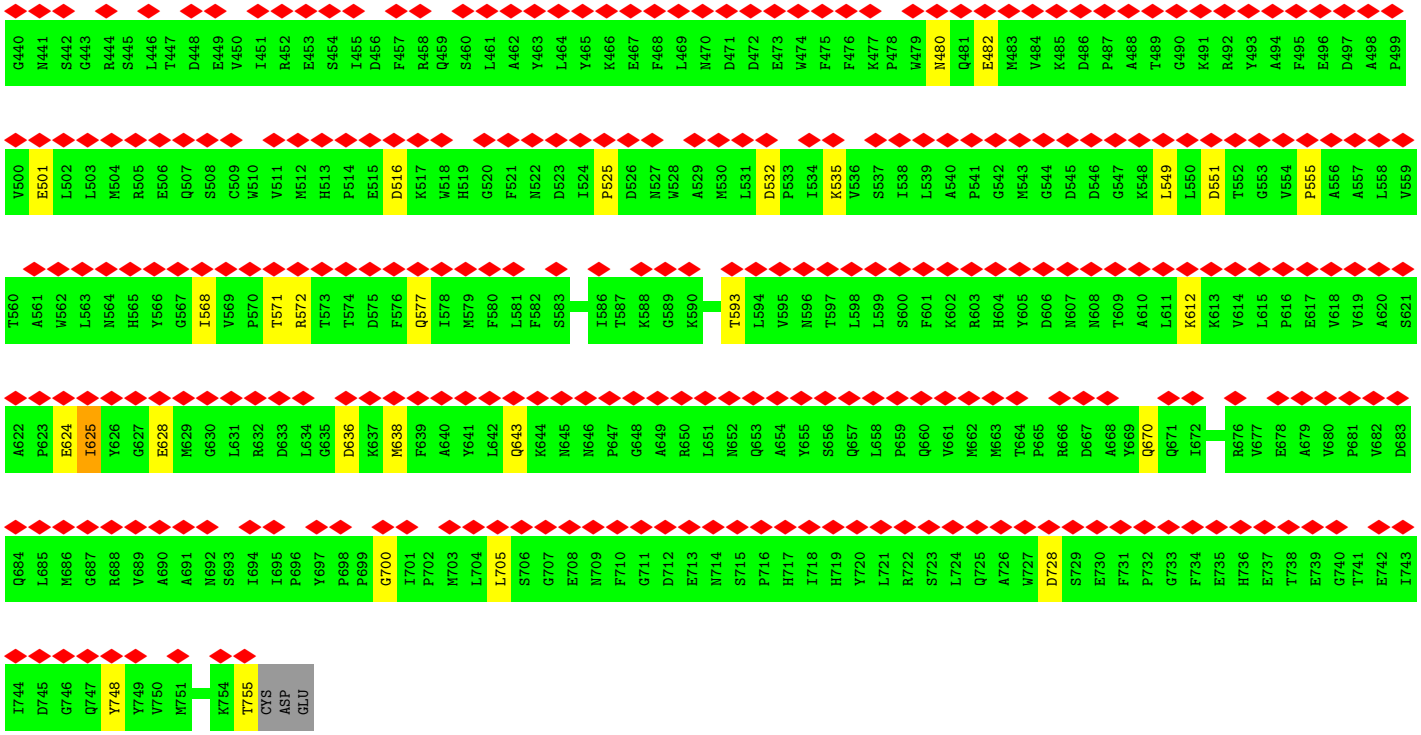
Chain F:



• Molecule 1: Biodegradative arginine decarboxylase

Chain J:




G440 N441 S442 G443 R444 S445 L446 T447 D448 E449 V450 I451 R452 E453 S454 I455 D456 F457 R458 Q459 S460 L461 A462 Y463 L464 Y465 K466 E467 F468 L469 N470 D471 D472 E473 W474 F475 F476 K477 P478 W479 N480 Q481 E482 M483 V484 K485 D486 P487 A488 T489 G490 K491 R492 Y493 A494 F495 E496 D497 A498 P499
V500 E501 L502 L503 M504 R505 E506 Q507 S508 C509 W510 V511 M512 H513 P514 E515 D516 K517 W518 H519 G520 F521 N522 D523 I524 P525 D526 N527 W528 A529 M530 L531 D532 P533 I534 K535 V536 S537 I538 L539 A540 P541 G542 M543 G544 D545 D546 G547 K548 L549 L550 D551 T552 G553 V554 P555 A556 A557 L558 V559
T560 A561 W562 L563 N564 H565 Y566 G567 I568 V569 P570 T571 R572 T573 T574 D575 F576 Q577 I578 M579 F580 L581 F582 S583 I586 T587 K588 G589 K590 T593 L594 V595 N596 T597 L598 L599 S600 F601 K602 R603 H604 Y605 D606 N607 N608 T609 A610 L611 K612 K613 V614 L615 P616 E617 V618 V619 A620 S621
A622 P623 E624 I625 Y626 G627 E628 M629 G630 L631 R632 D633 L634 G635 D636 K637 M638 F639 A640 Y641 L642 Q643 K644 N645 N646 P647 G648 A649 R650 L651 N652 Q653 A654 Y655 S656 Q657 L658 P659 Q660 V661 M662 M663 T664 P665 R666 D667 A668 Y669 Q670 Q671 I672 R676 V677 E678 A679 V680 P681 V682 D683
Q684 L685 M686 G687 R688 V689 A690 A691 N692 S693 I694 I695 P696 Y697 P698 P699 G700 I701 P702 M703 L704 L705 S706 G707 E708 N709 F710 G711 D712 E713 N714 S715 P716 H717 I718 H719 Y720 L721 R722 S723 L724 Q725 A726 W727 D728 S729 E730 F731 P732 G733 F734 E735 H736 E737 T738 E739 G740 T741 E742 I743
I744 D745 G746 Q747 Y748 Y749 V750 M751 K754 T755 CYS ASP GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D5	Depositor
Number of particles used	268579	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	215000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.809	Depositor
Minimum map value	-0.701	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	374.4, 374.4, 374.4	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.65, 0.65, 0.65	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.30	0/6148	0.44	0/8340
1	B	0.30	0/6148	0.44	0/8340
1	C	0.30	0/6148	0.44	0/8340
1	D	0.30	0/6148	0.44	0/8340
1	E	0.30	0/6148	0.44	0/8340
1	F	0.30	0/6148	0.44	0/8340
1	G	0.30	0/6148	0.44	0/8340
1	H	0.30	0/6148	0.44	0/8340
1	I	0.30	0/6148	0.44	0/8340
1	J	0.30	0/6148	0.44	0/8340
1	K	0.30	0/6148	0.44	0/8340
1	L	0.30	0/6148	0.44	0/8340
1	M	0.30	0/6148	0.44	0/8340
1	N	0.30	0/6148	0.44	0/8340
1	O	0.30	0/6148	0.44	0/8340
1	P	0.30	0/6148	0.44	0/8340
1	Q	0.30	0/6148	0.44	0/8340
1	R	0.30	0/6148	0.44	0/8340
1	S	0.30	0/6148	0.44	0/8340
1	T	0.30	0/6148	0.44	0/8340
All	All	0.30	0/122960	0.44	0/166800

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	A	6029	0	5849	54	0
1	B	6029	0	5849	60	0
1	C	6029	0	5849	53	0
1	D	6029	0	5849	51	0
1	E	6029	0	5849	50	0
1	F	6029	0	5849	56	0
1	G	6029	0	5849	55	0
1	H	6029	0	5849	52	0
1	I	6029	0	5849	53	0
1	J	6029	0	5849	54	0
1	K	6029	0	5849	56	0
1	L	6029	0	5849	56	0
1	M	6029	0	5849	51	0
1	N	6029	0	5849	55	0
1	O	6029	0	5849	53	0
1	P	6029	0	5849	57	0
1	Q	6029	0	5849	50	0
1	R	6029	0	5849	48	0
1	S	6029	0	5849	57	0
1	T	6029	0	5849	56	0
All	All	120580	0	116980	980	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 4.

The worst 5 of 980 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:593:THR:OG1	1:Q:111:GLU:OE1	1.86	0.92
1:O:244:ASP:OD2	1:T:670:GLN:NE2	2.06	0.88
1:B:111:GLU:OE1	1:N:593:THR:OG1	1.92	0.88
1:T:111:GLU:OE1	1:F:593:THR:OG1	1.89	0.88
1:G:593:THR:OG1	1:H:111:GLU:OE1	1.95	0.85

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	752/758 (99%)	737 (98%)	15 (2%)	0	100	100
1	B	752/758 (99%)	737 (98%)	15 (2%)	0	100	100
1	C	752/758 (99%)	737 (98%)	15 (2%)	0	100	100
1	D	752/758 (99%)	737 (98%)	15 (2%)	0	100	100
1	E	752/758 (99%)	737 (98%)	15 (2%)	0	100	100
1	F	752/758 (99%)	737 (98%)	15 (2%)	0	100	100
1	G	752/758 (99%)	737 (98%)	15 (2%)	0	100	100
1	H	752/758 (99%)	737 (98%)	15 (2%)	0	100	100
1	I	752/758 (99%)	737 (98%)	15 (2%)	0	100	100
1	J	752/758 (99%)	737 (98%)	15 (2%)	0	100	100
1	K	752/758 (99%)	737 (98%)	15 (2%)	0	100	100
1	L	752/758 (99%)	737 (98%)	15 (2%)	0	100	100
1	M	752/758 (99%)	737 (98%)	15 (2%)	0	100	100
1	N	752/758 (99%)	737 (98%)	15 (2%)	0	100	100
1	O	752/758 (99%)	737 (98%)	15 (2%)	0	100	100
1	P	752/758 (99%)	737 (98%)	15 (2%)	0	100	100
1	Q	752/758 (99%)	737 (98%)	15 (2%)	0	100	100
1	R	752/758 (99%)	737 (98%)	15 (2%)	0	100	100
1	S	752/758 (99%)	737 (98%)	15 (2%)	0	100	100
1	T	752/758 (99%)	737 (98%)	15 (2%)	0	100	100
All	All	15040/15160 (99%)	14740 (98%)	300 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	645/648 (100%)	623 (97%)	22 (3%)	37	35
1	B	645/648 (100%)	623 (97%)	22 (3%)	37	35
1	C	645/648 (100%)	623 (97%)	22 (3%)	37	35
1	D	645/648 (100%)	623 (97%)	22 (3%)	37	35
1	E	645/648 (100%)	623 (97%)	22 (3%)	37	35
1	F	645/648 (100%)	623 (97%)	22 (3%)	37	35
1	G	645/648 (100%)	623 (97%)	22 (3%)	37	35
1	H	645/648 (100%)	623 (97%)	22 (3%)	37	35
1	I	645/648 (100%)	623 (97%)	22 (3%)	37	35
1	J	645/648 (100%)	623 (97%)	22 (3%)	37	35
1	K	645/648 (100%)	623 (97%)	22 (3%)	37	35
1	L	645/648 (100%)	623 (97%)	22 (3%)	37	35
1	M	645/648 (100%)	623 (97%)	22 (3%)	37	35
1	N	645/648 (100%)	623 (97%)	22 (3%)	37	35
1	O	645/648 (100%)	623 (97%)	22 (3%)	37	35
1	P	645/648 (100%)	623 (97%)	22 (3%)	37	35
1	Q	645/648 (100%)	623 (97%)	22 (3%)	37	35
1	R	645/648 (100%)	623 (97%)	22 (3%)	37	35
1	S	645/648 (100%)	623 (97%)	22 (3%)	37	35
1	T	645/648 (100%)	623 (97%)	22 (3%)	37	35
All	All	12900/12960 (100%)	12460 (97%)	440 (3%)	40	35

5 of 440 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	306	LYS
1	G	15	SER
1	J	636	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	93	ASP
1	O	571	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	401	ASN
1	F	389	ASN
1	H	389	ASN
1	E	401	ASN
1	J	389	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	LLP	H	386	1	23,24,25	0.70	0	25,32,34	0.73	0
1	LLP	G	386	1	23,24,25	0.70	0	25,32,34	0.72	0
1	LLP	K	386	1	23,24,25	0.70	0	25,32,34	0.72	0
1	LLP	D	386	1	23,24,25	0.70	0	25,32,34	0.73	0
1	LLP	L	386	1	23,24,25	0.71	0	25,32,34	0.73	0
1	LLP	F	386	1	23,24,25	0.71	0	25,32,34	0.73	0
1	LLP	S	386	1	23,24,25	0.71	0	25,32,34	0.73	0
1	LLP	C	386	1	23,24,25	0.70	0	25,32,34	0.73	0
1	LLP	M	386	1	23,24,25	0.70	0	25,32,34	0.73	0
1	LLP	O	386	1	23,24,25	0.70	0	25,32,34	0.73	0
1	LLP	E	386	1	23,24,25	0.70	0	25,32,34	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	LLP	P	386	1	23,24,25	0.70	0	25,32,34	0.73	0
1	LLP	T	386	1	23,24,25	0.70	0	25,32,34	0.73	0
1	LLP	Q	386	1	23,24,25	0.70	0	25,32,34	0.73	0
1	LLP	B	386	1	23,24,25	0.70	0	25,32,34	0.73	0
1	LLP	J	386	1	23,24,25	0.70	0	25,32,34	0.72	0
1	LLP	N	386	1	23,24,25	0.71	0	25,32,34	0.72	0
1	LLP	I	386	1	23,24,25	0.71	0	25,32,34	0.72	0
1	LLP	R	386	1	23,24,25	0.70	0	25,32,34	0.72	0
1	LLP	A	386	1	23,24,25	0.71	0	25,32,34	0.73	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	H	386	1	-	5/16/17/19	0/1/1/1
1	LLP	G	386	1	-	5/16/17/19	0/1/1/1
1	LLP	K	386	1	-	5/16/17/19	0/1/1/1
1	LLP	D	386	1	-	5/16/17/19	0/1/1/1
1	LLP	L	386	1	-	5/16/17/19	0/1/1/1
1	LLP	F	386	1	-	5/16/17/19	0/1/1/1
1	LLP	S	386	1	-	5/16/17/19	0/1/1/1
1	LLP	C	386	1	-	5/16/17/19	0/1/1/1
1	LLP	M	386	1	-	5/16/17/19	0/1/1/1
1	LLP	O	386	1	-	5/16/17/19	0/1/1/1
1	LLP	E	386	1	-	5/16/17/19	0/1/1/1
1	LLP	P	386	1	-	5/16/17/19	0/1/1/1
1	LLP	T	386	1	-	5/16/17/19	0/1/1/1
1	LLP	Q	386	1	-	5/16/17/19	0/1/1/1
1	LLP	B	386	1	-	5/16/17/19	0/1/1/1
1	LLP	J	386	1	-	5/16/17/19	0/1/1/1
1	LLP	N	386	1	-	5/16/17/19	0/1/1/1
1	LLP	I	386	1	-	5/16/17/19	0/1/1/1
1	LLP	R	386	1	-	5/16/17/19	0/1/1/1
1	LLP	A	386	1	-	5/16/17/19	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 100 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	386	LLP	C4-C4'-NZ-CE
1	A	386	LLP	C-CA-CB-CG
1	A	386	LLP	CG-CD-CE-NZ
1	B	386	LLP	C4-C4'-NZ-CE
1	B	386	LLP	C-CA-CB-CG

There are no ring outliers.

20 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	386	LLP	1	0
1	G	386	LLP	1	0
1	K	386	LLP	1	0
1	D	386	LLP	1	0
1	L	386	LLP	1	0
1	F	386	LLP	1	0
1	S	386	LLP	1	0
1	C	386	LLP	1	0
1	M	386	LLP	1	0
1	O	386	LLP	1	0
1	E	386	LLP	1	0
1	P	386	LLP	1	0
1	T	386	LLP	1	0
1	Q	386	LLP	1	0
1	B	386	LLP	1	0
1	J	386	LLP	1	0
1	N	386	LLP	1	0
1	I	386	LLP	1	0
1	R	386	LLP	1	0
1	A	386	LLP	1	0

5.5 Carbohydrates (i)

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

There are no chain breaks in this entry.

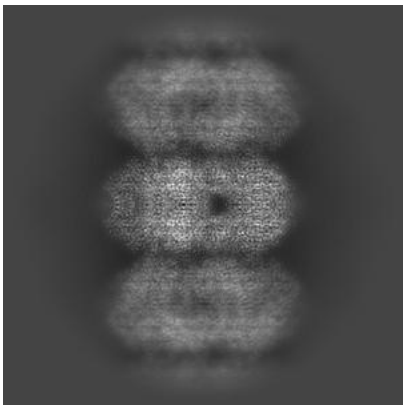
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13466. These allow visual inspection of the internal detail of the map and identification of artifacts.

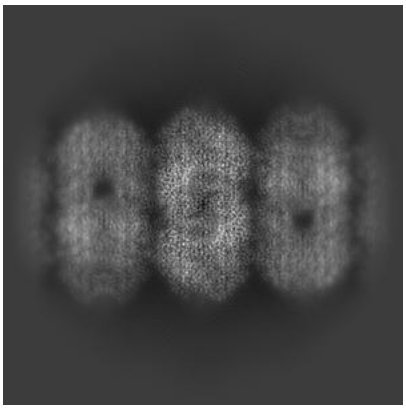
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

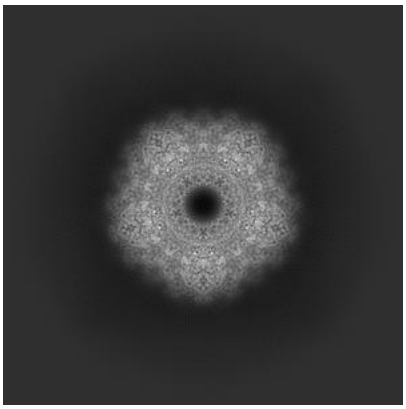
6.1.1 Primary map



X

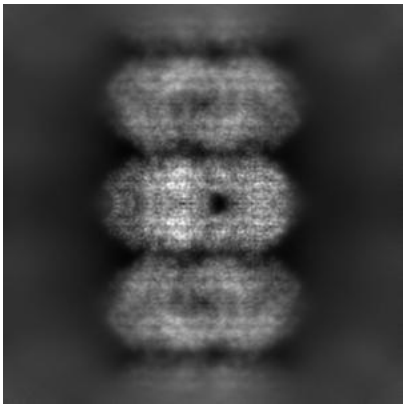


Y

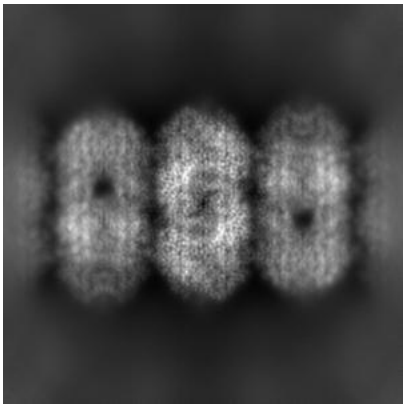


Z

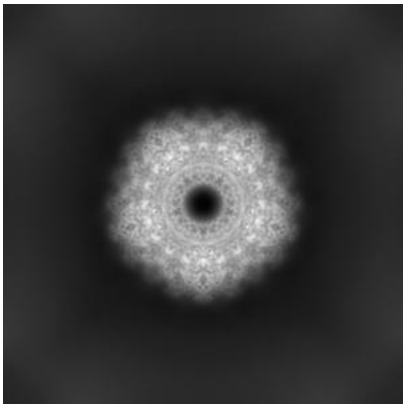
6.1.2 Raw map



X



Y

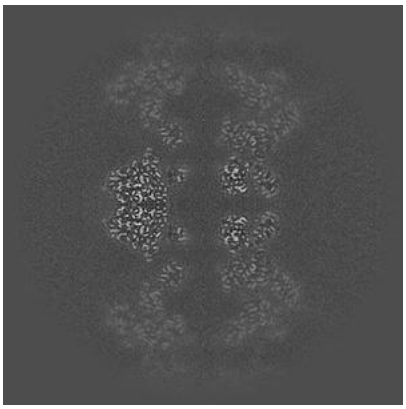


Z

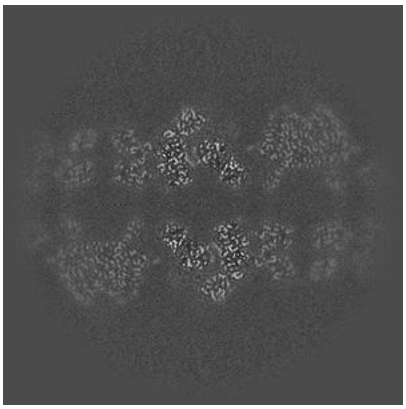
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

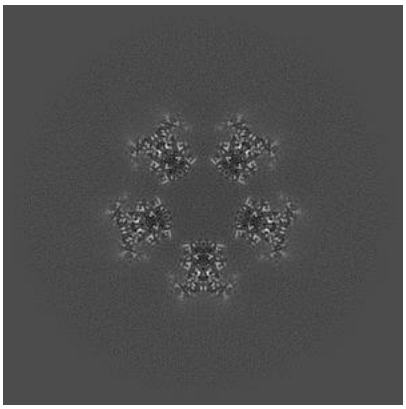
6.2.1 Primary map



X Index: 288

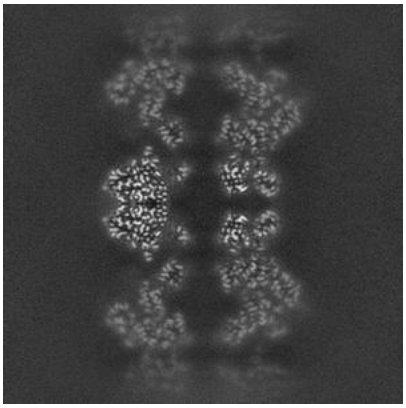


Y Index: 288

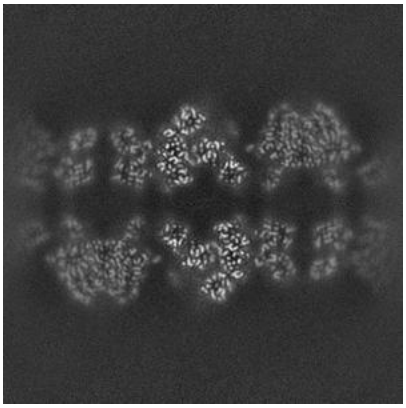


Z Index: 288

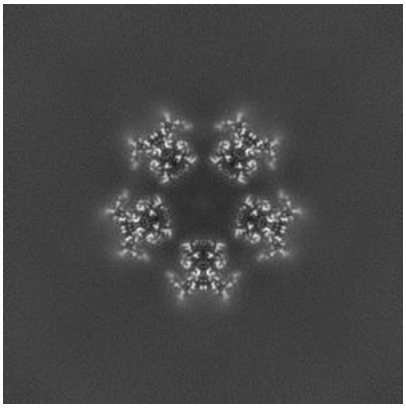
6.2.2 Raw map



X Index: 288



Y Index: 288

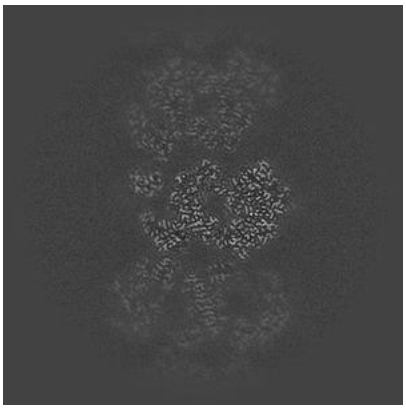


Z Index: 288

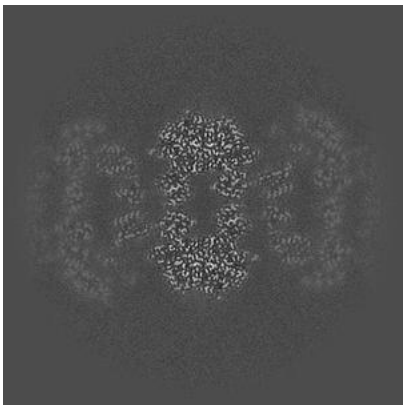
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

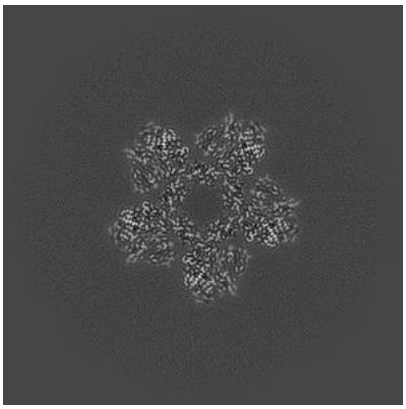
6.3.1 Primary map



X Index: 231

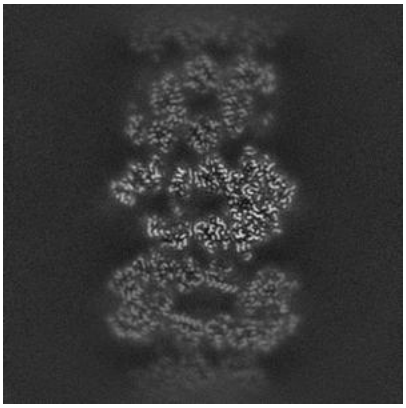


Y Index: 260

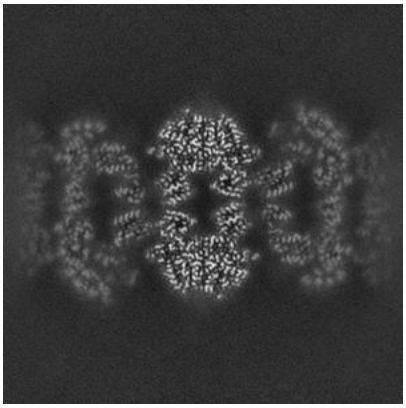


Z Index: 259

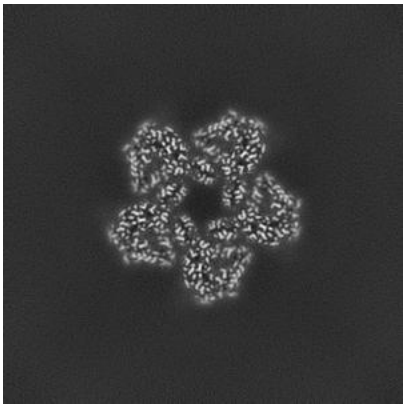
6.3.2 Raw map



X Index: 243



Y Index: 260

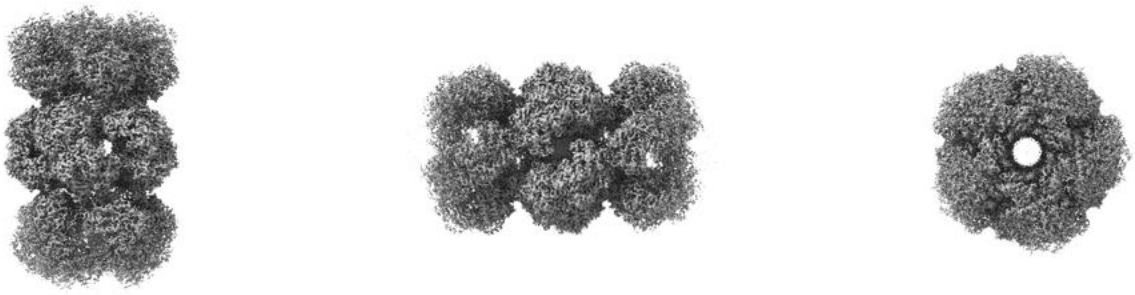


Z Index: 265

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

6.4 Orthogonal surface views (i)

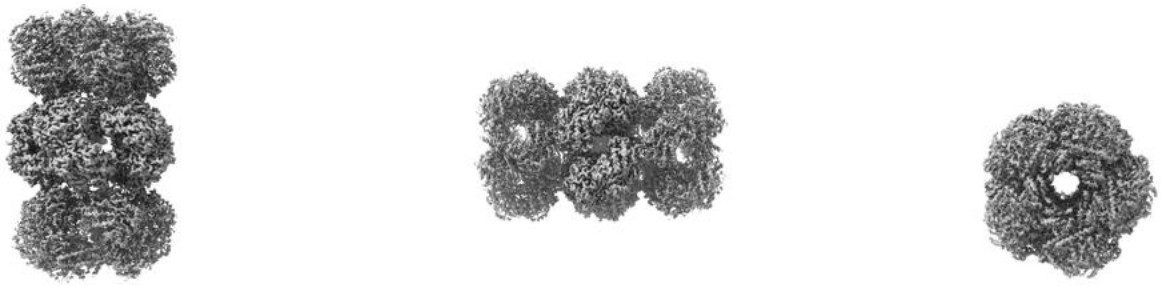
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

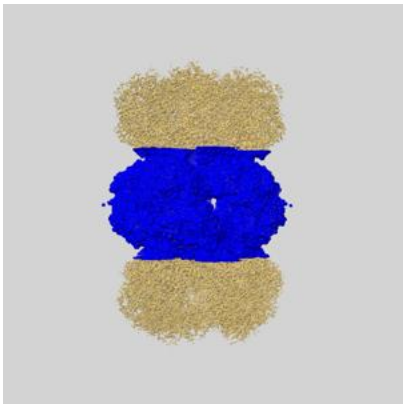
6.5 Mask visualisation (i)

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

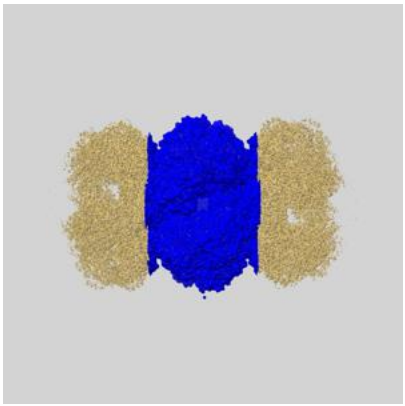
A mask typically either:

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

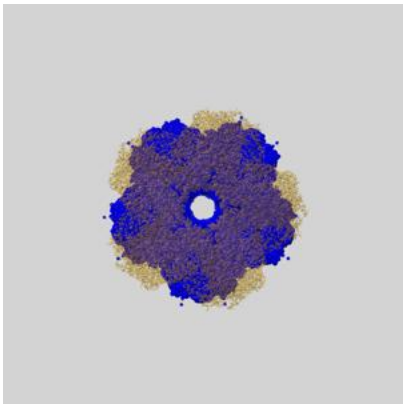
6.5.1 emd_13466_msk_1.map (i)



X



Y

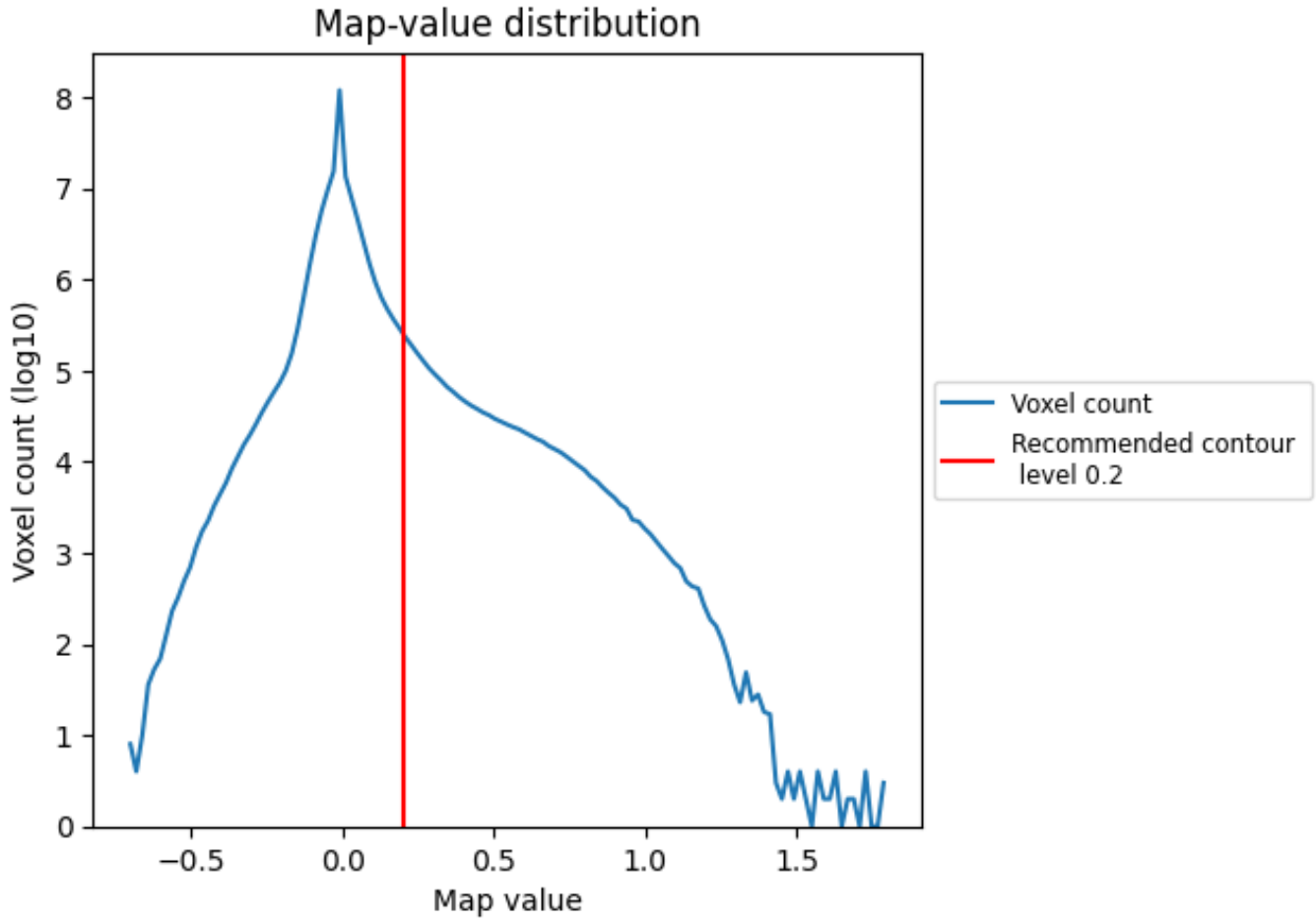


Z

7 Map analysis

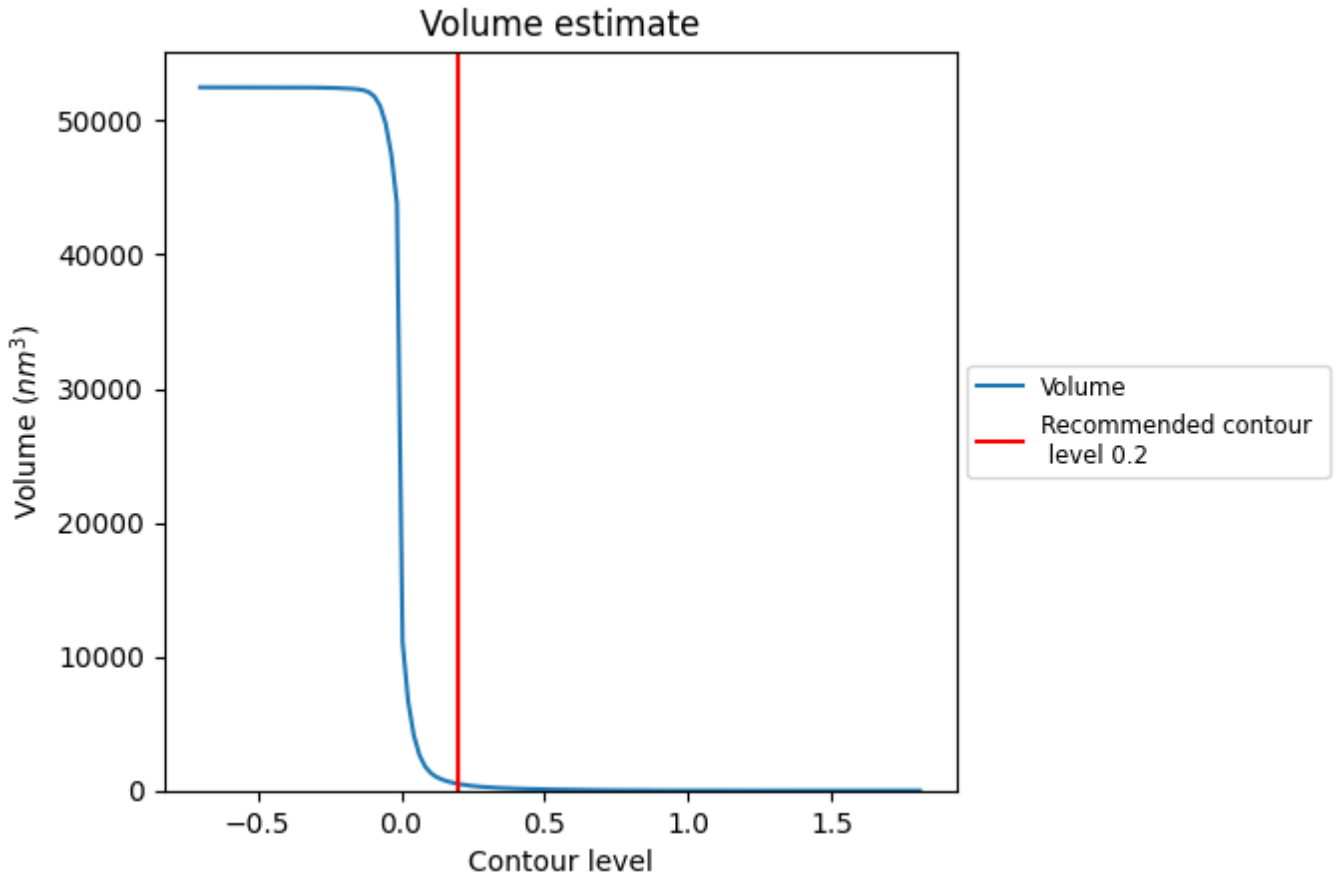
This section contains the results of statistical analysis of the map.

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.

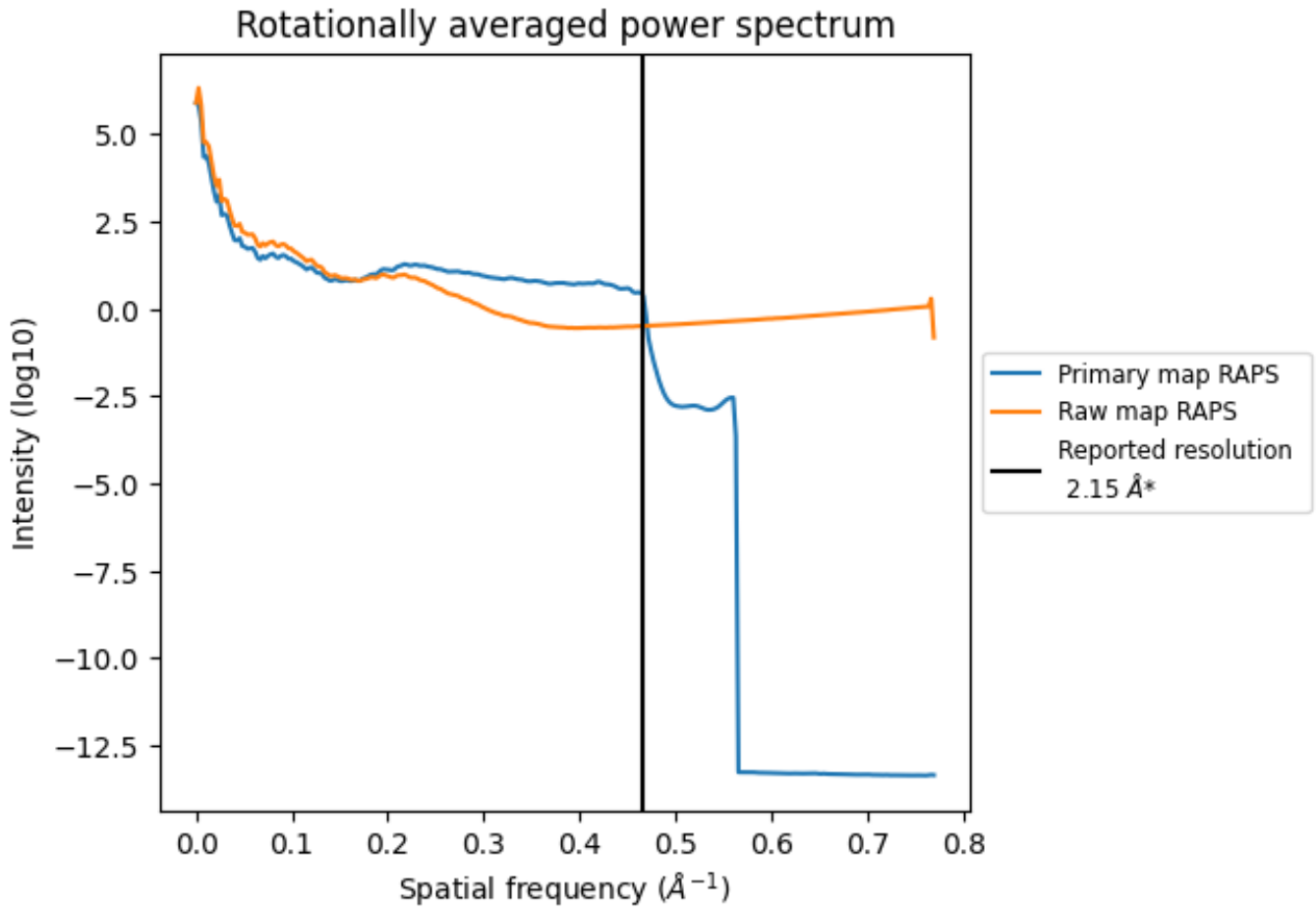
7.2 Volume estimate (i)



The volume at the recommended contour level is 494 nm^3; this corresponds to an approximate mass of 446 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)

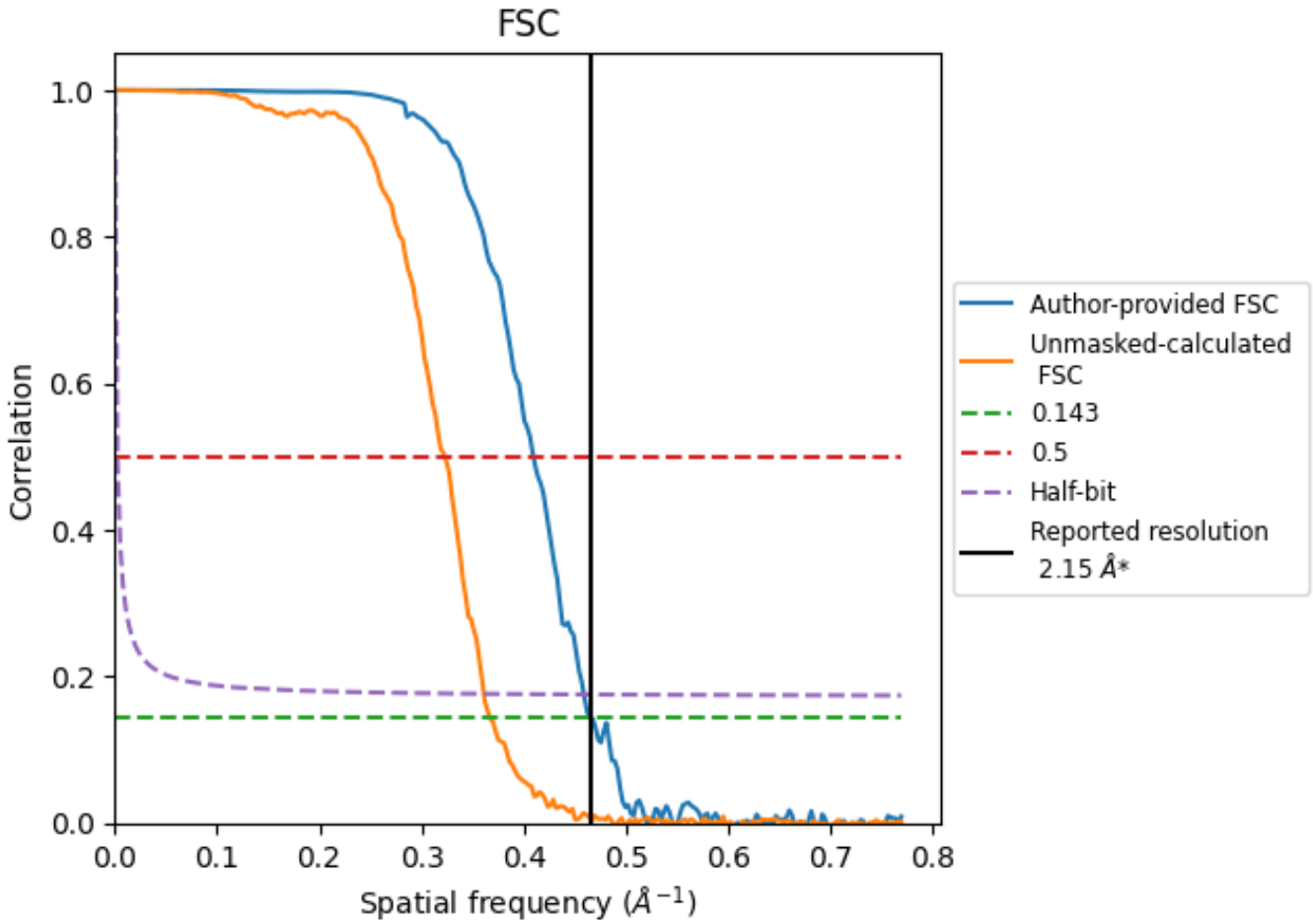


*Reported resolution corresponds to spatial frequency of 0.465 $Å^{-1}$

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 0.465 $Å^{-1}$

8.2 Resolution estimates (i)

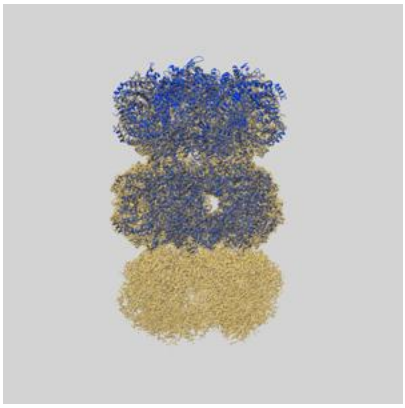
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.15	-	-
Author-provided FSC curve	2.15	2.44	2.18
Unmasked-calculated*	2.72	3.10	2.77

*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 2.72 differs from the reported value 2.15 by more than 10 %

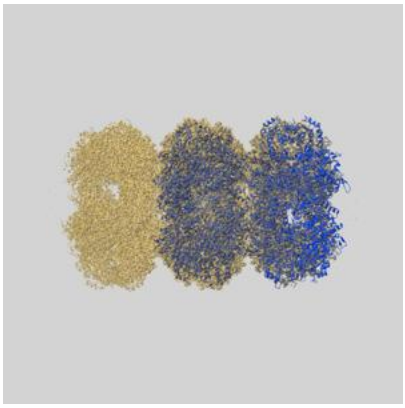
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13466 and PDB model 7PK6. Per-residue inclusion information can be found in section 3 on page 6.

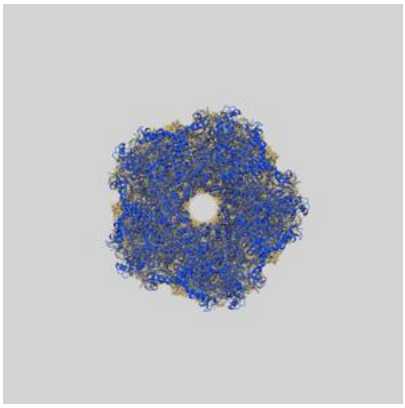
9.1 Map-model overlay



X



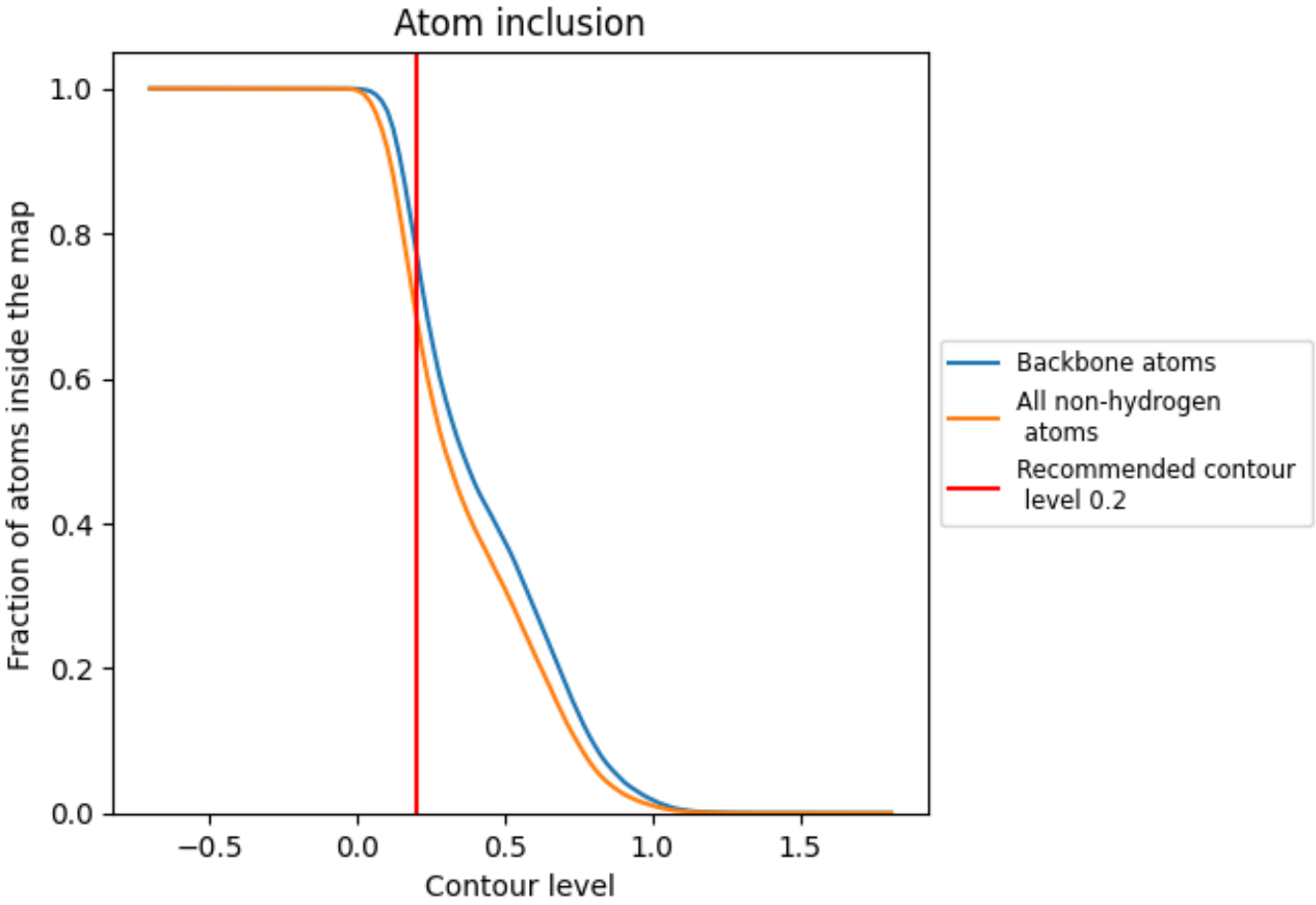
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.