wwPDB EM Validation Summary Report

Mar 11, 2024 – 07:30 AM EDT

PDB ID	:	6PVQ
EMDB ID	:	EMD-20497
Title	:	Cryo-EM structure of mouse TRPV3-Y564A in intermediate state at 37 degrees Celsius
Authors	:	Singh, A.K.; McGoldrick, L.L.; Sobolevsky, A.I.
Deposited on	:	2019-07-21
Resolution	:	4.75 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

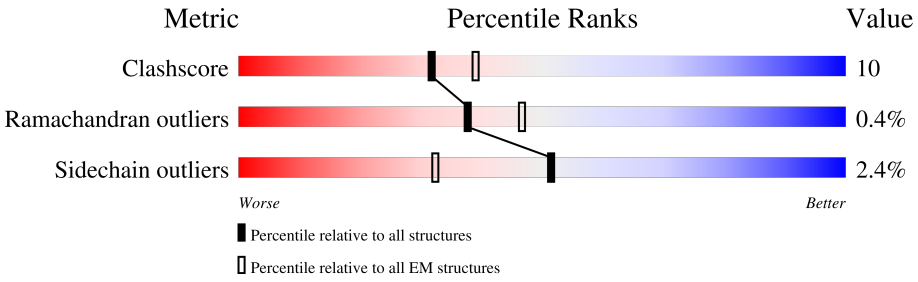
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.75 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	808	16% 51% 17% · 30%
1	B	808	15% 47% 16% · 36%
1	C	808	16% 51% 18% 30%
1	D	808	15% 46% 17% · 36%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 17640 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 Transient receptor potential cation channel subfamily V member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	562	Total	C	N	O	S	0	0
			4581	2938	781	837	25		
1	B	518	Total	C	N	O	S	0	0
			4239	2736	717	761	25		
1	C	562	Total	C	N	O	S	0	0
			4581	2938	781	837	25		
1	D	518	Total	C	N	O	S	0	0
			4239	2736	717	761	25		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	564	ALA	TYR	engineered mutation	UNP Q8K424
A	792	LEU	-	expression tag	UNP Q8K424
A	793	VAL	-	expression tag	UNP Q8K424
A	794	PRO	-	expression tag	UNP Q8K424
A	795	ARG	-	expression tag	UNP Q8K424
A	796	GLY	-	expression tag	UNP Q8K424
A	797	SER	-	expression tag	UNP Q8K424
A	798	ALA	-	expression tag	UNP Q8K424
A	799	ALA	-	expression tag	UNP Q8K424
A	800	ALA	-	expression tag	UNP Q8K424
A	801	TRP	-	expression tag	UNP Q8K424
A	802	SER	-	expression tag	UNP Q8K424
A	803	HIS	-	expression tag	UNP Q8K424
A	804	PRO	-	expression tag	UNP Q8K424
A	805	GLN	-	expression tag	UNP Q8K424
A	806	PHE	-	expression tag	UNP Q8K424
A	807	GLU	-	expression tag	UNP Q8K424
A	808	LYS	-	expression tag	UNP Q8K424
B	564	ALA	TYR	engineered mutation	UNP Q8K424
B	792	LEU	-	expression tag	UNP Q8K424
B	793	VAL	-	expression tag	UNP Q8K424

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Chain	Residue	Modelled	Actual	Comment	Reference
B	794	PRO	-	expression tag	UNP Q8K424
B	795	ARG	-	expression tag	UNP Q8K424
B	796	GLY	-	expression tag	UNP Q8K424
B	797	SER	-	expression tag	UNP Q8K424
B	798	ALA	-	expression tag	UNP Q8K424
B	799	ALA	-	expression tag	UNP Q8K424
B	800	ALA	-	expression tag	UNP Q8K424
B	801	TRP	-	expression tag	UNP Q8K424
B	802	SER	-	expression tag	UNP Q8K424
B	803	HIS	-	expression tag	UNP Q8K424
B	804	PRO	-	expression tag	UNP Q8K424
B	805	GLN	-	expression tag	UNP Q8K424
B	806	PHE	-	expression tag	UNP Q8K424
B	807	GLU	-	expression tag	UNP Q8K424
B	808	LYS	-	expression tag	UNP Q8K424
C	564	ALA	TYR	engineered mutation	UNP Q8K424
C	792	LEU	-	expression tag	UNP Q8K424
C	793	VAL	-	expression tag	UNP Q8K424
C	794	PRO	-	expression tag	UNP Q8K424
C	795	ARG	-	expression tag	UNP Q8K424
C	796	GLY	-	expression tag	UNP Q8K424
C	797	SER	-	expression tag	UNP Q8K424
C	798	ALA	-	expression tag	UNP Q8K424
C	799	ALA	-	expression tag	UNP Q8K424
C	800	ALA	-	expression tag	UNP Q8K424
C	801	TRP	-	expression tag	UNP Q8K424
C	802	SER	-	expression tag	UNP Q8K424
C	803	HIS	-	expression tag	UNP Q8K424
C	804	PRO	-	expression tag	UNP Q8K424
C	805	GLN	-	expression tag	UNP Q8K424
C	806	PHE	-	expression tag	UNP Q8K424
C	807	GLU	-	expression tag	UNP Q8K424
C	808	LYS	-	expression tag	UNP Q8K424
D	564	ALA	TYR	engineered mutation	UNP Q8K424
D	792	LEU	-	expression tag	UNP Q8K424
D	793	VAL	-	expression tag	UNP Q8K424
D	794	PRO	-	expression tag	UNP Q8K424
D	795	ARG	-	expression tag	UNP Q8K424
D	796	GLY	-	expression tag	UNP Q8K424
D	797	SER	-	expression tag	UNP Q8K424
D	798	ALA	-	expression tag	UNP Q8K424
D	799	ALA	-	expression tag	UNP Q8K424

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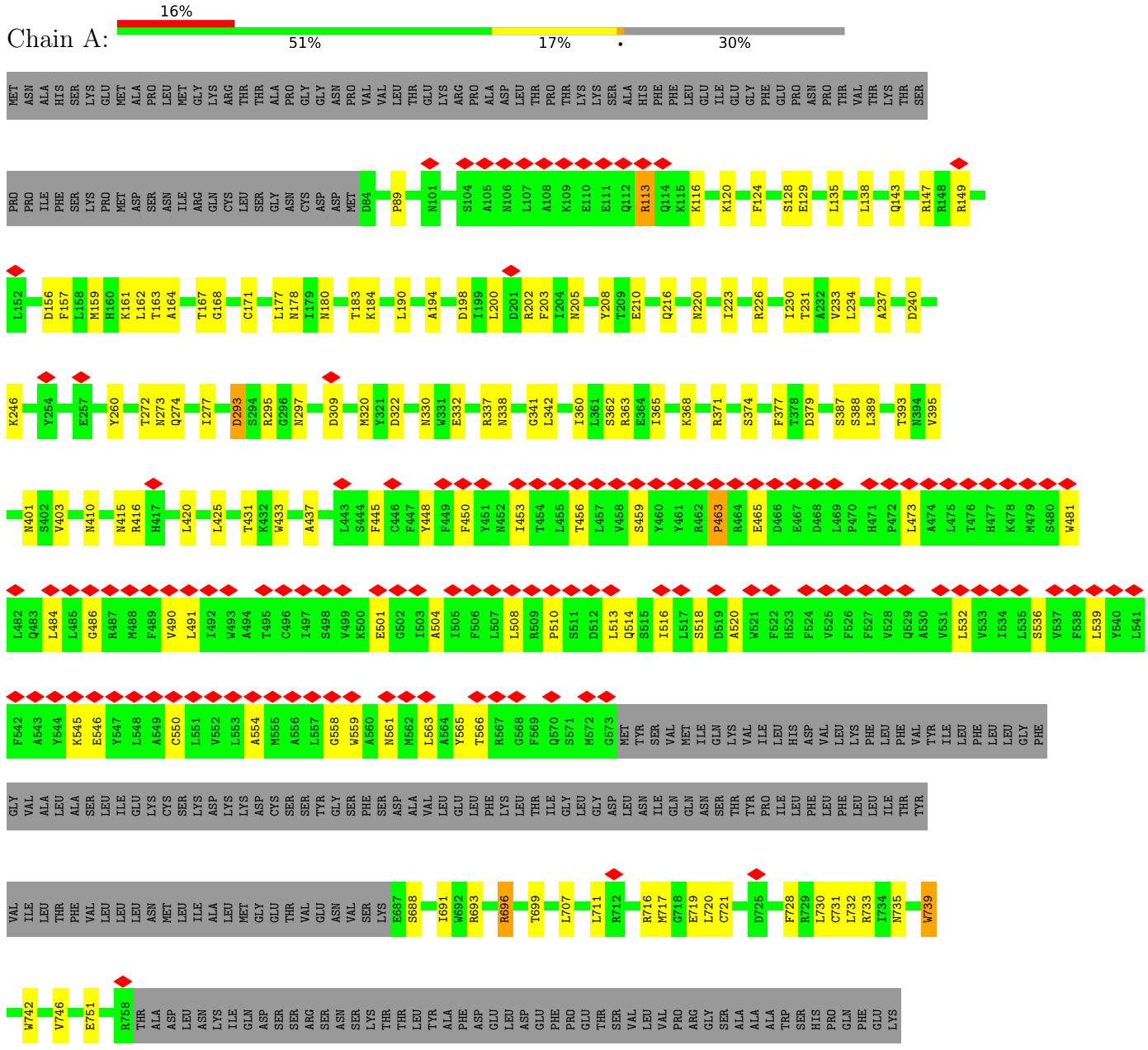
Chain	Residue	Modelled	Actual	Comment	Reference
D	800	ALA	-	expression tag	UNP Q8K424
D	801	TRP	-	expression tag	UNP Q8K424
D	802	SER	-	expression tag	UNP Q8K424
D	803	HIS	-	expression tag	UNP Q8K424
D	804	PRO	-	expression tag	UNP Q8K424
D	805	GLN	-	expression tag	UNP Q8K424
D	806	PHE	-	expression tag	UNP Q8K424
D	807	GLU	-	expression tag	UNP Q8K424
D	808	LYS	-	expression tag	UNP Q8K424

3 Residue-property plots (i)

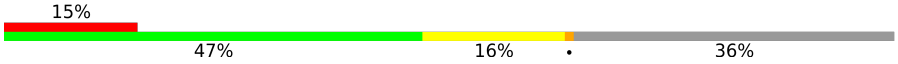
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

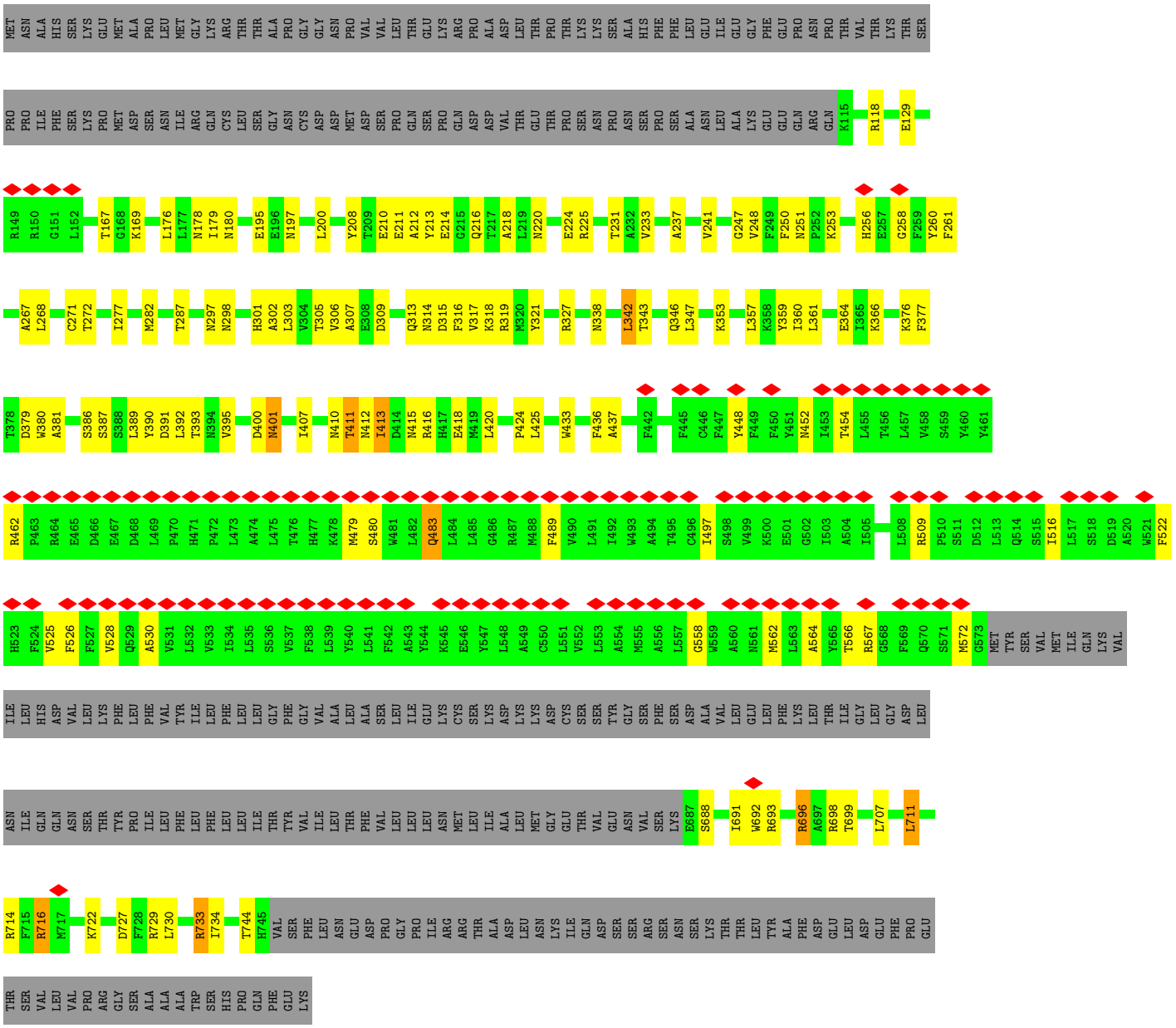
- Molecule 1: Transient receptor potential cation channel subfamily V member 3



• Molecule 1: Transient receptor potential cation channel subfamily V member 3

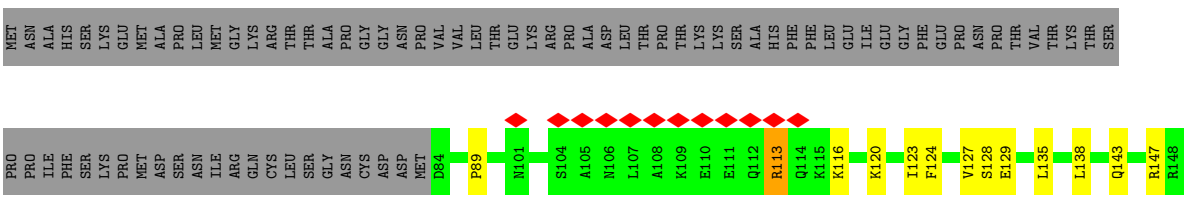
Chain B:

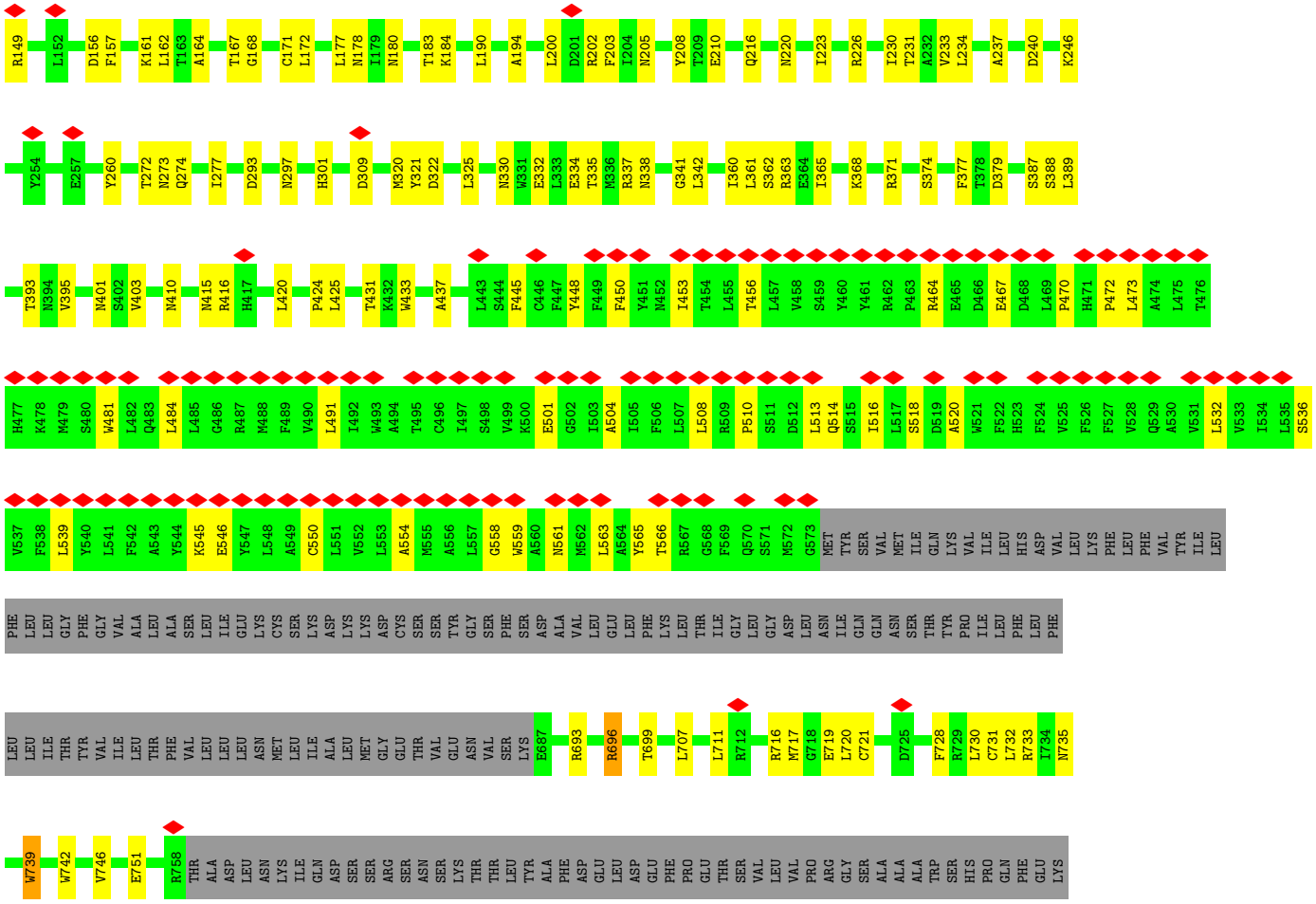




• Molecule 1: Transient receptor potential cation channel subfamily V member 3

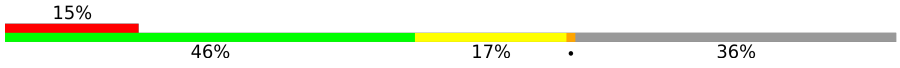
Chain C:

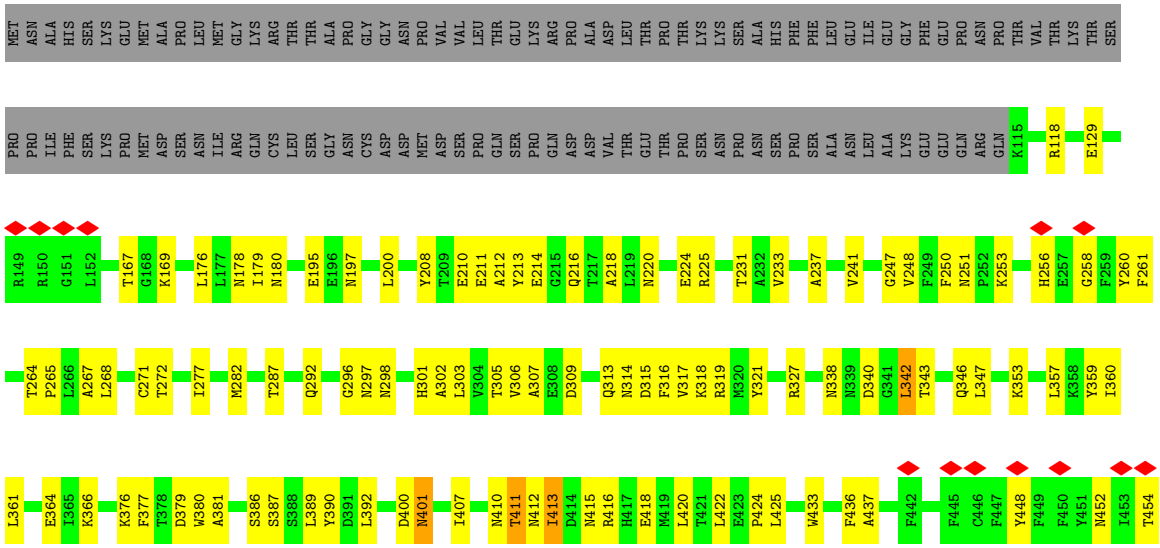


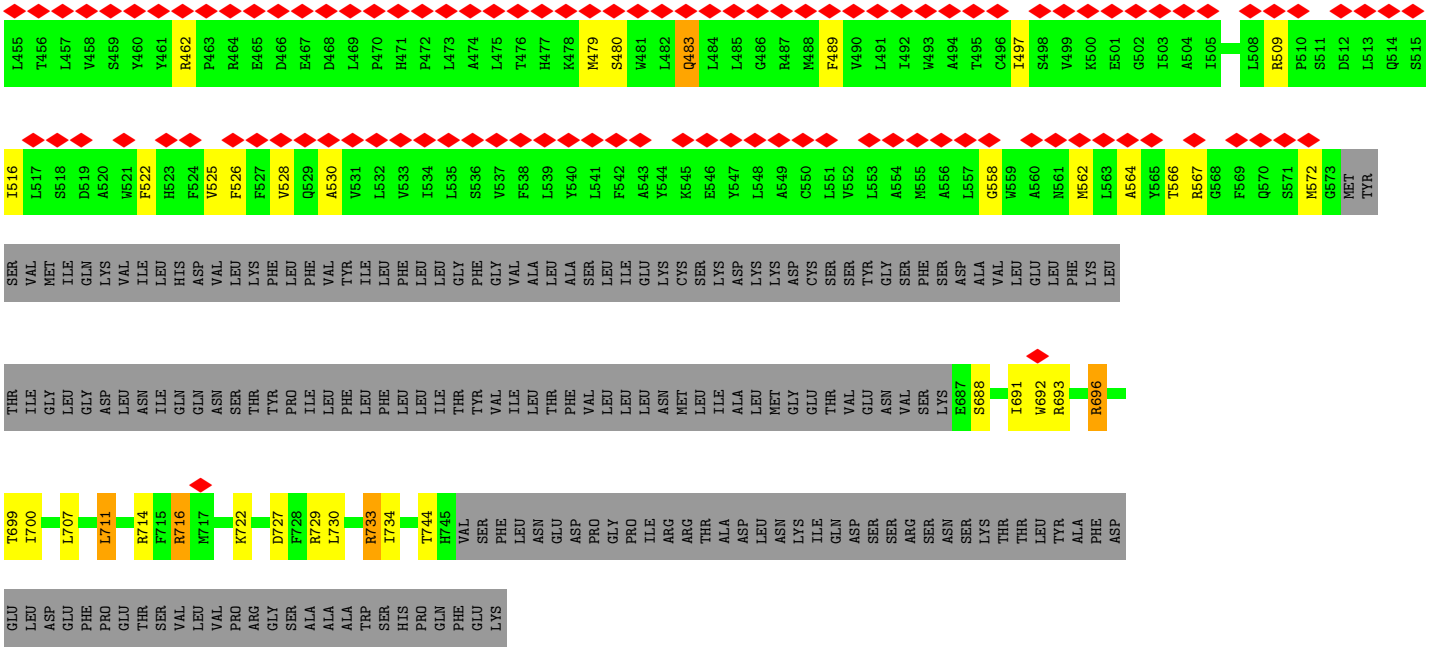


• Molecule 1: Transient receptor potential cation channel subfamily V member 3

Chain D:






L455 T456 L457 V458 S459 Y460 Y461 R462 P463 R464 E465 D466 E467 D468 L469 P470 H471 P472 L473 A474 L475 T476 H477 K478 M479 S480 W481 L482 Q483 L484 L485 G486 R487 M488 F489 V490 L491 I492 W493 A494 T495 C496 I497 S498 V499 K500 E501 G502 I503 A504 I505 L508 R509 P510 S511 D512 L513 Q514 S515
I516 L517 S518 D519 A520 W521 F522 H523 F524 V525 F526 F527 V528 Q529 A530 V531 L532 V533 I534 L535 S536 V537 F538 L539 Y540 L541 F542 A543 Y544 K545 E546 Y547 L548 A549 C550 L551 V552 L553 A554 N555 A556 L557 G558 W559 A560 N561 M562 L563 A564 Y565 T566 R567 G568 F569 Q570 S571 M572 G573 MET TYR
SER VAL MET ILE GLN LYS VAL ILE LEU HIS ASP VAL LEU LYS PHE LEU PHE VAL TYR ILE LEU PHE LEU LEU LEU GLY PHE GLY VAL ALA LEU ALA SER LEU ILE GLU LYS CYS SER LYS ASP LYS LYS ASP CYS SER SER TYR GLY SER PHE SER ASP ALA VAL LEU GLU LEU PHE LYS LEU
THR ILE GLY LEU GLY ASP LEU ASN ILE GLN GLN ASN SER THR TYR PRO ILE LEU PHE LEU PHE LEU LEU ILE THR TYR VAL ILE LEU LEU THR PHE VAL LEU LEU LEU ASN MET LEU ILE ALA ALA LEU MET GLY GLU THR VAL GLU ASN VAL SER LYS E687 S688 I691 W692 R693 R696
T699 I700 L707 L711 R714 F715 R716 M717 K722 D727 F728 R729 L730 R733 I734 T744 H745 VAL SER PHE LEU ASN GLU ASP PRO GLY PRO ILE ARG ARG THR ALA ASP LEU ASN LYS ILE GLN ASP SER SER ARG SER ASN SER LYS THR THR LEU TYR ALA PHE ASP
GLU LEU ASP GLU PHE PRO GLU THR SER VAL LEU VAL PRO ARG GLY SER ALA ALA ALA TRP SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	101814	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 ($e^-/Å^2$)	57.0	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	0.087	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0176	Depositor
Map size (Å)	233.19998, 233.19998, 233.19998	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.43	0/4682	0.66	2/6339 (0.0%)
1	B	0.42	0/4332	0.67	1/5859 (0.0%)
1	C	0.43	0/4682	0.66	2/6339 (0.0%)
1	D	0.42	0/4332	0.67	2/5859 (0.0%)
All	All	0.42	0/18028	0.67	7/24396 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	3
1	C	0	2
1	D	0	3
All	All	0	13

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	190	LEU	CB-CG-CD2	-6.15	100.55	111.00
1	A	190	LEU	CB-CG-CD2	-6.10	100.63	111.00
1	C	513	LEU	CA-CB-CG	5.46	127.87	115.30
1	A	513	LEU	CA-CB-CG	5.46	127.85	115.30
1	D	711	LEU	CA-CB-CG	5.41	127.75	115.30

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	293	ASP	Peptide
1	A	463	PRO	Peptide
1	A	465	GLU	Peptide
1	A	739	TRP	Peptide
1	A	89	PRO	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	4581	0	4575	86	0
1	B	4239	0	4261	84	0
1	C	4581	0	4575	91	0
1	D	4239	0	4261	84	0
All	All	17640	0	17672	337	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 10.

The worst 5 of 337 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:A:368:LYS:HA	1:A:371:ARG:HE	1.57	0.70
1:B:722:LYS:HD2	1:B:727:ASP:HB3	1.74	0.69
1:D:722:LYS:HD2	1:D:727:ASP:HB3	1.74	0.68
1:C:368:LYS:HA	1:C:371:ARG:HE	1.57	0.68
1:A:293:ASP:H	1:A:297:ASN:H	1.42	0.67

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	558/808 (69%)	475 (85%)	82 (15%)	1 (0%)	47 81
1	B	514/808 (64%)	438 (85%)	73 (14%)	3 (1%)	25 65
1	C	558/808 (69%)	476 (85%)	81 (14%)	1 (0%)	47 81
1	D	514/808 (64%)	438 (85%)	73 (14%)	3 (1%)	25 65
All	All	2144/3232 (66%)	1827 (85%)	309 (14%)	8 (0%)	38 72

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	412	ASN
1	D	412	ASN
1	A	113	ARG
1	C	113	ARG
1	B	411	THR

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	499/720 (69%)	491 (98%)	8 (2%)	62 79
1	B	458/720 (64%)	443 (97%)	15 (3%)	38 61
1	C	499/720 (69%)	491 (98%)	8 (2%)	62 79
1	D	458/720 (64%)	443 (97%)	15 (3%)	38 61
All	All	1914/2880 (66%)	1868 (98%)	46 (2%)	51 69

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	545	LYS
1	D	272	THR
1	C	696	ARG

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Mol	Chain	Res	Type
1	D	178	ASN
1	D	314	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	205	ASN
1	C	401	ASN
1	D	314	ASN
1	C	297	ASN
1	D	178	ASN

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

There are no chain breaks in this entry.

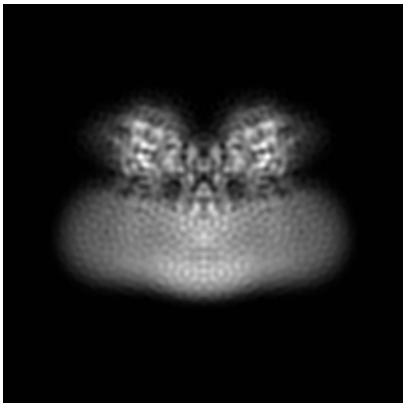
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20497. These allow visual inspection of the internal detail of the map and identification of artifacts.

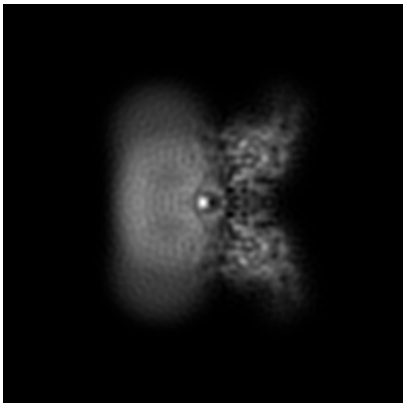
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

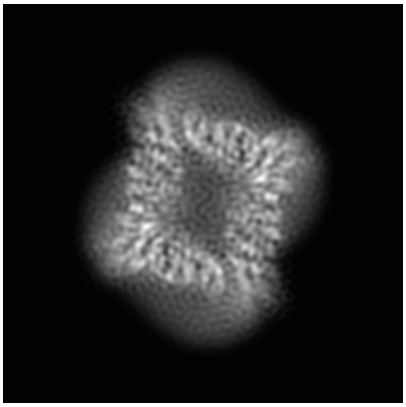
6.1.1 Primary map



X



Y

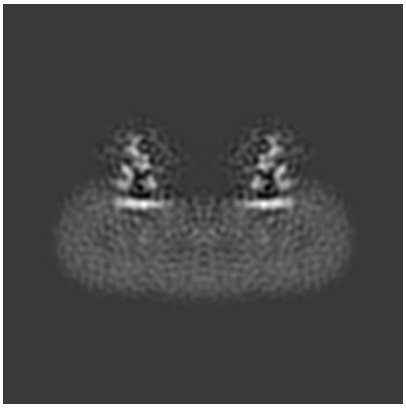


Z

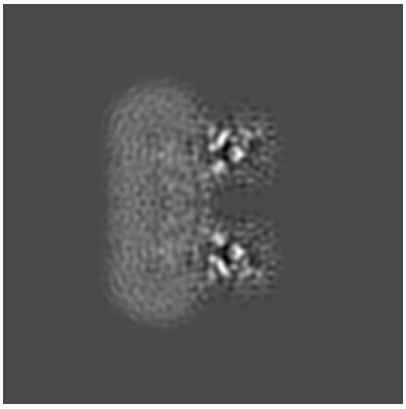
The images above show the map projected in three orthogonal directions.

6.2 Central slices

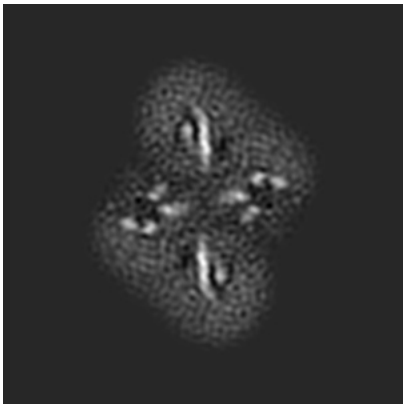
6.2.1 Primary map



X Index: 110



Y Index: 110

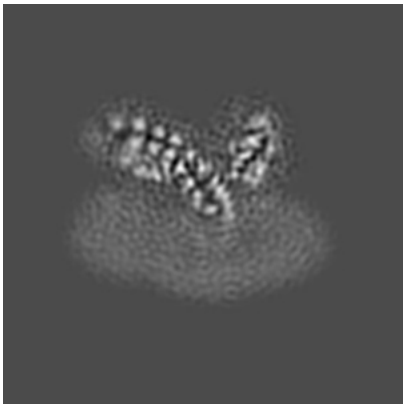


Z Index: 110

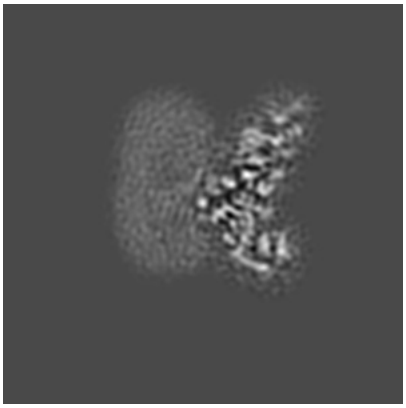
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 138



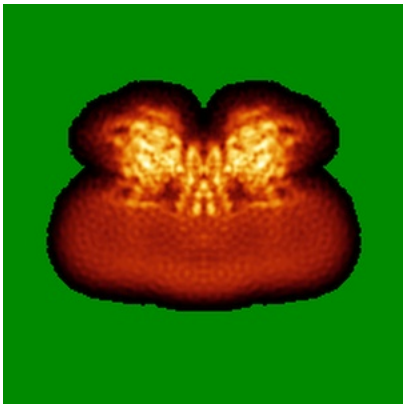
Y Index: 144

Z Index: 135

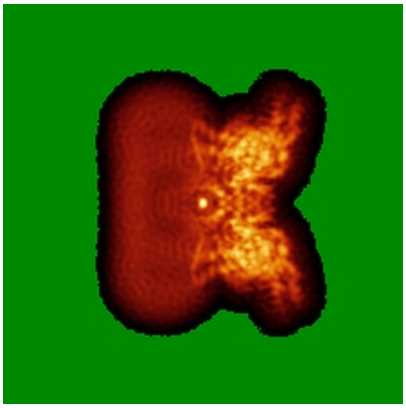
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



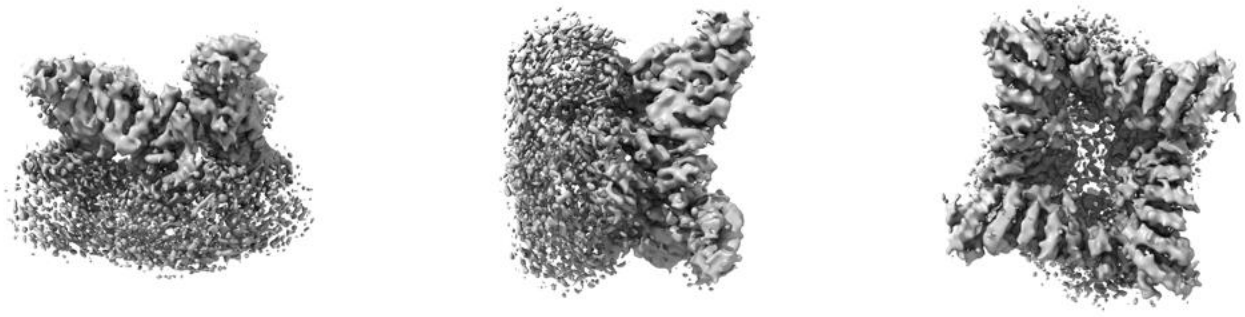
Y

Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0176. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

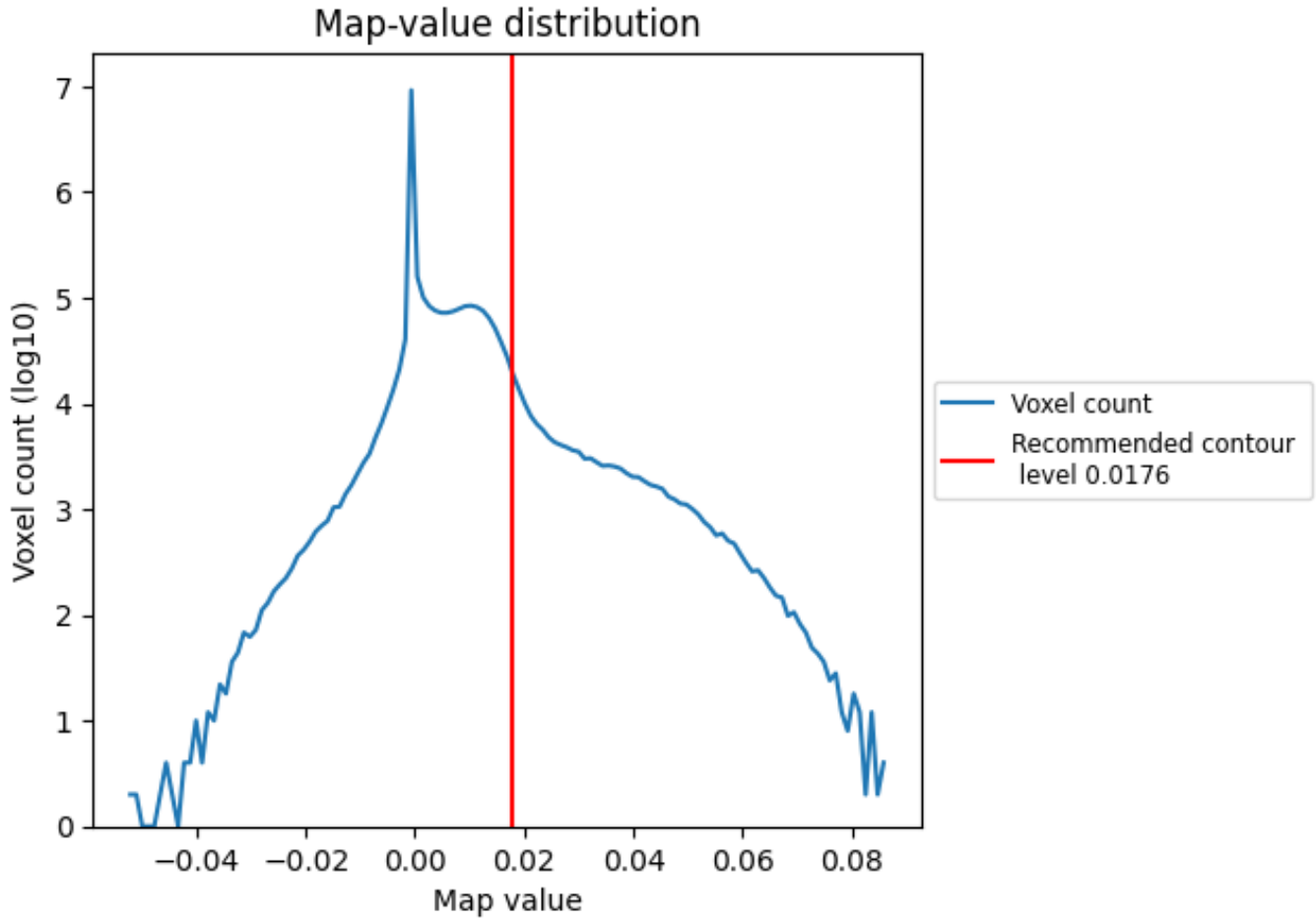
6.6 Mask visualisation (i)

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

7 Map analysis

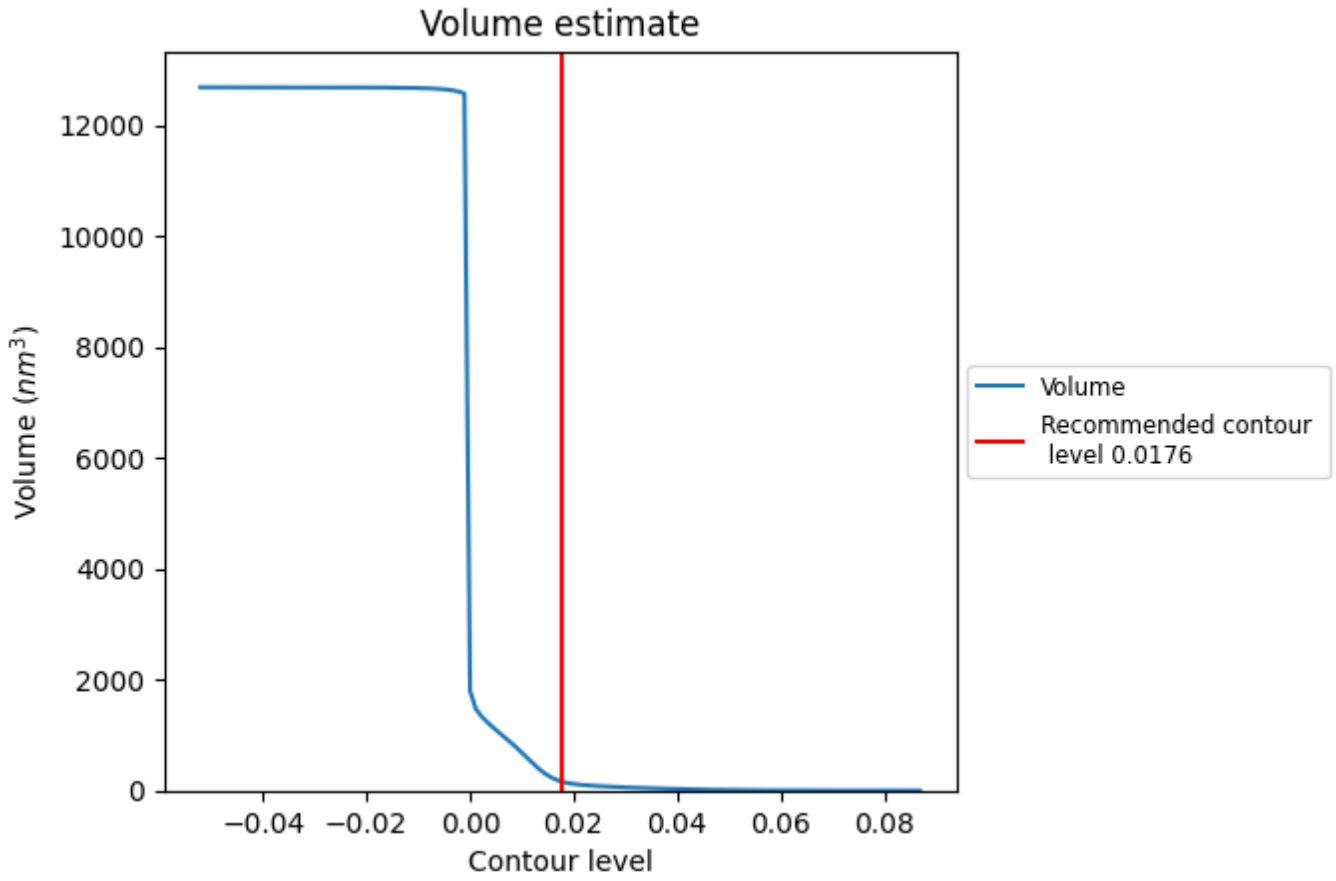
This section contains the results of statistical analysis of the map.

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.

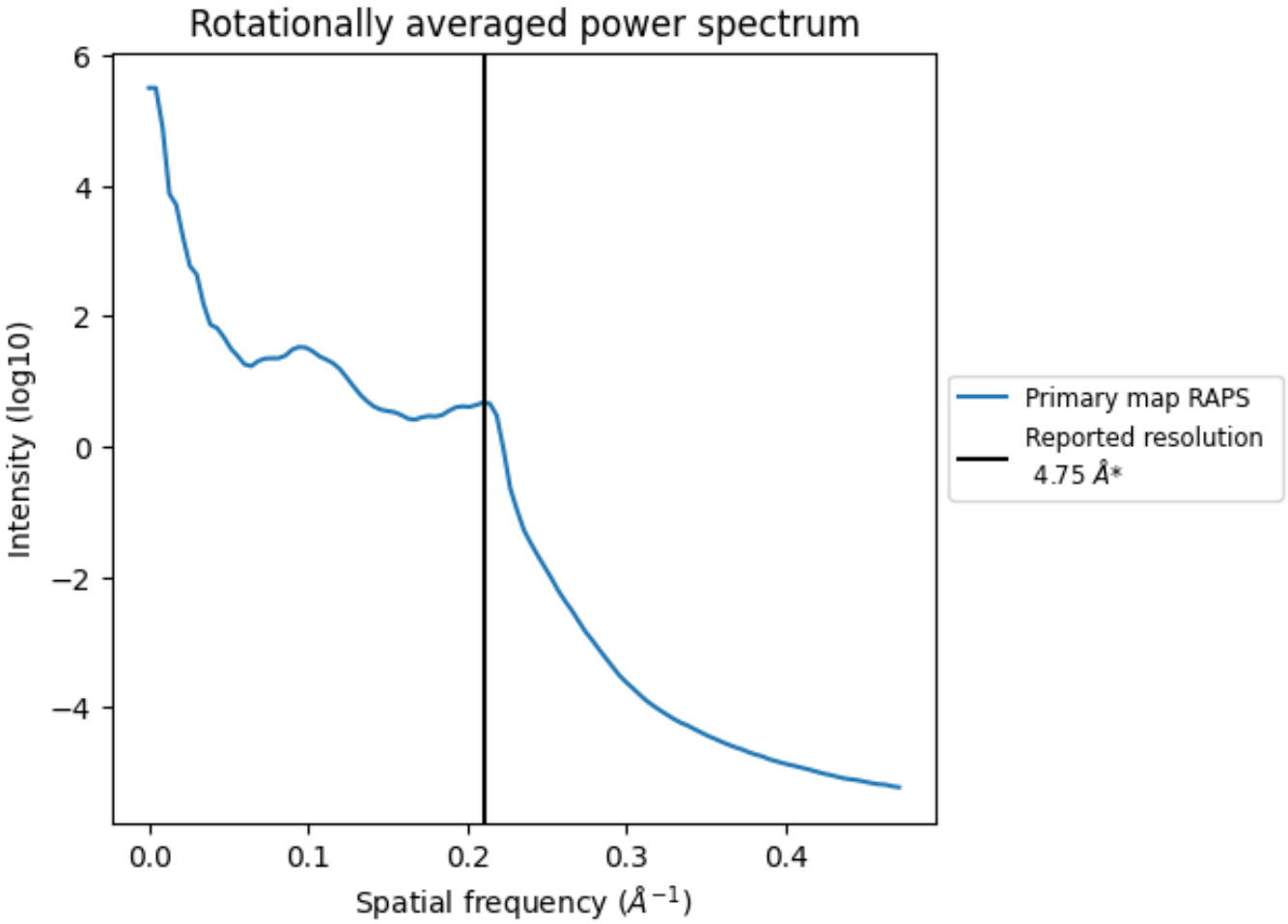
7.2 Volume estimate (i)



The volume at the recommended contour level is 166 nm^3; this corresponds to an approximate mass of 150 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 0.211 $Å^{-1}$

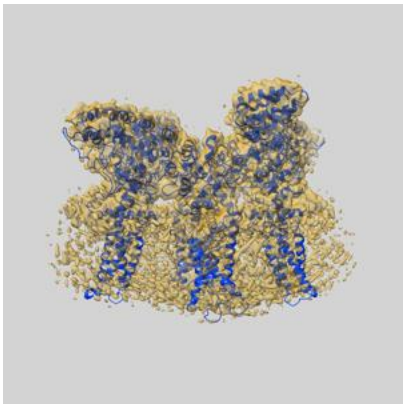
8 Fourier-Shell correlation

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

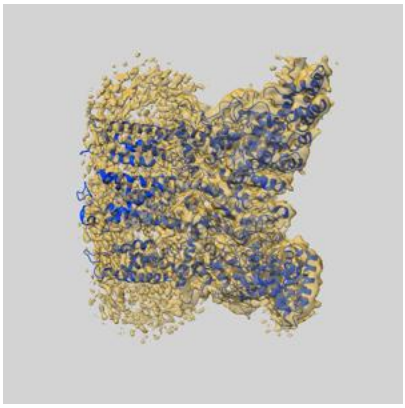
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20497 and PDB model 6PVQ. Per-residue inclusion information can be found in section 3 on page 6.

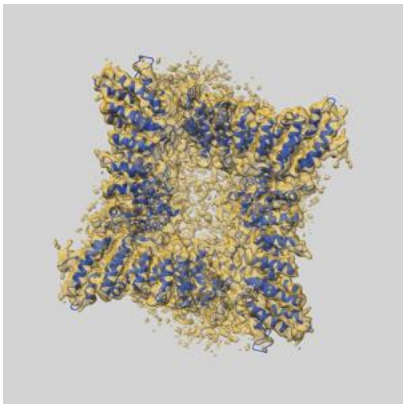
9.1 Map-model overlay



X



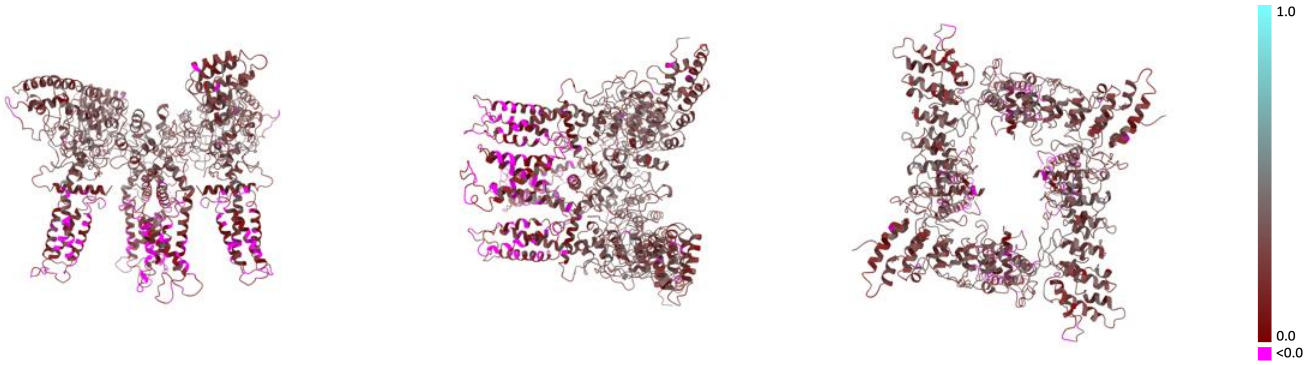
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0176 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.

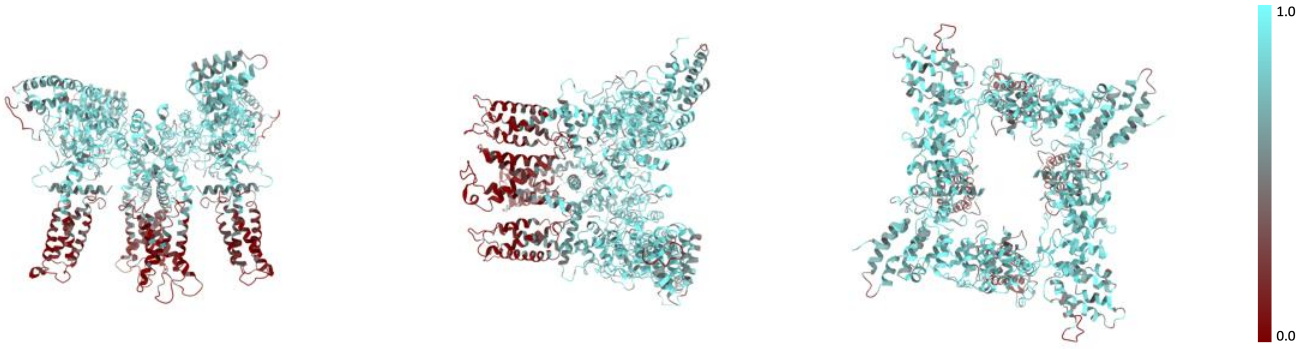
9.2 Q-score mapped to coordinate model (i)



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.

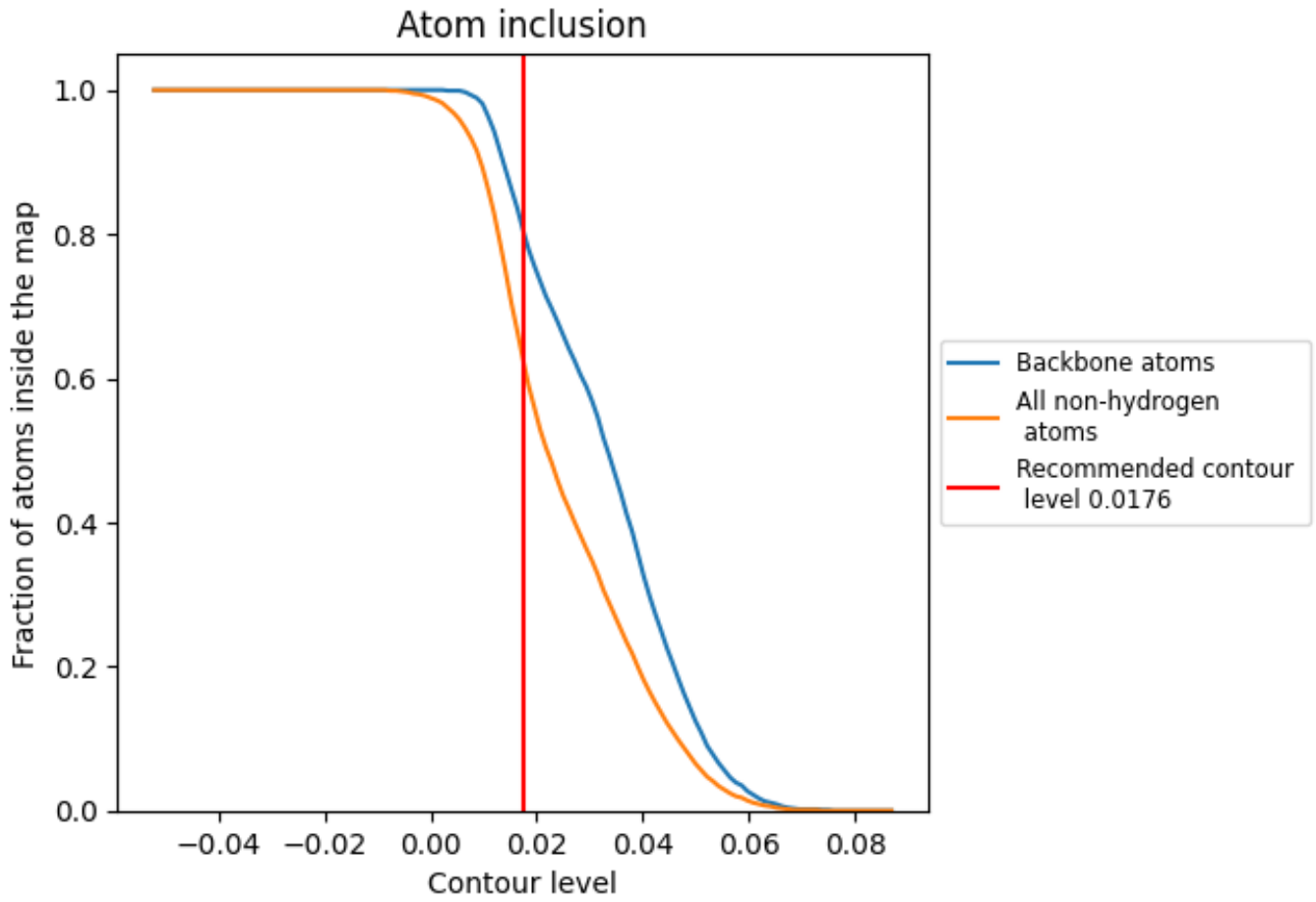
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0176).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 62% 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 (0.0176) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6200	0.2400
A	0.6200	0.2420
B	0.6190	0.2380
C	0.6210	0.2430
D	0.6190	0.2370