wwPDB EM Validation Summary Report

Oct 24, 2022 – 06:18 PM JST

PDB ID	:	7W6T
EMDB ID	:	EMD-32335
Title	:	CryoEM structure of human KChIP1-Kv4.3-DPP6 complex
Authors	:	Ma, D.M.; Guo, J.T.
Deposited on	:	2021-12-02
Resolution	:	3.85 Å(reported)

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

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

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

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

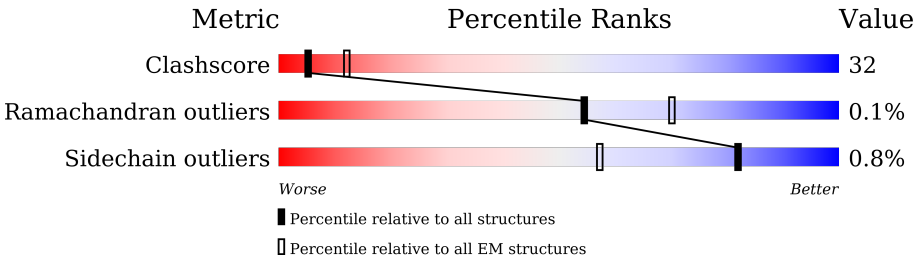
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.85 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	228	19% 40% 38% 21%
1	C	228	5% 29% 49% 21%
1	E	228	17% 40% 39% 21%
1	G	228	10% 38% 40% 21%
2	B	636	34% 34% 32%
2	D	636	31% 37% 32%
2	F	636	36% 32% 32%
2	H	636	35% 32% 32%

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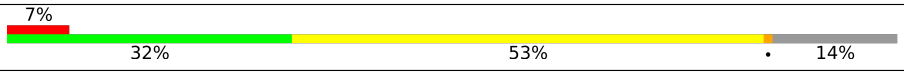
Mol	Chain	Length	Quality of chain
3	I	873	
3	J	873	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 31768 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 Kv channel-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	179	Total	C	N	O	S	0	0
			1474	942	240	284	8		
1	C	179	Total	C	N	O	S	0	0
			1474	942	240	284	8		
1	E	179	Total	C	N	O	S	0	0
			1474	942	240	284	8		
1	G	179	Total	C	N	O	S	0	0
			1474	942	240	284	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q9NZI2
C	0	SER	-	expression tag	UNP Q9NZI2
E	0	SER	-	expression tag	UNP Q9NZI2
G	0	SER	-	expression tag	UNP Q9NZI2

- Molecule 2 is a protein called Isoform 2 of Potassium voltage-gated channel subfamily D member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	430	Total	C	N	O	S	0	0
			3456	2245	579	607	25		
2	D	430	Total	C	N	O	S	0	0
			3456	2245	579	607	25		
2	F	430	Total	C	N	O	S	0	0
			3456	2245	579	607	25		
2	H	430	Total	C	N	O	S	0	0
			3456	2245	579	607	25		

- Molecule 3 is a protein called Dipeptidyl aminopeptidase-like protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	749	Total	C	N	O	S	0	0
			6024	3842	1025	1134	23		
3	J	749	Total	C	N	O	S	0	0
			6024	3842	1025	1134	23		

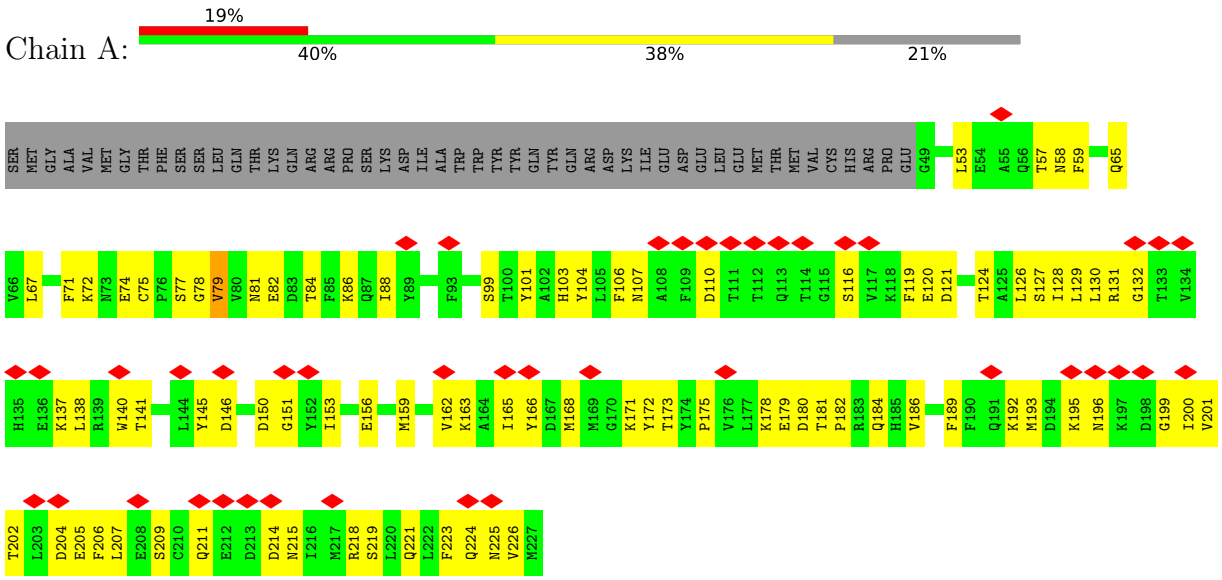
There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	805	LEU	-	expression tag	UNP E9PWX1
I	806	GLU	-	expression tag	UNP E9PWX1
I	807	GLY	-	expression tag	UNP E9PWX1
I	808	GLY	-	expression tag	UNP E9PWX1
I	809	SER	-	expression tag	UNP E9PWX1
I	810	SER	-	expression tag	UNP E9PWX1
I	811	ASP	-	expression tag	UNP E9PWX1
I	812	TYR	-	expression tag	UNP E9PWX1
I	813	LYS	-	expression tag	UNP E9PWX1
I	814	ASP	-	expression tag	UNP E9PWX1
I	815	ASP	-	expression tag	UNP E9PWX1
I	816	ASP	-	expression tag	UNP E9PWX1
I	817	ASP	-	expression tag	UNP E9PWX1
I	818	LYS	-	expression tag	UNP E9PWX1
J	805	LEU	-	expression tag	UNP E9PWX1
J	806	GLU	-	expression tag	UNP E9PWX1
J	807	GLY	-	expression tag	UNP E9PWX1
J	808	GLY	-	expression tag	UNP E9PWX1
J	809	SER	-	expression tag	UNP E9PWX1
J	810	SER	-	expression tag	UNP E9PWX1
J	811	ASP	-	expression tag	UNP E9PWX1
J	812	TYR	-	expression tag	UNP E9PWX1
J	813	LYS	-	expression tag	UNP E9PWX1
J	814	ASP	-	expression tag	UNP E9PWX1
J	815	ASP	-	expression tag	UNP E9PWX1
J	816	ASP	-	expression tag	UNP E9PWX1
J	817	ASP	-	expression tag	UNP E9PWX1
J	818	LYS	-	expression tag	UNP E9PWX1

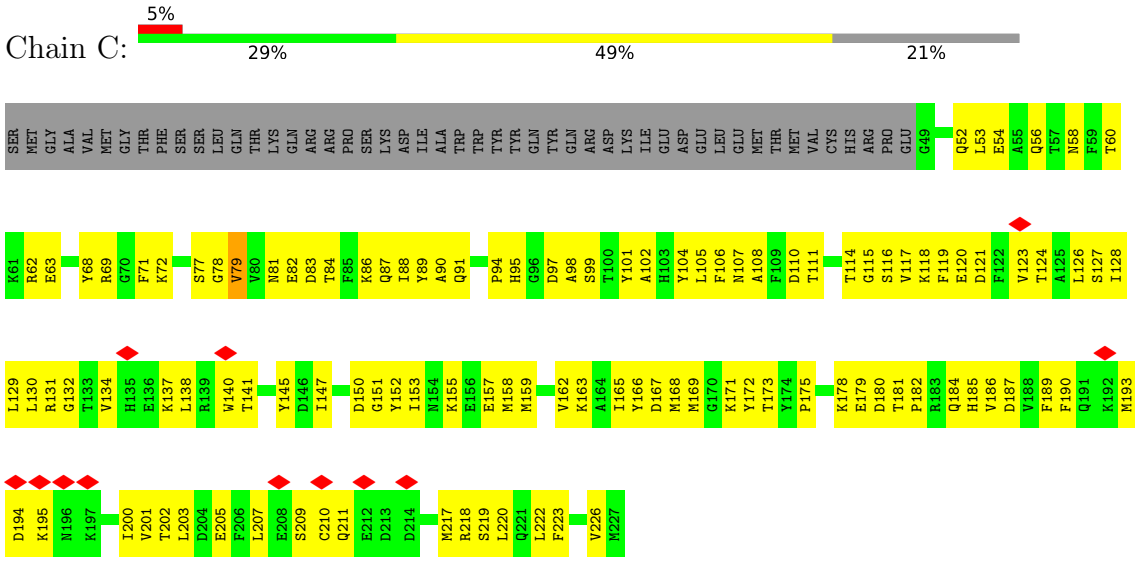
3 Residue-property plots (i)

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: Kv channel-interacting protein 1

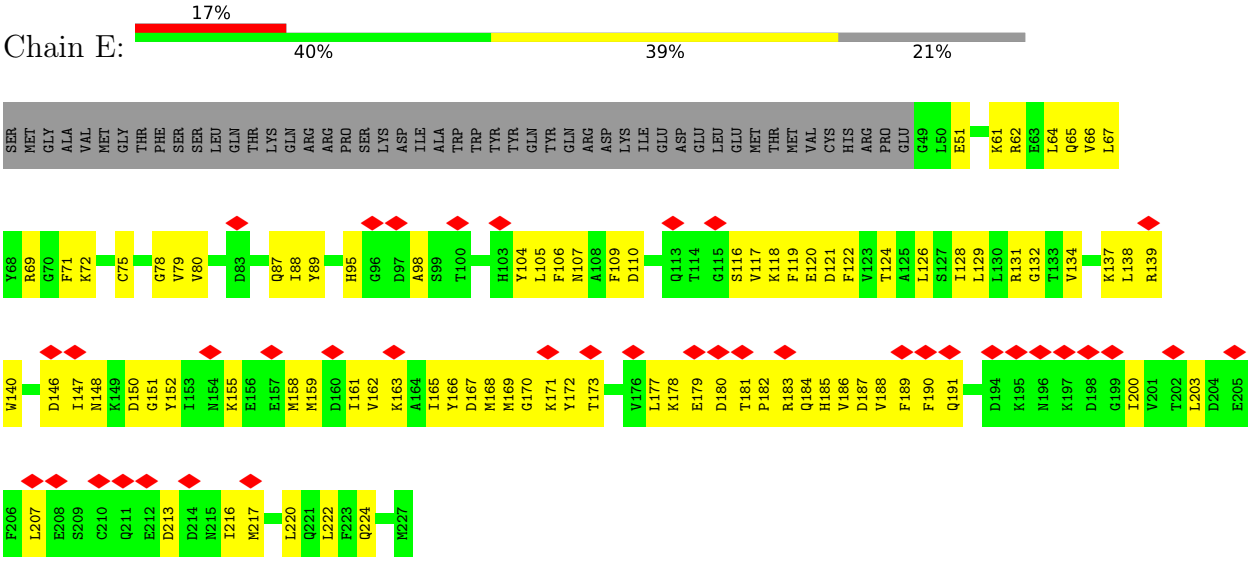


• Molecule 1: Kv channel-interacting protein 1



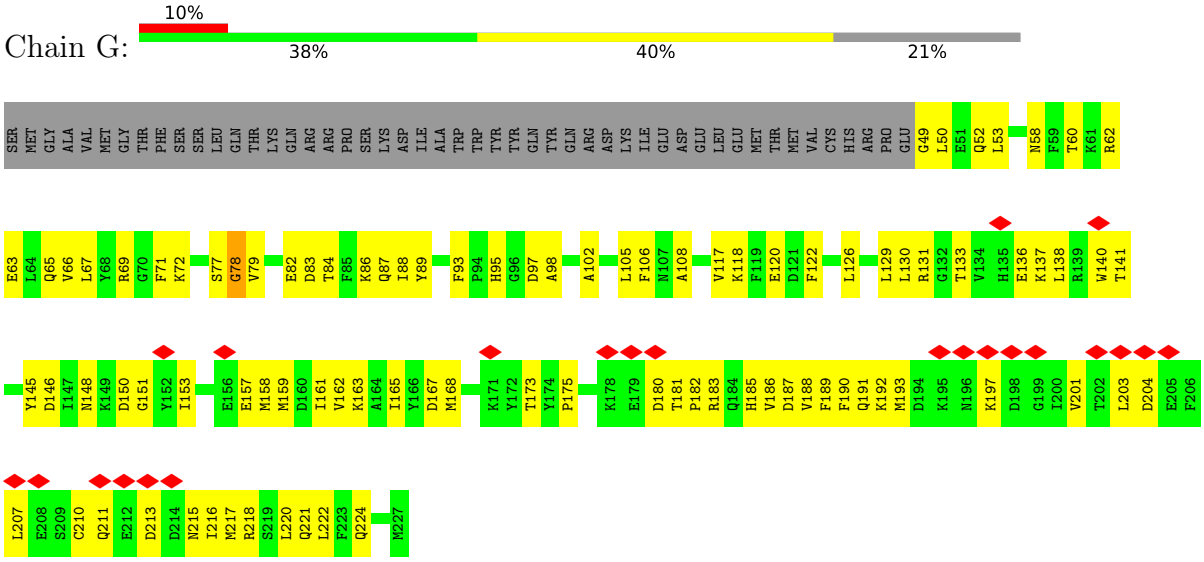
• Molecule 1: Kv channel-interacting protein 1

Chain E:



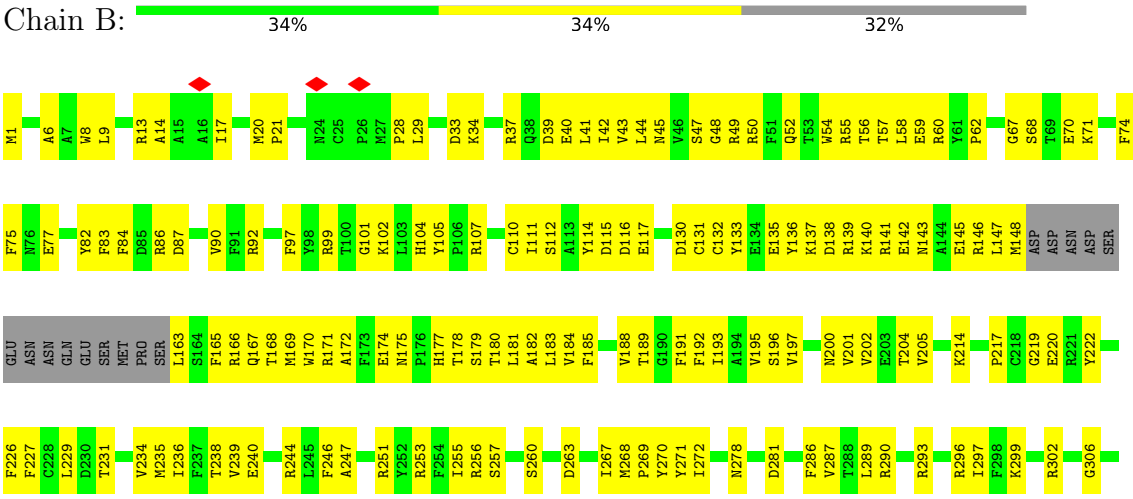
• Molecule 1: Kv channel-interacting protein 1

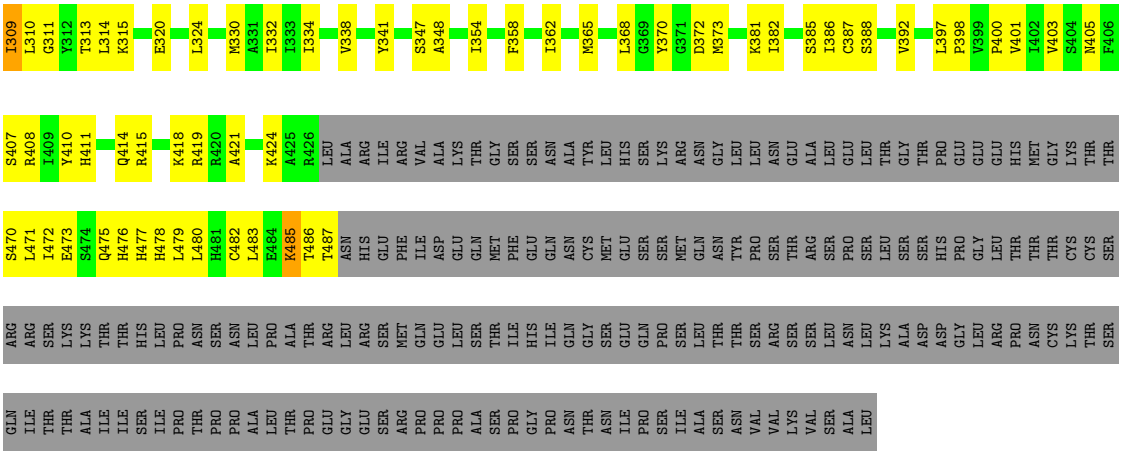
Chain G:



• Molecule 2: Isoform 2 of Potassium voltage-gated channel subfamily D member 3

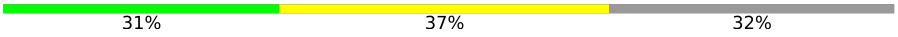
Chain B:

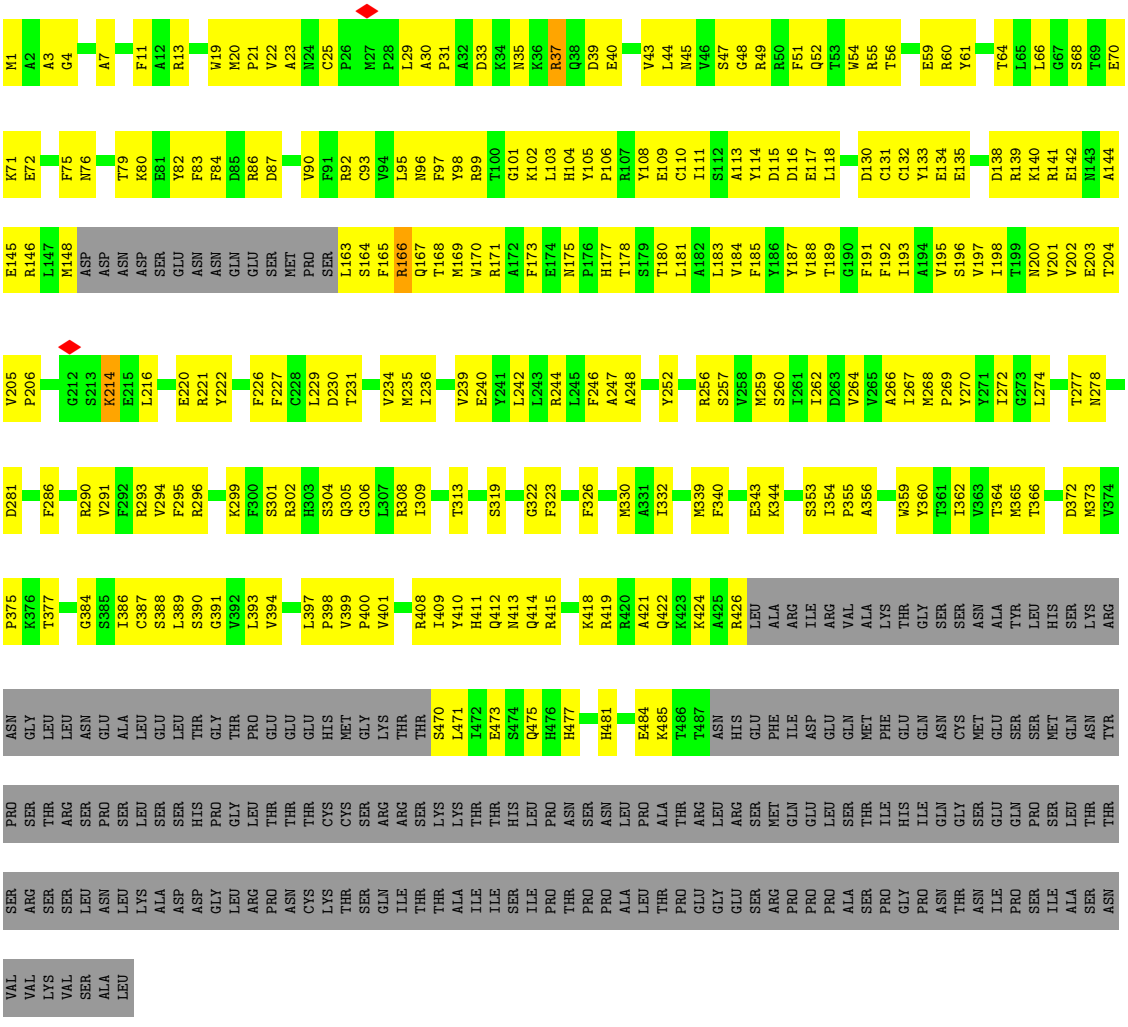




• Molecule 2: Isoform 2 of Potassium voltage-gated channel subfamily D member 3

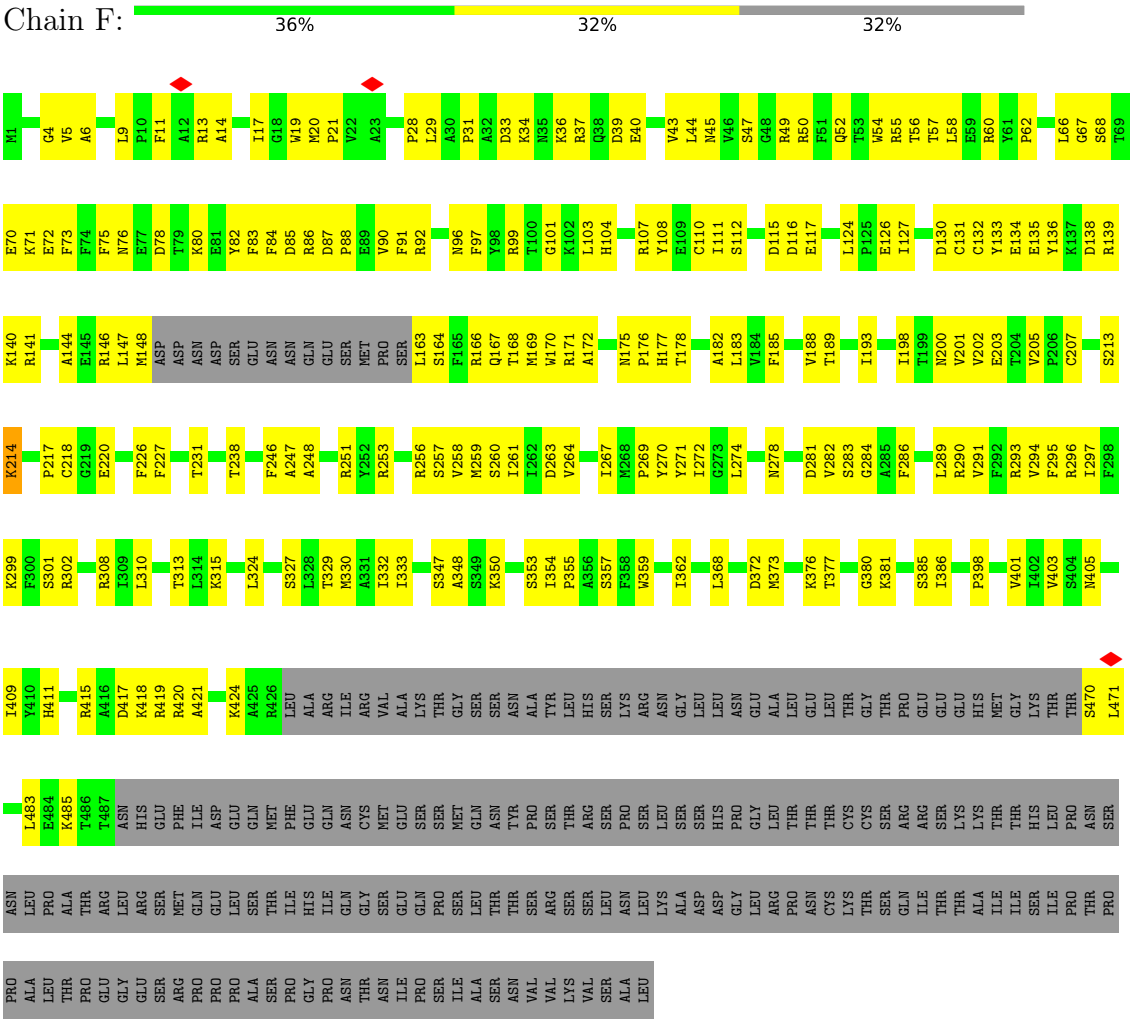
Chain D:





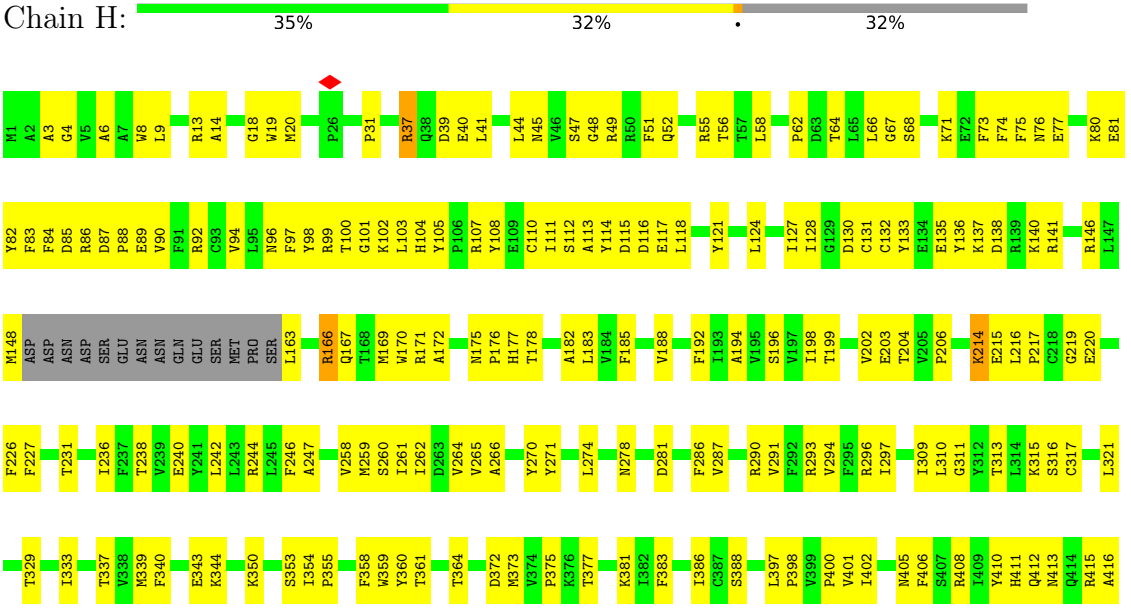
• Molecule 2: Isoform 2 of Potassium voltage-gated channel subfamily D member 3

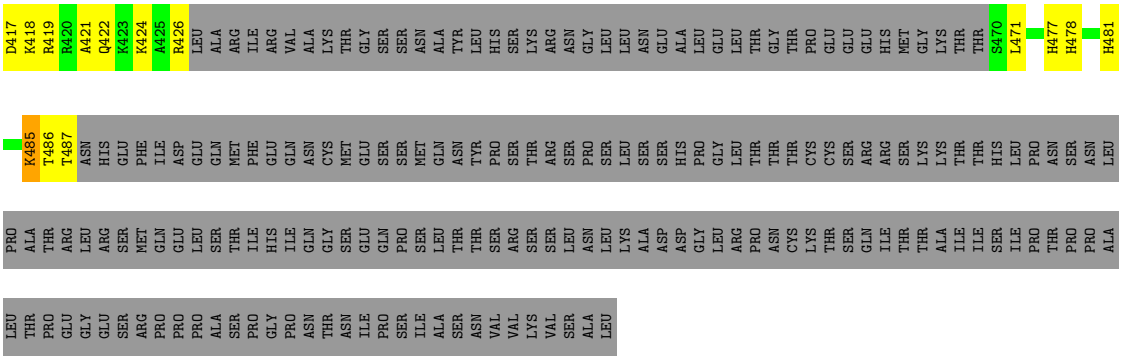
Chain F:



• Molecule 2: Isoform 2 of Potassium voltage-gated channel subfamily D member 3

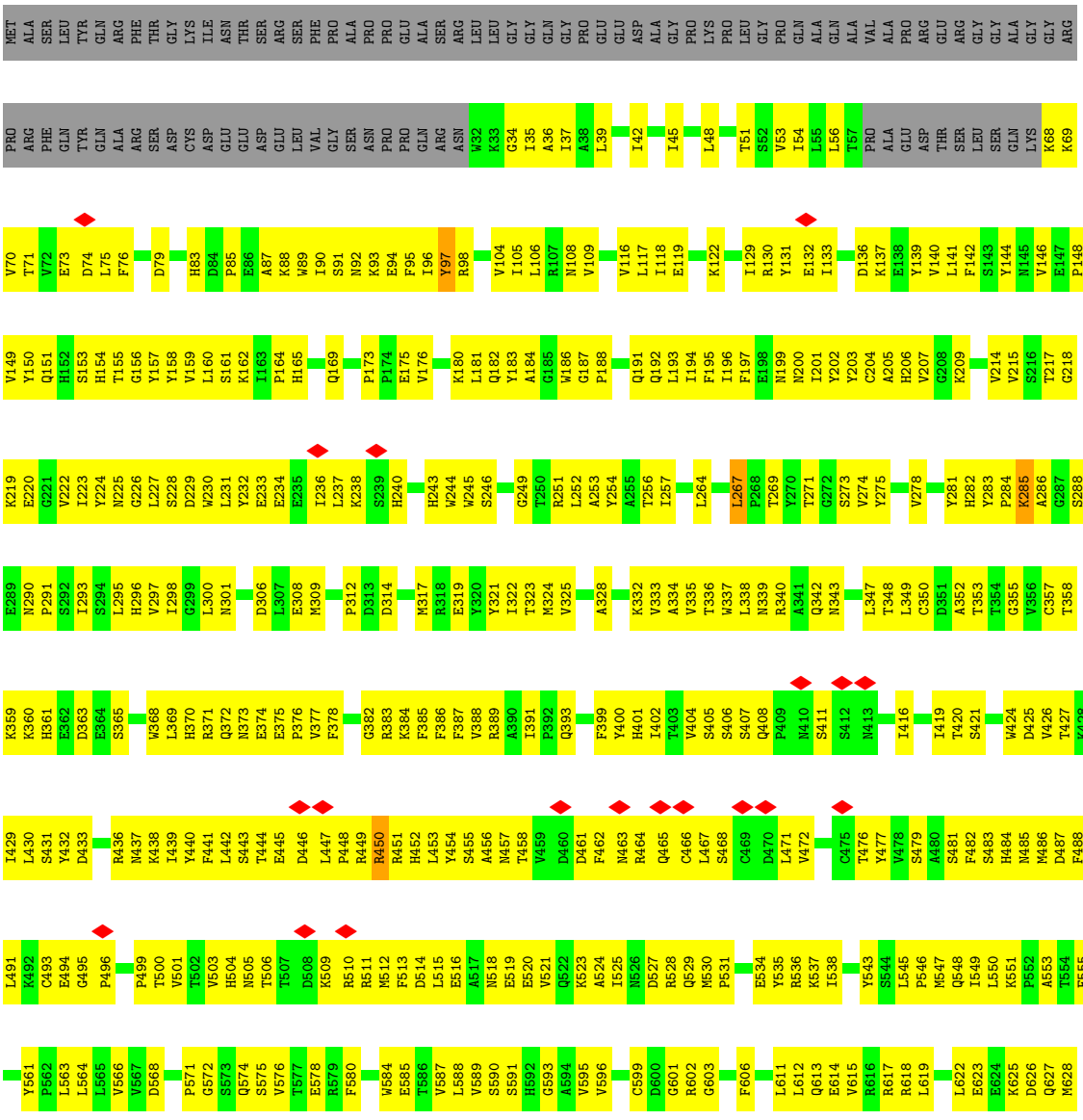
Chain H:

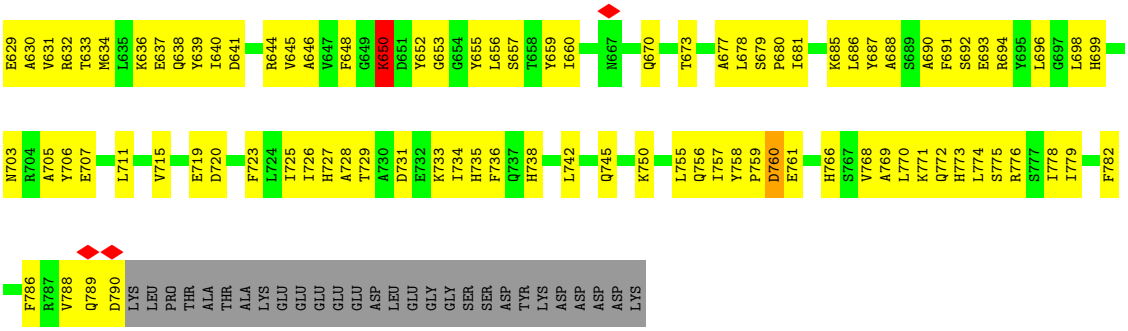




• Molecule 3: Dipeptidyl aminopeptidase-like protein 6

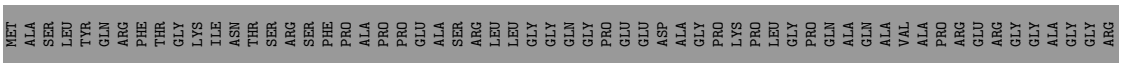
Chain I:

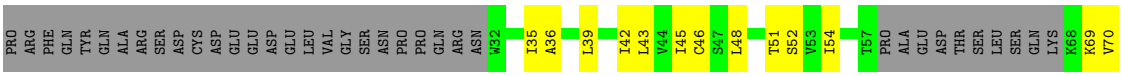


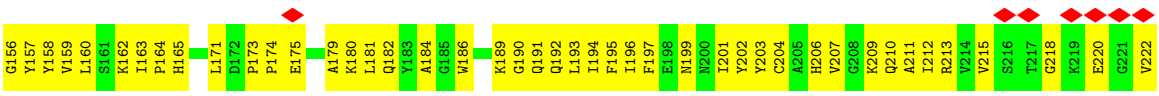


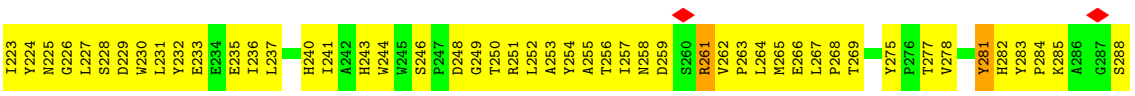
• Molecule 3: Dipeptidyl aminopeptidase-like protein 6

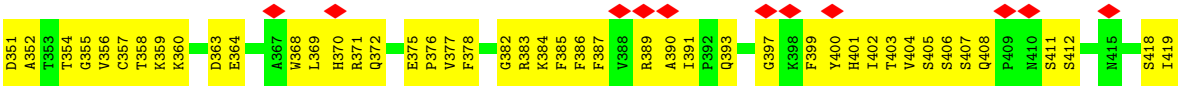
Chain J:

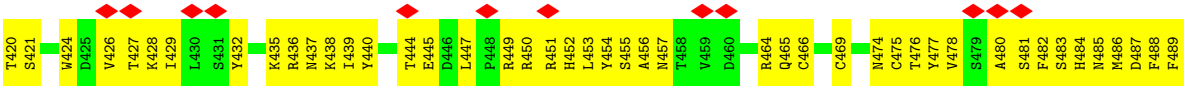


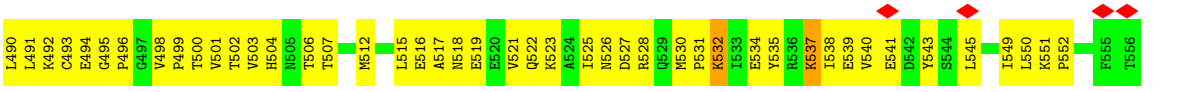


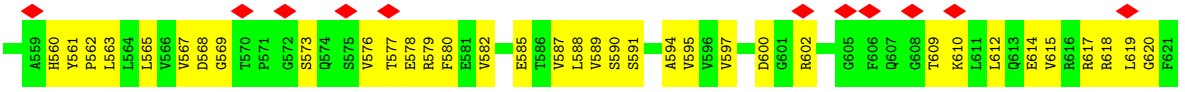


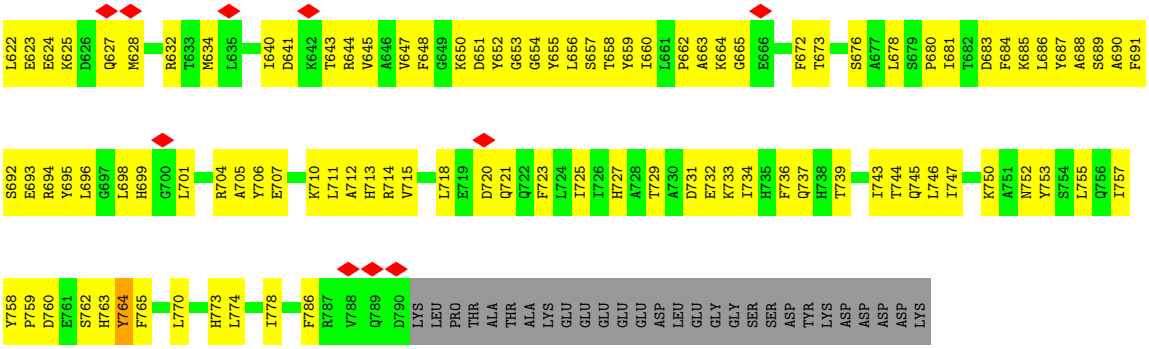











L622 E623 E624 K625 D626 Q627 M628 R632 T633 M634 L635 I640 D641 K642 T643 R644 V645 A646 V647 F648 G649 K650 D651 Y652 G653 G654 Y655 L656 S657 T658 Y659 I660 L661 P662 A663 K664 G665 E666 F672 T673 S676 A677 L678 S679 P680 I681 T682 D683 F684 K685 L686 Y687 A688 S689 A690 F691
S692 E693 R694 Y695 L696 G697 L698 H699 G700 L701 R704 A705 Y706 E707 K710 L711 A712 H713 R714 V715 L718 E719 D720 Q721 Q722 F723 L724 T725 I726 H727 A728 T729 A730 D731 E732 K733 I734 H735 F736 Q737 H738 T739 I743 T744 Q745 L746 I747 K750 A751 N752 Y753 S754 L755 Q756 I757
Y758 P759 D760 E761 S762 H763 Y764 F765 L770 H773 L774 I778 F786 R787 V788 Q789 D790 LYS LEU PRO THR ALA THR ALA LYS GLU GLU GLU GLU GLU GLU ASP LEU GLU GLY GLY SER SER ASP TYR LYS ASP ASP ASP ASP LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	263176	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 ($e^-/Å^2$)	65	Depositor
Minimum defocus (nm)	-1100	Depositor
Maximum defocus (nm)	-1300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.080	Depositor
Minimum map value	-0.457	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.0956	Depositor
Map size (Å)	273.78003, 273.78003, 273.78003	wwPDB
Map dimensions	270, 270, 270	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.014, 1.014, 1.014	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	0.26	0/1506	0.44	0/2032
1	C	0.28	0/1506	0.47	0/2032
1	E	0.28	0/1506	0.48	0/2032
1	G	0.27	0/1506	0.47	0/2032
2	B	0.39	0/3544	0.47	0/4800
2	D	0.37	0/3544	0.46	0/4800
2	F	0.37	0/3544	0.47	0/4800
2	H	0.38	0/3544	0.47	0/4800
3	I	0.35	0/6171	0.54	0/8370
3	J	0.35	0/6171	0.53	0/8370
All	All	0.35	0/32542	0.50	0/44068

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	G	0	1
3	I	0	4
3	J	0	2
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	78	GLY	Peptide
3	I	267	LEU	Peptide
3	I	285	LYS	Peptide

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Mol	Chain	Res	Type	Group
3	I	650	LYS	Peptide
3	I	760	ASP	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	1474	0	1415	72	0
1	C	1474	0	1415	104	0
1	E	1474	0	1415	73	0
1	G	1474	0	1415	75	0
2	B	3456	0	3462	200	0
2	D	3456	0	3462	226	0
2	F	3456	0	3462	182	0
2	H	3456	0	3462	192	0
3	I	6024	0	5922	528	0
3	J	6024	0	5922	516	0
All	All	31768	0	31352	2013	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 32.

The worst 5 of 2013 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:C:186:VAL:O	1:C:189:PHE:HB3	1.60	1.01
1:A:186:VAL:O	1:A:189:PHE:HB3	1.61	0.99
3:J:265:MET:HB2	3:J:283:TYR:HB2	1.42	0.98
3:J:92:ASN:HA	3:J:484:HIS:HB2	1.50	0.94
3:J:264:LEU:HA	3:J:282:HIS:HA	1.51	0.92

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	177/228 (78%)	165 (93%)	12 (7%)	0	100 100
1	C	177/228 (78%)	161 (91%)	15 (8%)	1 (1%)	25 62
1	E	177/228 (78%)	160 (90%)	17 (10%)	0	100 100
1	G	177/228 (78%)	164 (93%)	13 (7%)	0	100 100
2	B	424/636 (67%)	380 (90%)	44 (10%)	0	100 100
2	D	424/636 (67%)	383 (90%)	40 (9%)	1 (0%)	47 78
2	F	424/636 (67%)	379 (89%)	45 (11%)	0	100 100
2	H	424/636 (67%)	389 (92%)	35 (8%)	0	100 100
3	I	745/873 (85%)	656 (88%)	89 (12%)	0	100 100
3	J	745/873 (85%)	638 (86%)	107 (14%)	0	100 100
All	All	3894/5202 (75%)	3475 (89%)	417 (11%)	2 (0%)	54 83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	484	GLU
1	C	79	VAL

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	162/208 (78%)	161 (99%)	1 (1%)	86 91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	162/208 (78%)	162 (100%)	0	100 100
1	E	162/208 (78%)	161 (99%)	1 (1%)	86 91
1	G	162/208 (78%)	162 (100%)	0	100 100
2	B	374/560 (67%)	370 (99%)	4 (1%)	73 84
2	D	374/560 (67%)	371 (99%)	3 (1%)	81 89
2	F	374/560 (67%)	371 (99%)	3 (1%)	81 89
2	H	374/560 (67%)	370 (99%)	4 (1%)	73 84
3	I	667/766 (87%)	662 (99%)	5 (1%)	84 90
3	J	667/766 (87%)	660 (99%)	7 (1%)	76 85
All	All	3478/4604 (76%)	3450 (99%)	28 (1%)	82 89

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	214	LYS
3	J	764	TYR
3	I	450	ARG
3	J	532	LYS
3	I	97	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
3	I	206	HIS
3	I	638	GLN
3	J	522	GLN
3	I	225	ASN
3	I	437	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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

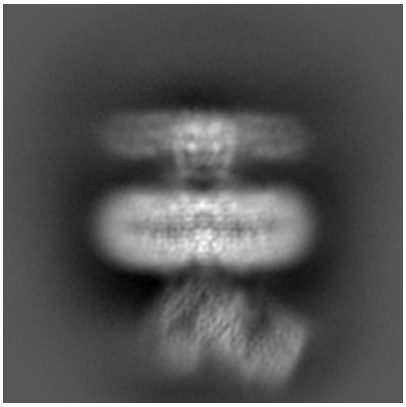
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32335. These allow visual inspection of the internal detail of the map and identification of artifacts.

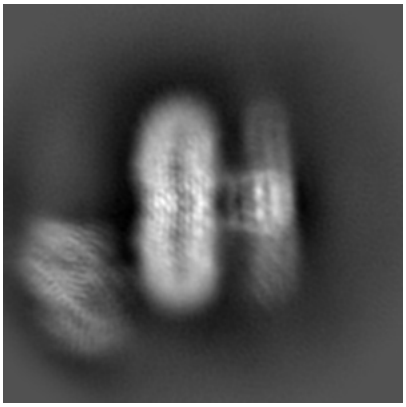
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

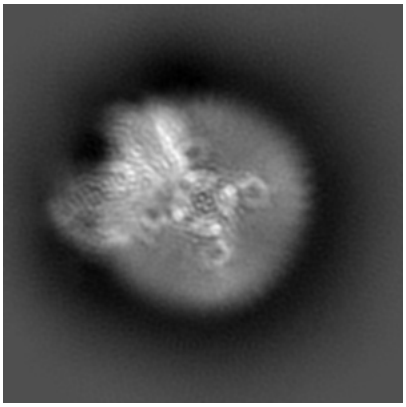
6.1.1 Primary map



X



Y

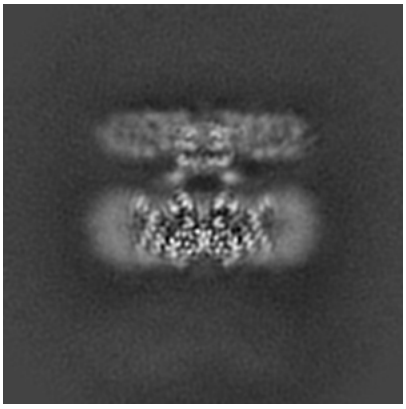


Z

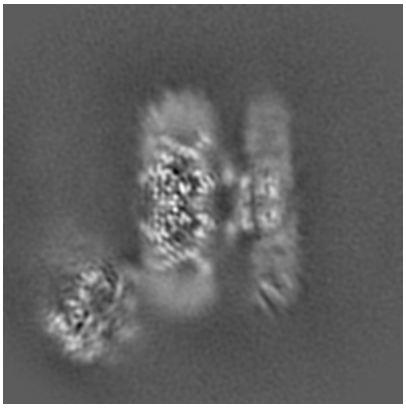
The images above show the map projected in three orthogonal directions.

6.2 Central slices

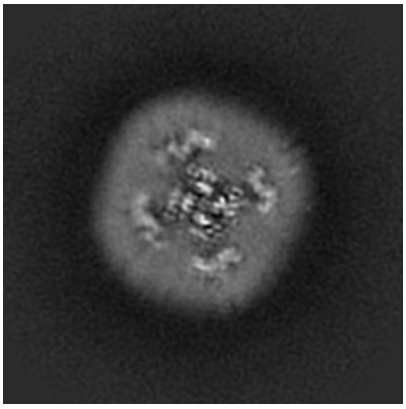
6.2.1 Primary map



X Index: 135



Y Index: 135

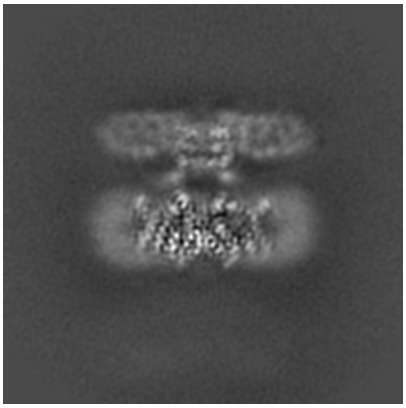


Z Index: 135

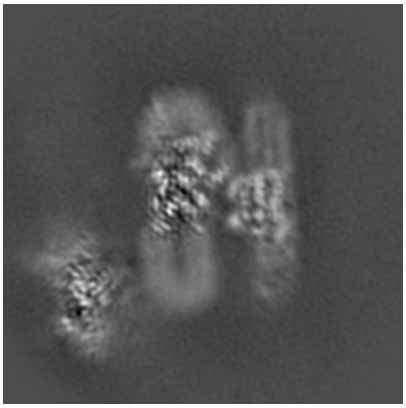
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

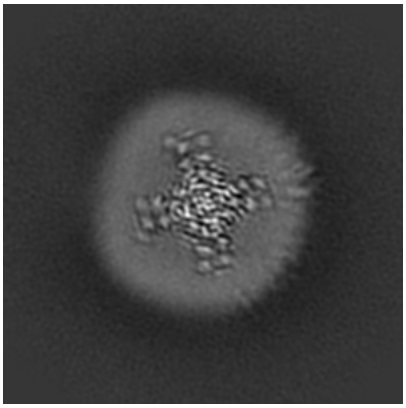
6.3.1 Primary map



X Index: 137



Y Index: 144



Z Index: 107

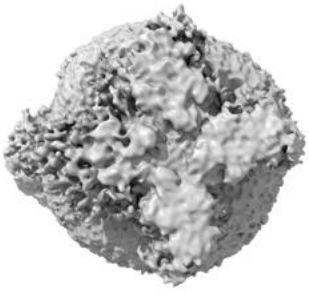
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.0956. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

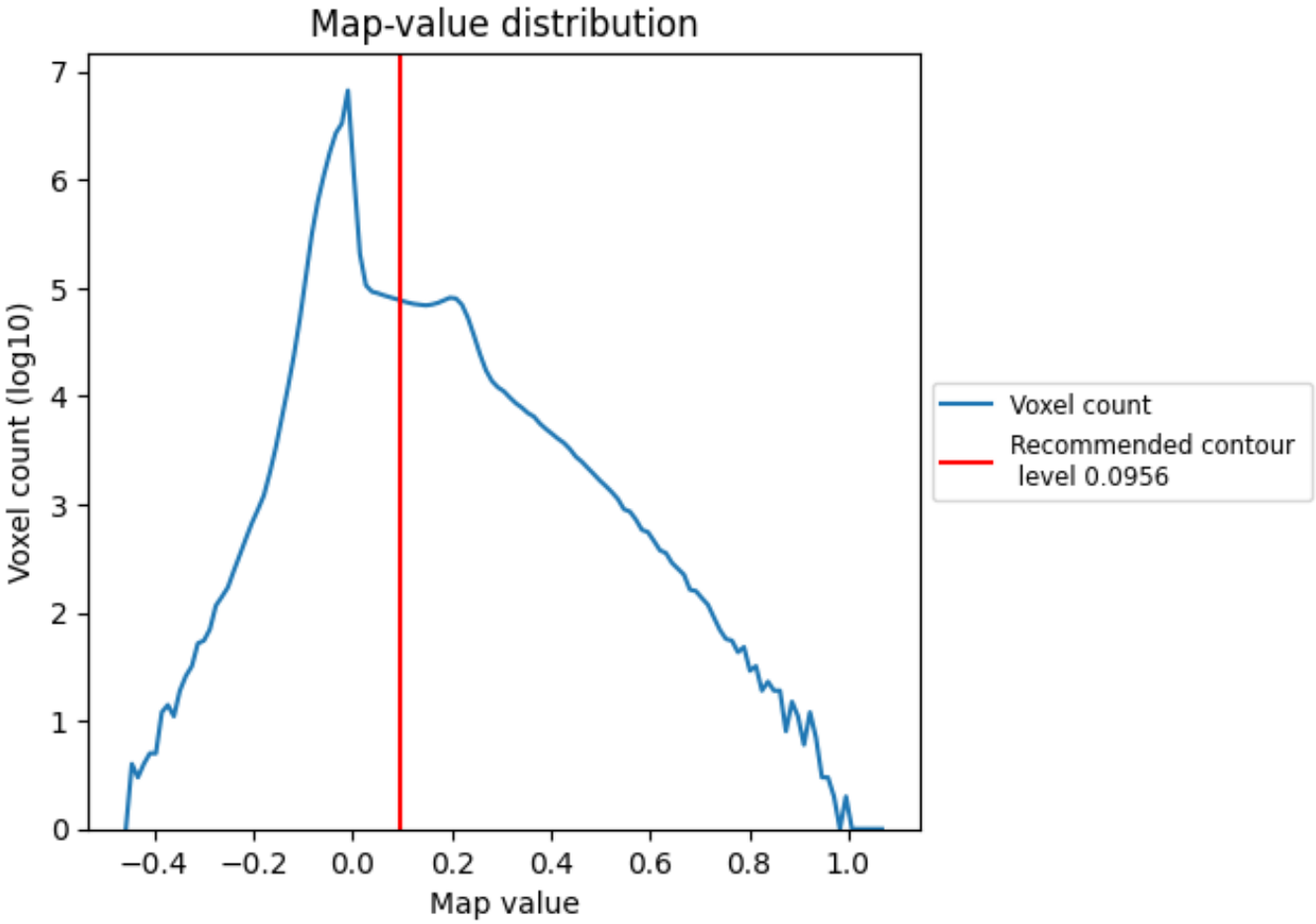
6.5 Mask visualisation (i)

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

7 Map analysis

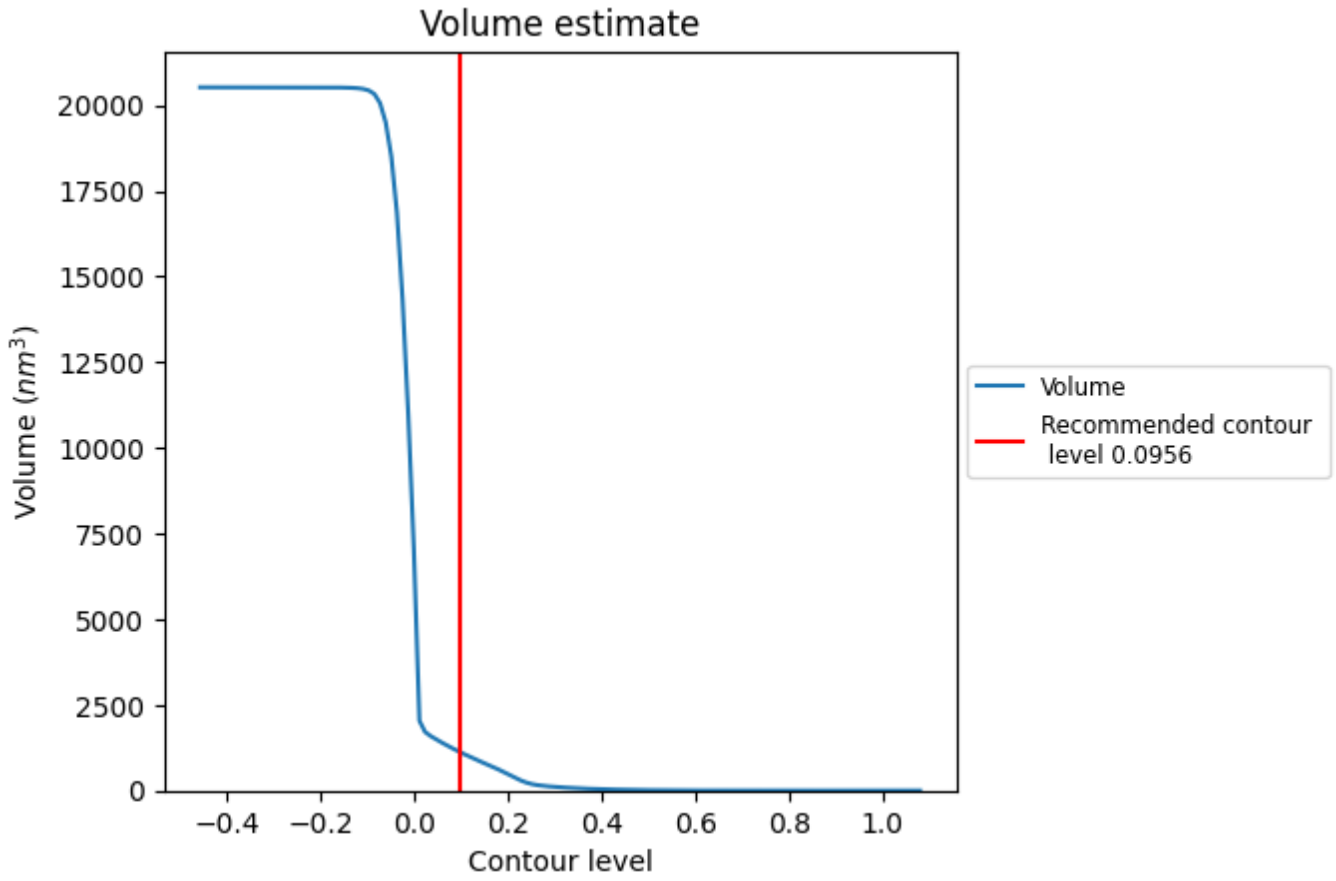
This section contains the results of statistical analysis of the map.

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.

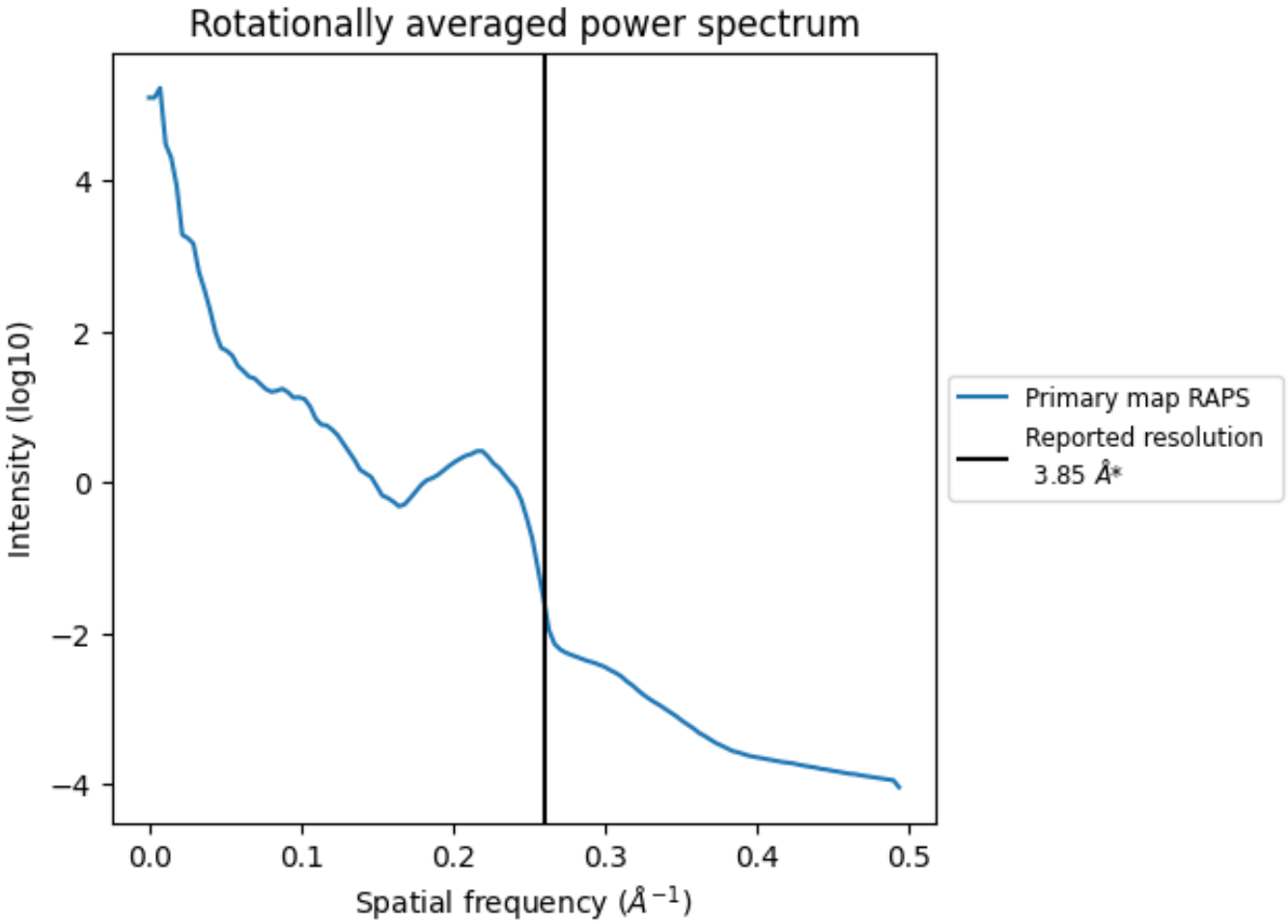
7.2 Volume estimate (i)



The volume at the recommended contour level is 1137 nm^3; this corresponds to an approximate mass of 1027 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 0.260 Å^{-1}

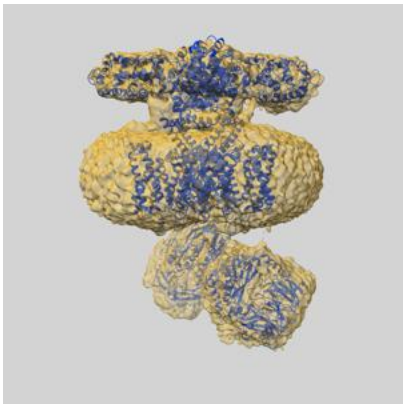
8 Fourier-Shell correlation

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

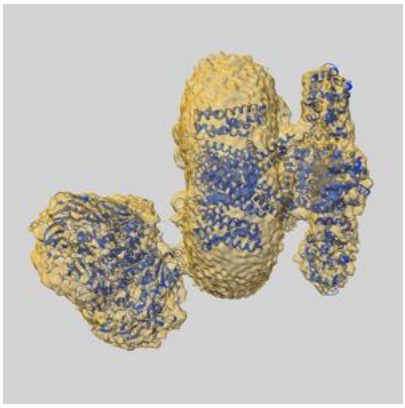
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32335 and PDB model 7W6T. Per-residue inclusion information can be found in section 3 on page 6.

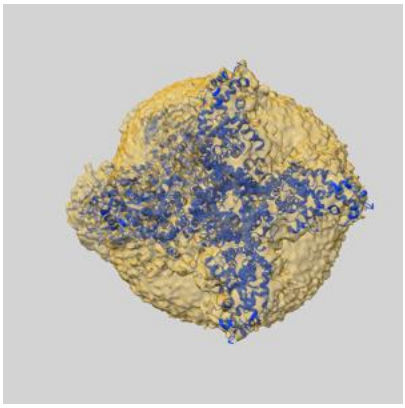
9.1 Map-model overlay



X



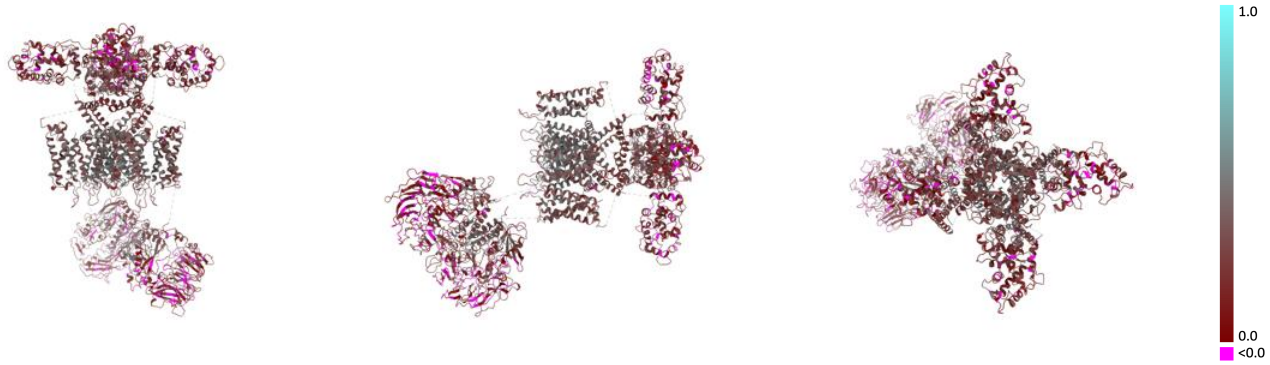
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0956 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.

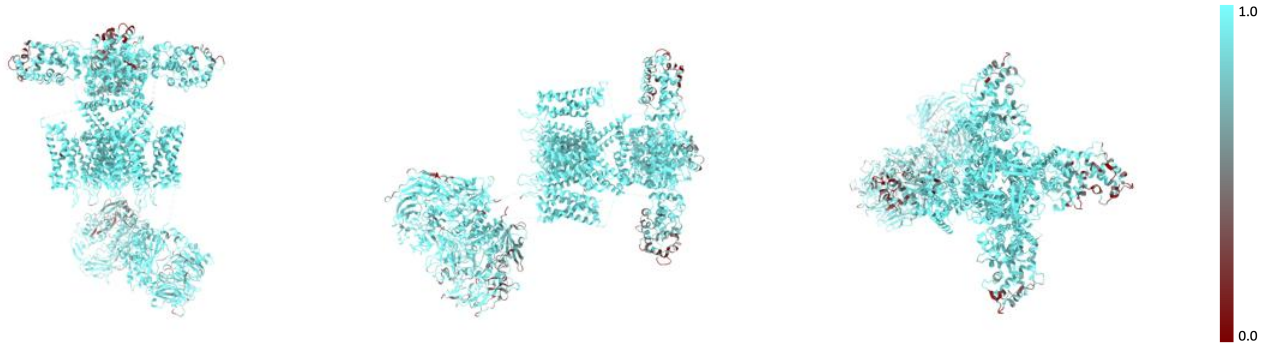
9.2 Q-score mapped to coordinate model (i)



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.

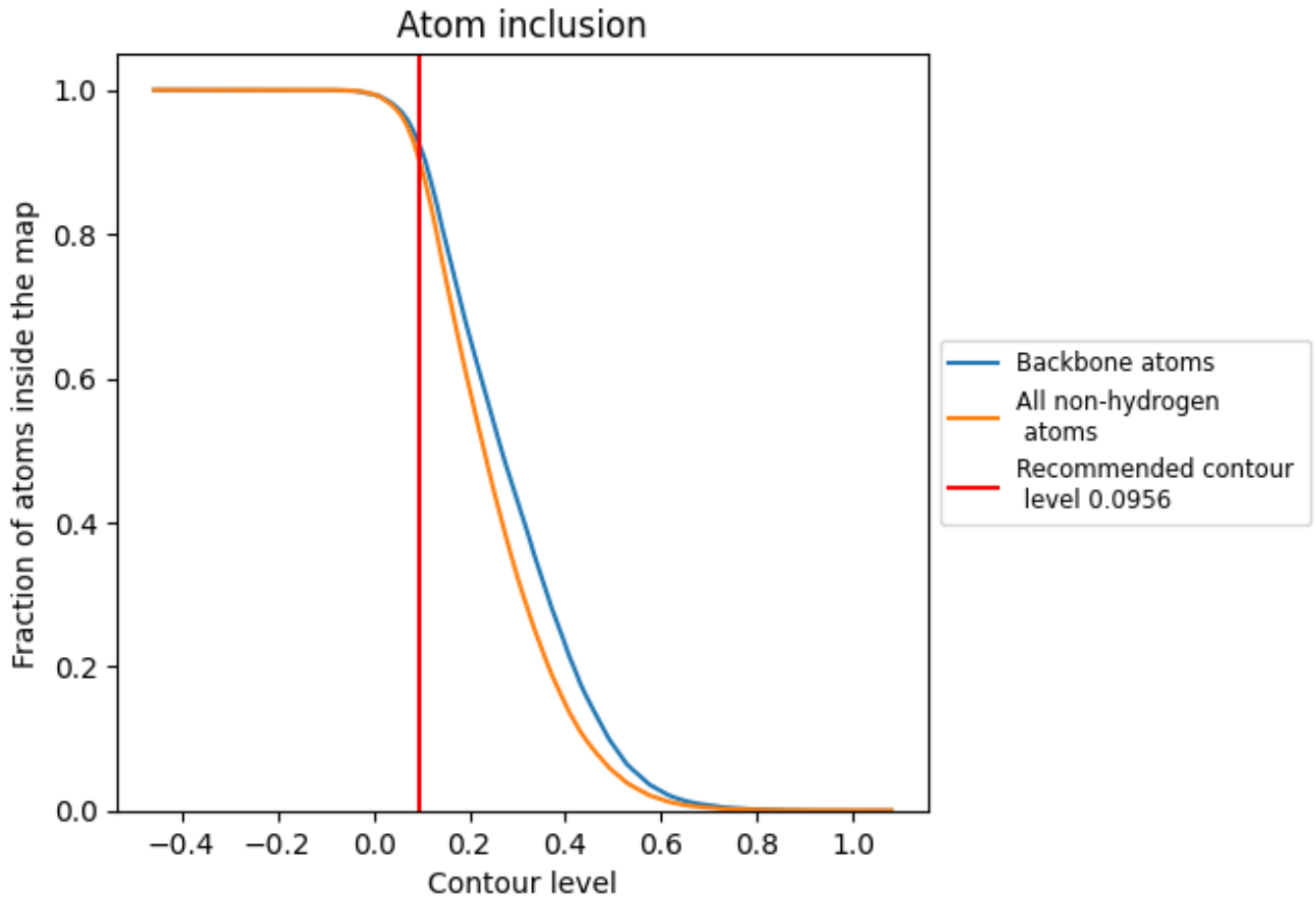
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0956).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 90% 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 (0.0956) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9024	0.2500
A	0.6921	0.1520
B	0.9769	0.3270
C	0.8609	0.1880
D	0.9795	0.3190
E	0.6777	0.1440
F	0.9739	0.3320
G	0.8017	0.1840
H	0.9772	0.3340
I	0.9329	0.1940
J	0.8440	0.2080