wwPDB EM Validation Summary Report (i)

Mar 20, 2024 – 12:01 PM JST

PDB ID	:	7C4J
EMDB ID	:	EMD-30285
Title	:	Cryo-EM structure of the yeast Swi/Snf complex in a nucleosome free state
Authors	:	Wang, C.C.; Guo, Z.Y.; Zhan, X.C.; Zhang, X.F.
Deposited on	:	2020-05-18
Resolution	:	2.89 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:

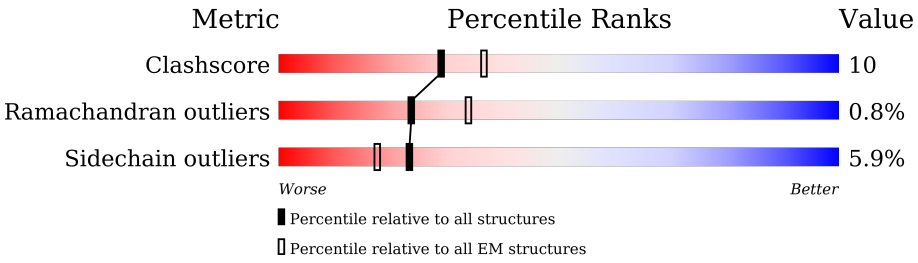
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.89 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	566	10% 51% 14% 34%
2	B	825	36% 11% 52%
2	D	825	5% 36% 14% 49%
3	C	332	10% 33% 11% 54%
4	E	623	32% 11% 54%
5	F	905	33% 9% 58%
6	H	1703	11% 86%
7	I	1314	33% 7% 60%

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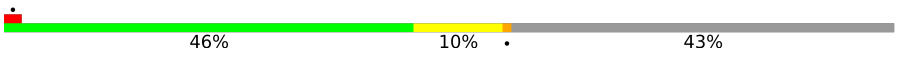
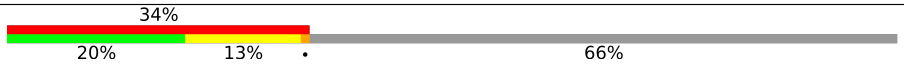
Mol	Chain	Length	Quality of chain
8	G	82	
9	J	157	
10	K	477	
11	L	467	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 29757 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 Transcription regulatory protein SNF12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	374	3048	1928	529	581	10	0	0

- Molecule 2 is a protein called SWI/SNF complex subunit SWI3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	395	3250	2082	560	597	11	0	0
2	D	421	3445	2203	592	638	12	0	0

- Molecule 3 is a protein called Transcription regulatory protein SNF6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	154	1266	793	232	236	5	0	0

- Molecule 4 is a protein called SWI/SNF global transcription activator complex subunit SWP82.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	288	2355	1529	412	411	3	0	0

- Molecule 5 is a protein called SWI/SNF chromatin-remodeling complex subunit SNF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	383	3134	1977	529	618	10	0	0

- Molecule 6 is a protein called Transcription regulatory protein SNF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	242	Total	C	N	O	S	0	0
			1966	1233	354	373	6		

- Molecule 7 is a protein called SWI/SNF chromatin-remodeling complex subunit SWI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	524	Total	C	N	O	S	0	0
			4242	2754	703	774	11		

- Molecule 8 is a protein called Unkown.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	G	47	Total	C	N	O	0	0
			271	166	56	49		

- Molecule 9 is a protein called Regulator of Ty1 transposition protein 102.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	53	Total	C	N	O	0	0
			482	308	83	91		

- Molecule 10 is a protein called Actin-related protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	387	Total	C	N	O	S	3	0
			3131	2020	516	591	4		

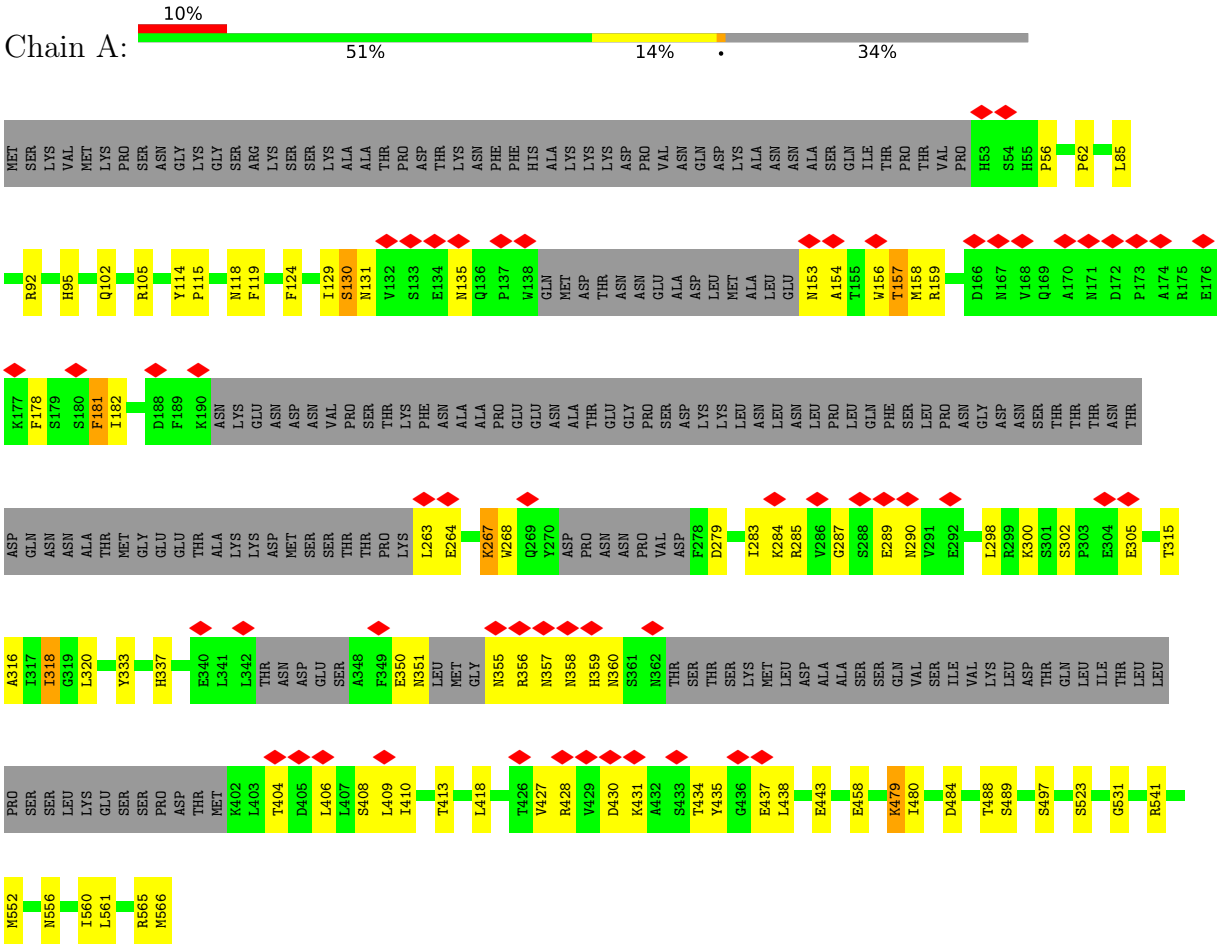
- Molecule 11 is a protein called Actin-like protein ARP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	392	Total	C	N	O	S	1	0
			3167	2033	519	611	4		

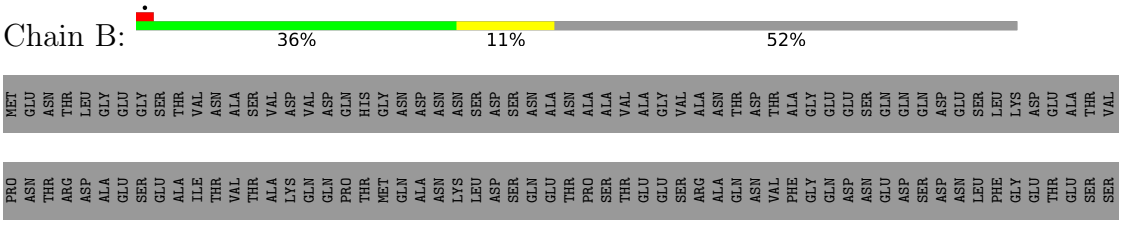
3 Residue-property plots (i)

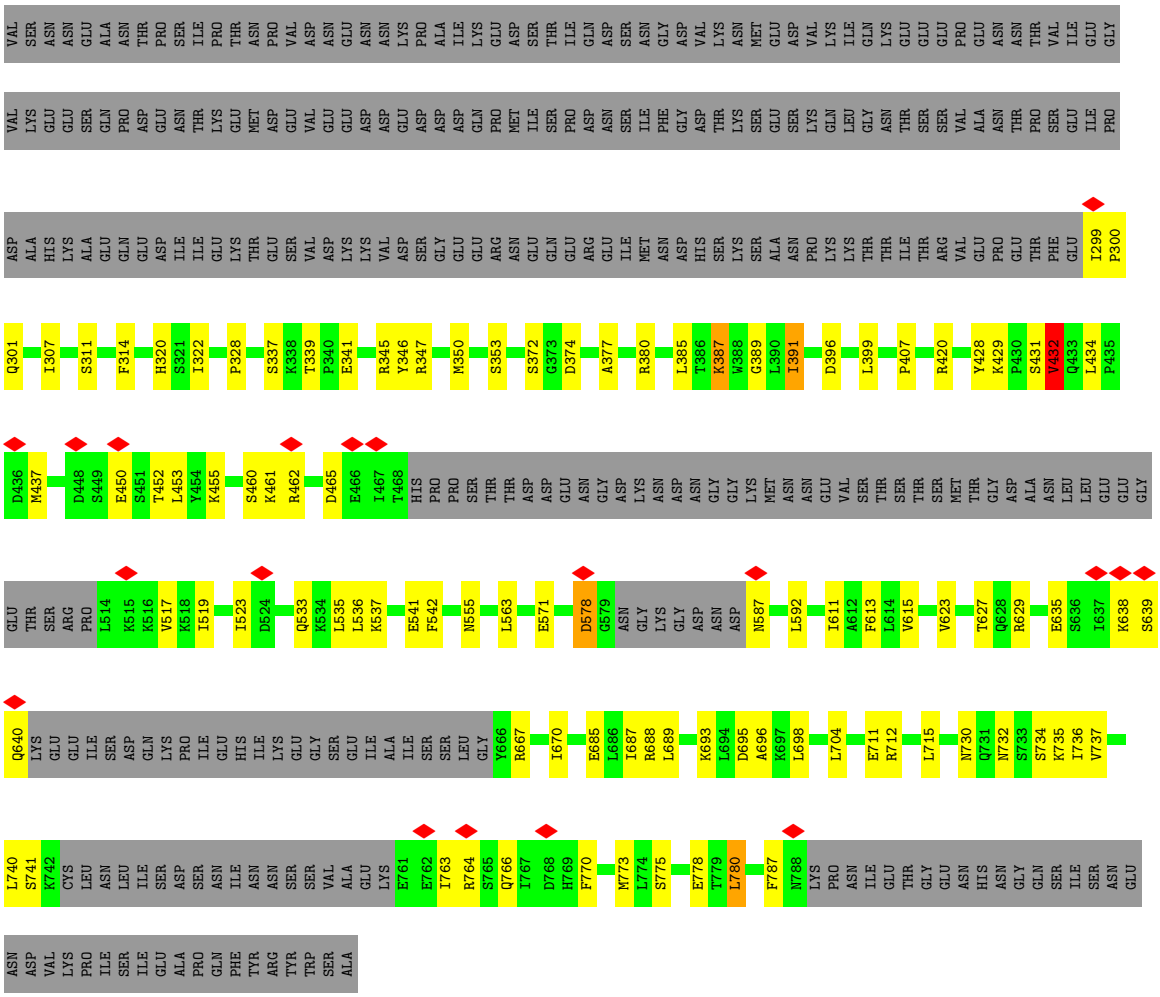
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Transcription regulatory protein SNF12



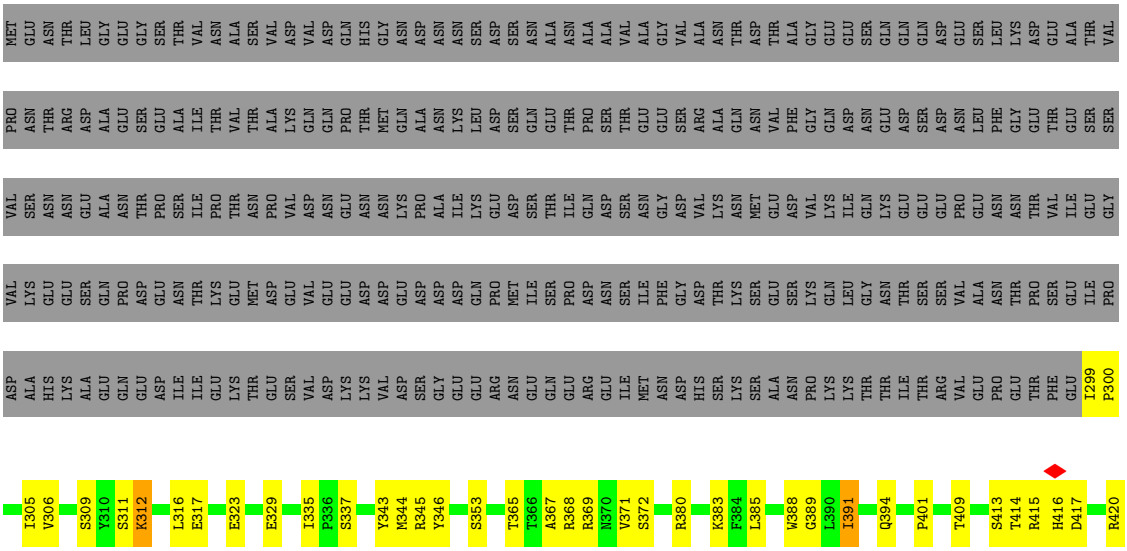
• Molecule 2: SWI/SNF complex subunit SWI3

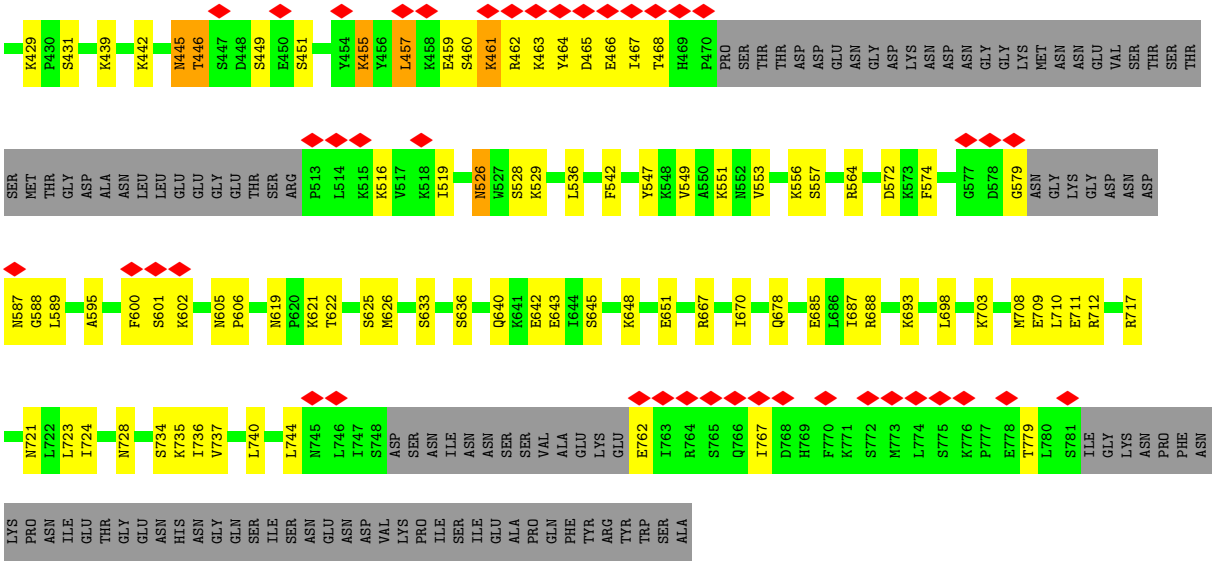




• Molecule 2: SWI/SNF complex subunit SWI3

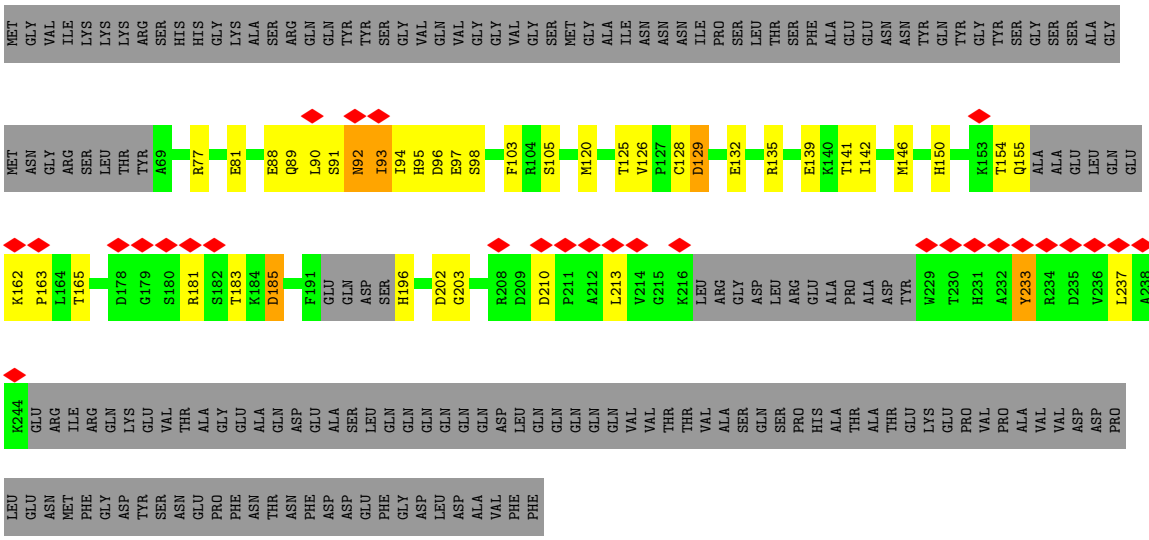
Chain D:





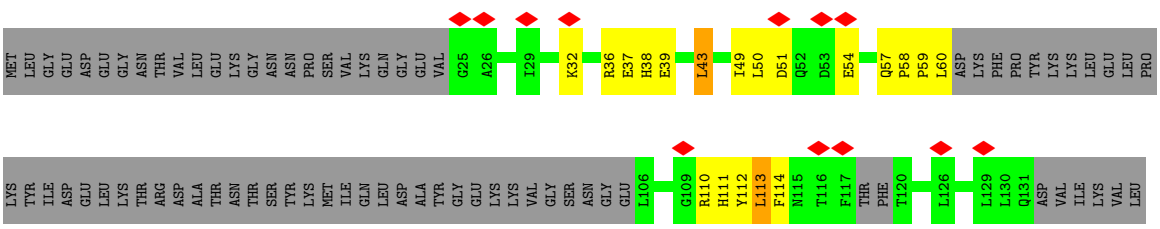
• Molecule 3: Transcription regulatory protein SNF6

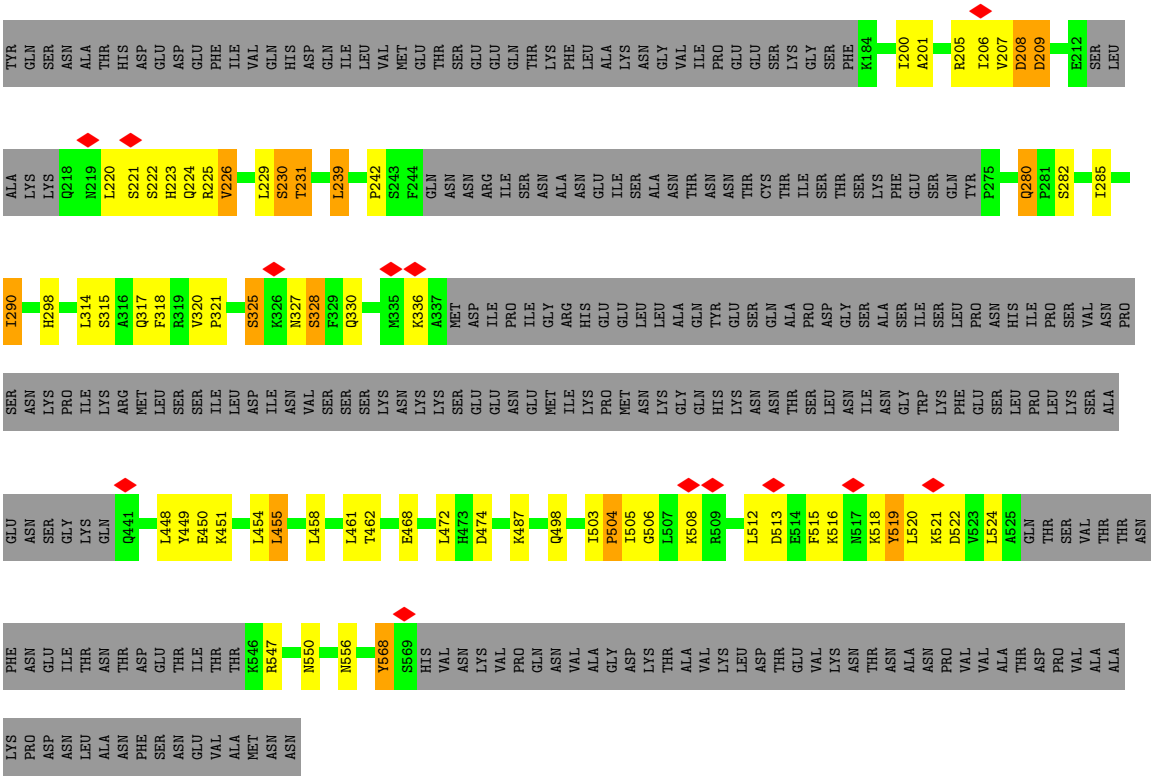
Chain C:



• Molecule 4: SWI/SNF global transcription activator complex subunit SWP82

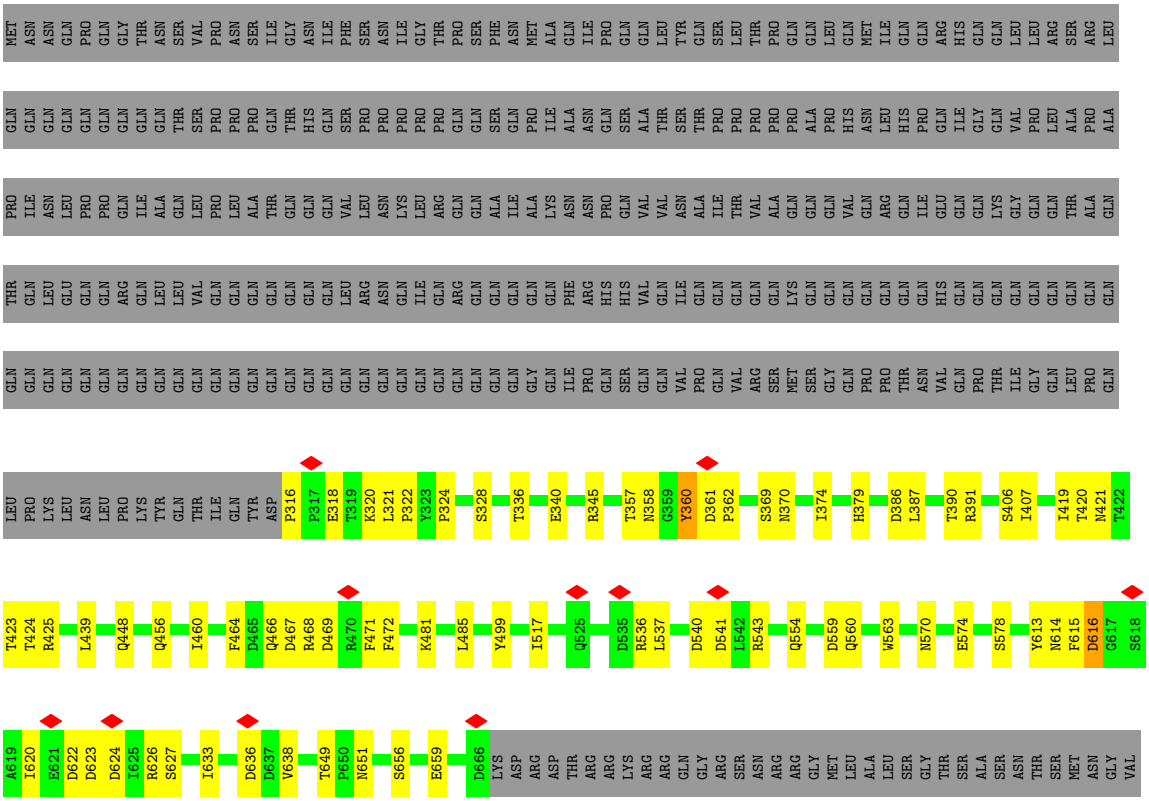
Chain E:

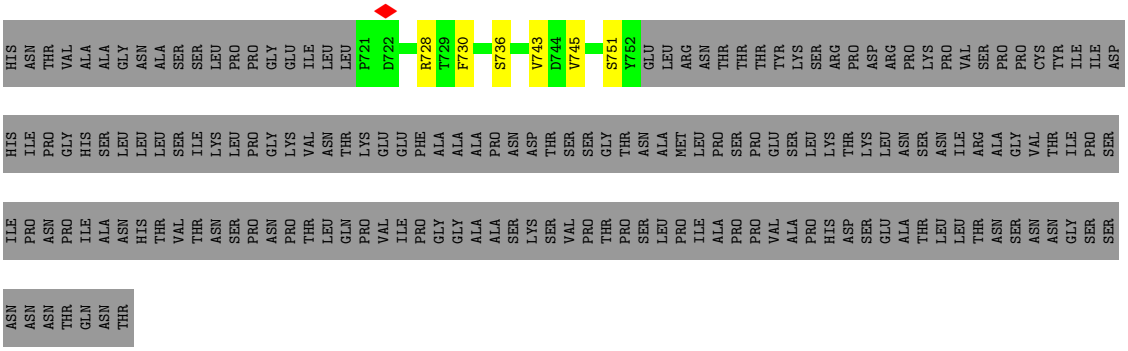




• Molecule 5: SWI/SNF chromatin-remodeling complex subunit SNF5

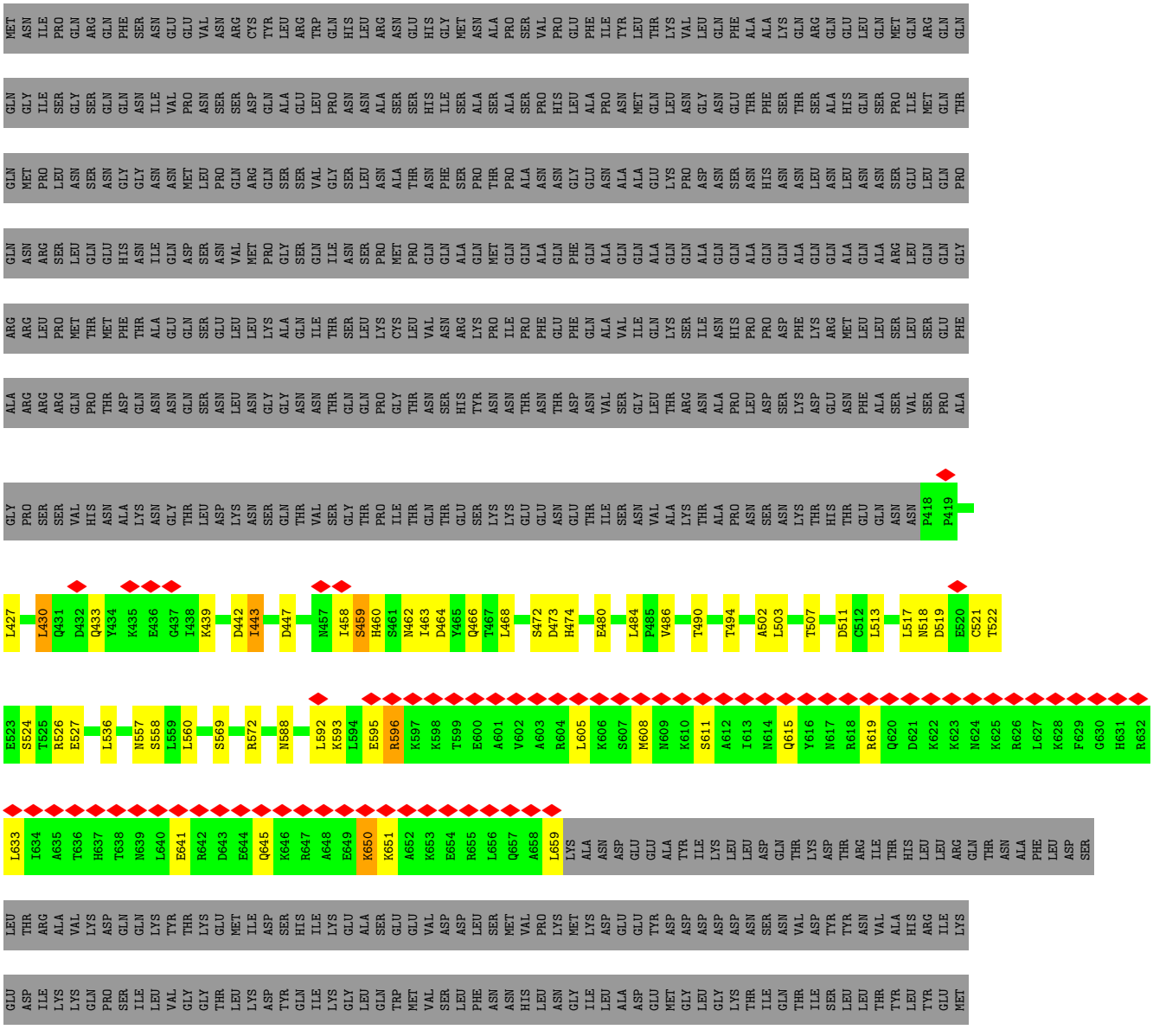
Chain F:

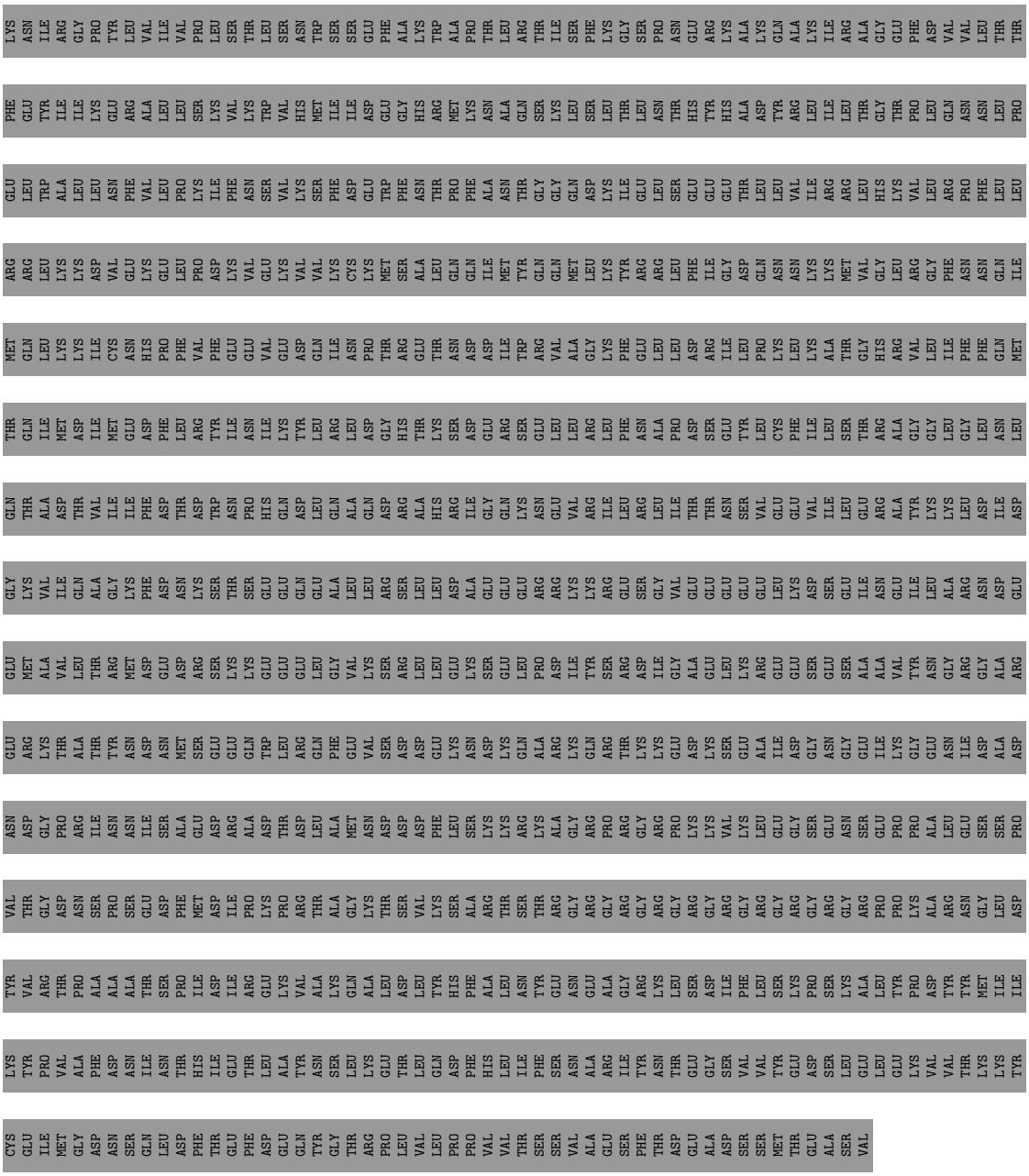




• Molecule 6: Transcription regulatory protein SNF2

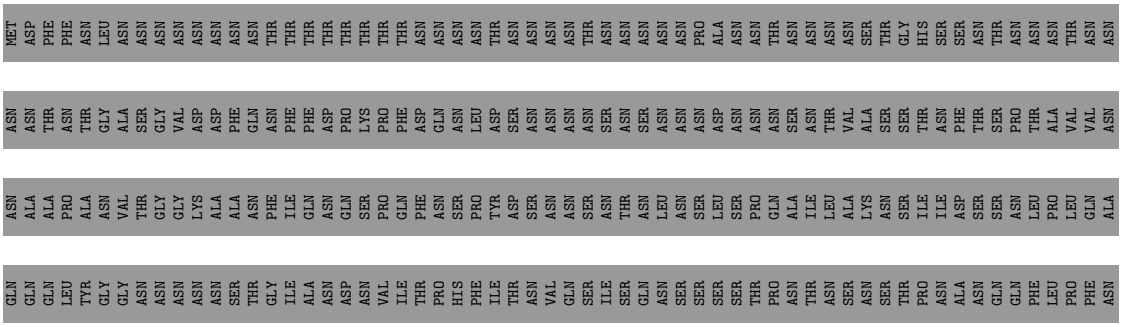
Chain H:

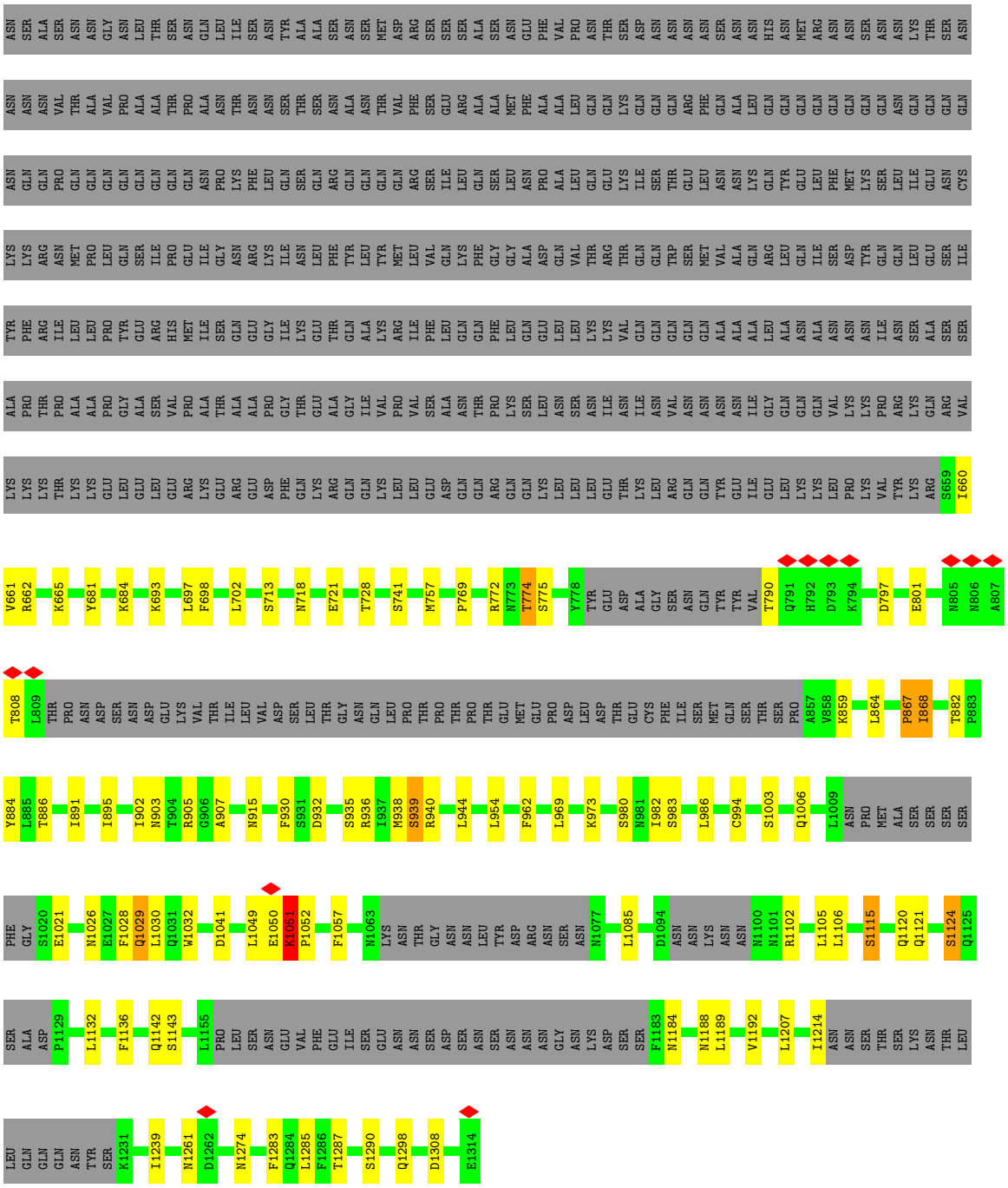




• Molecule 7: SWI/SNF chromatin-remodeling complex subunit SWI1

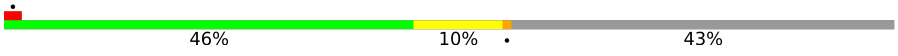
Chain I:

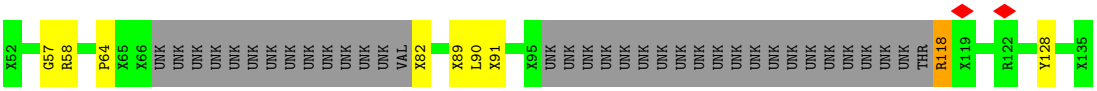




• Molecule 8: Unkown

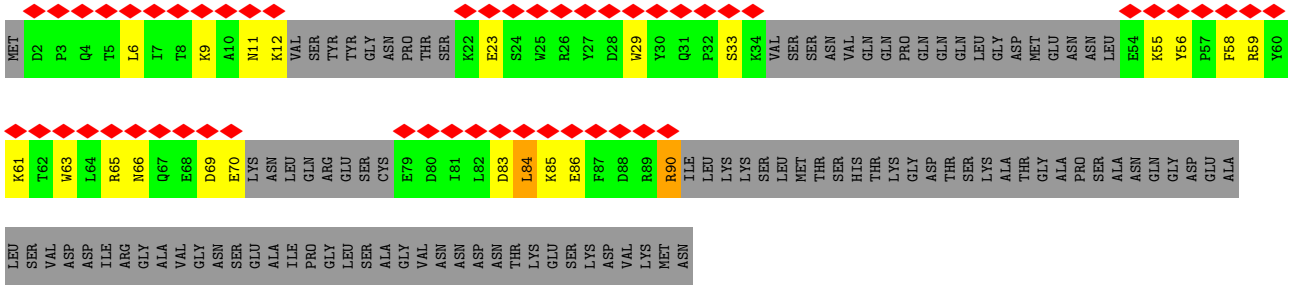
Chain G:





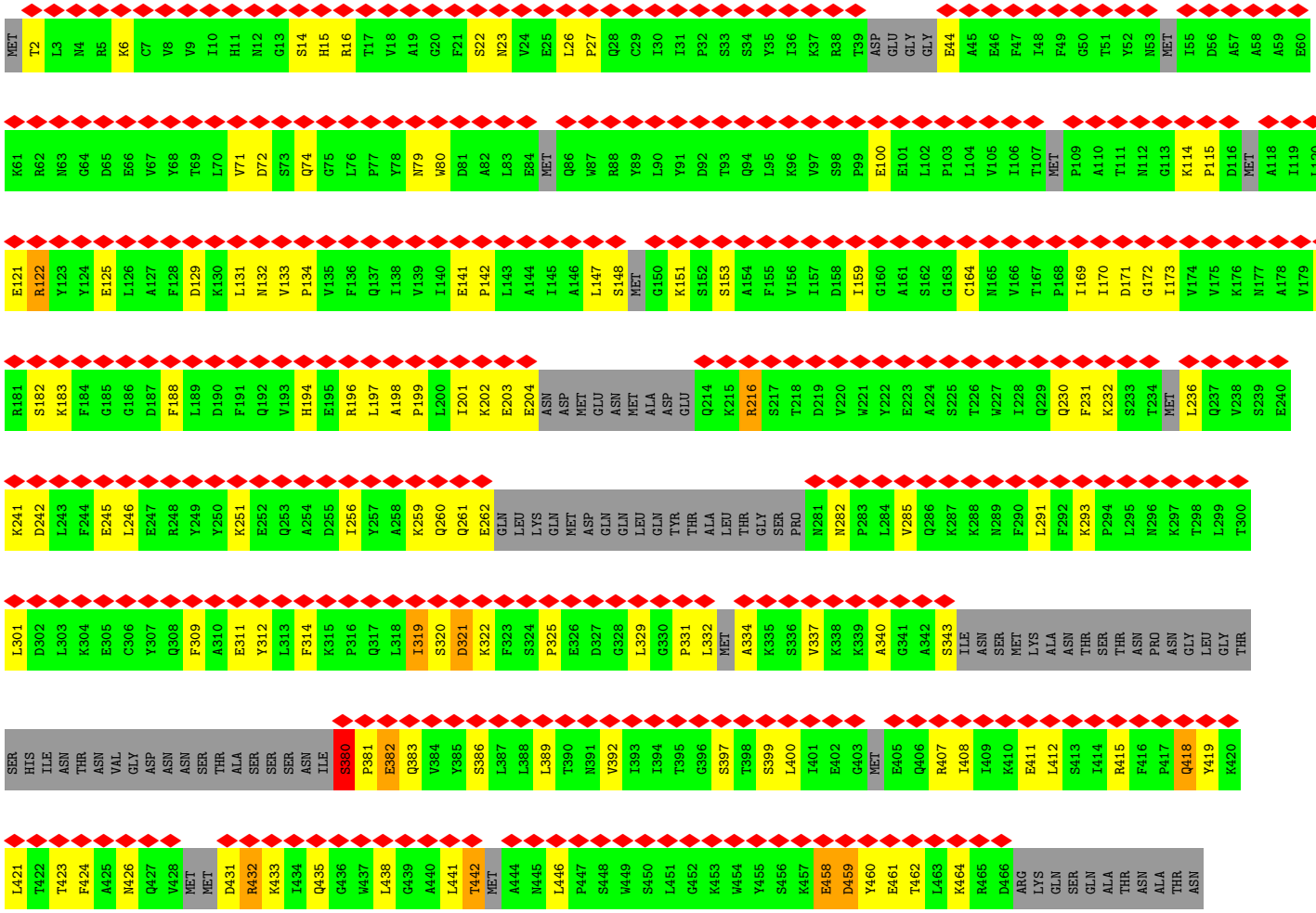
• Molecule 9: Regulator of Ty1 transposition protein 102

Chain J:



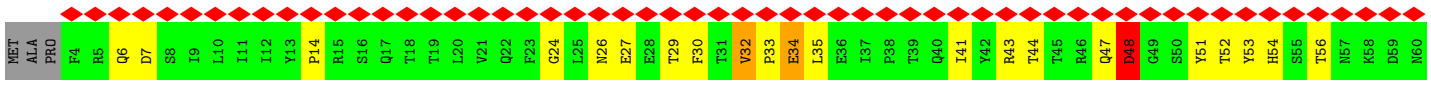
• Molecule 10: Actin-related protein 7

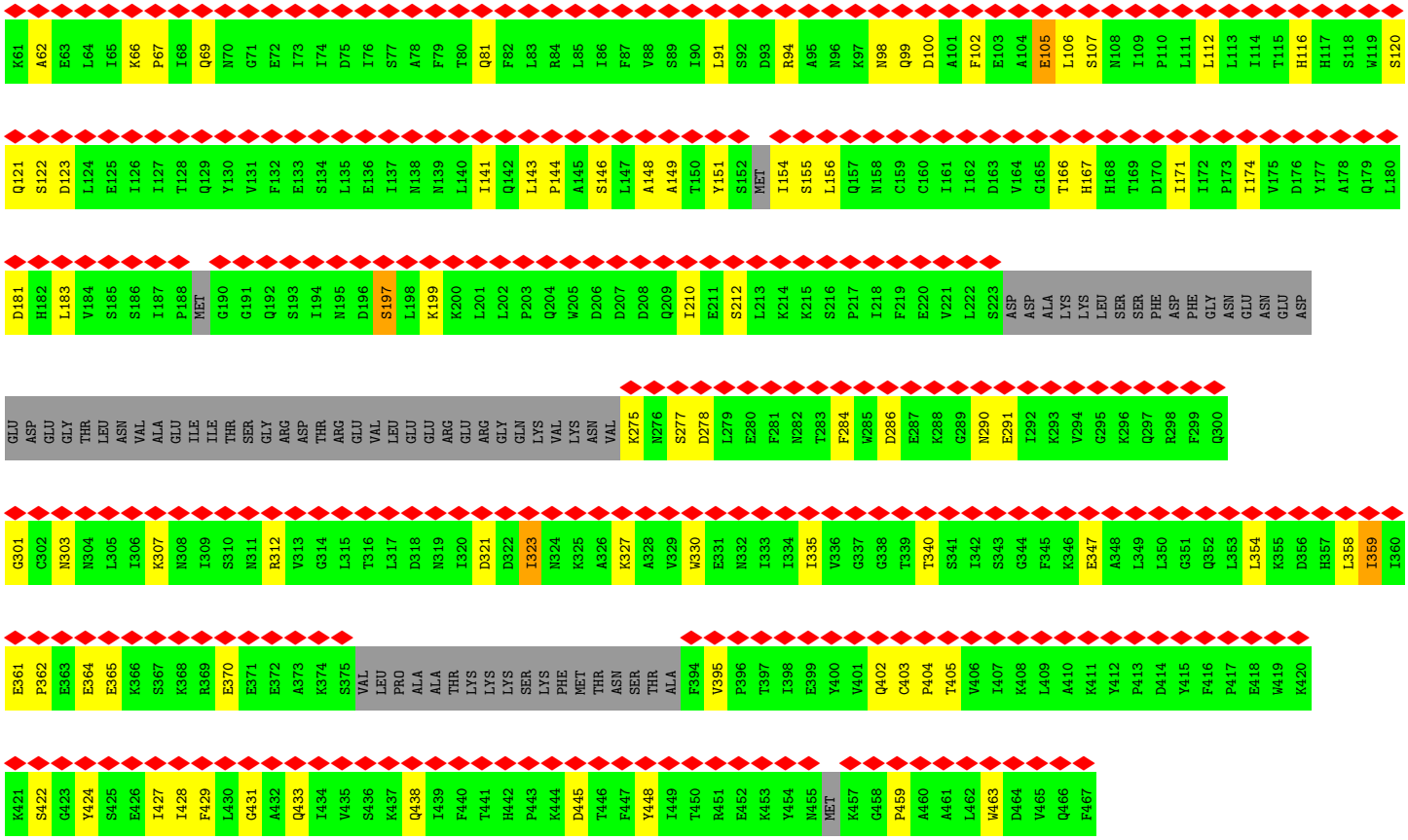
Chain K:



• Molecule 11: Actin-like protein ARP9

Chain L:




K61 A62 E63 L64 I65 K66 P67 I68 Q69 N70 G71 E72 I73 I74 D75 I76 S77 A78 F79 T80 Q81 F82 L83 R84 L85 I86 F87 V88 S89 I90 L91 S92 D93 R94 A95 N96 K97 N98 Q99 D100 A101 F102 E103 A104 E105 L106 S107 N108 I109 P110 L111 L112 L113 I114 T115 H116 H117 S118 W119 S120
Q121 S122 D123 L124 E125 I126 I127 T128 Q129 Y130 V131 F132 E133 S134 L135 E136 I137 N138 N139 L140 I141 Q142 L143 P144 A145 S146 L147 A148 A149 T150 Y151 S152 MET I154 S155 L156 Q157 N158 C159 C160 I161 I162 D163 V164 G165 T166 H167 H168 T169 D170 I171 I172 P173 I174 V175 D176 Y177 A178 Q179 L180
D181 H182 L183 V184 S185 S186 I187 P188 MET G190 G191 Q192 S193 I194 N195 D196 S197 L198 K199 K200 L201 L202 P203 Q204 W205 D206 D207 D208 Q209 I210 E211 S212 L213 K214 K215 S216 P217 I218 F219 E220 V221 L222 S223 ASP ASP ALA LYS LYS LEU SER SER PHE ASP PHE GLY ASN GLU ASN GLU ASP
GLU ASP GLU GLY THR LEU ASN VAL ALA GLU ILE ILE THR SER GLY ARG ASP THR ARG GLU VAL LEU GLU GLU ARG GLU ARG GLY GLN LYS VAL LYS ASN VAL K275 N276 S277 D278 L279 E280 F281 N282 T283 F284 W285 D286 E287 K288 G289 N290 E291 I292 K293 V294 G295 K296 Q297 R298 F299 Q300
G301 C302 N303 N304 L305 I306 K307 N308 I309 S310 N311 R312 V313 G314 L315 T316 L317 D318 N319 I320 D321 D322 I323 N324 K325 A326 K327 A328 V329 W330 E331 N332 I333 I334 I335 V336 G337 G338 T339 T340 S341 I342 S343 G344 F345 K346 E347 A348 L349 L350 G351 Q352 L353 L354 K355 D356 H357 L358 I359 I360
E361 P362 E363 E364 E365 K366 S367 K368 R369 E370 E371 E372 A373 K374 S375 VAL LEU PRO ALA ALA THR LYS LYS LYS SER LYS PHE MET THR ASN SER THR ALA F394 V395 P396 T397 I398 E399 Y400 V401 Q402 C403 P404 T405 V406 I407 K408 L409 A410 K411 Y412 P413 D414 Y415 F416 P417 E418 W419 K420
K421 S422 G423 Y424 S425 E426 I427 I428 F429 L430 G431 A432 Q433 I434 V435 S436 K437 Q438 I439 F440 T441 H442 P443 K444 D445 T446 F447 Y448 I449 T450 R451 E452 K453 Y454 N455 MET K457 G458 P459 A460 A461 L462 W463 D464 V465 Q466 F467

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	386469	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.094	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	347.84, 347.84, 347.84	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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	0.33	0/3104	0.44	0/4188
2	B	0.37	0/3318	0.47	0/4465
2	D	0.39	0/3517	0.47	0/4735
3	C	0.34	0/1287	0.46	0/1729
4	E	0.37	0/2404	0.50	1/3237 (0.0%)
5	F	0.39	0/3201	0.51	0/4336
6	H	0.39	0/2000	0.52	0/2706
7	I	0.38	0/4316	0.48	0/5843
8	G	0.38	0/101	0.59	0/123
9	J	0.41	0/493	0.58	0/659
10	K	0.44	0/3197	0.61	1/4313 (0.0%)
11	L	0.45	0/3234	0.59	0/4382
All	All	0.39	0/30172	0.51	2/40716 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	K	380	SER	C-N-CD	5.92	140.84	128.40
4	E	461	LEU	C-N-CA	5.82	136.25	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3048	0	3012	56	0
2	B	3250	0	3302	74	0
2	D	3445	0	3505	86	0
3	C	1266	0	1264	36	0
4	E	2355	0	2416	67	0
5	F	3134	0	3045	54	0
6	H	1966	0	1991	61	0
7	I	4242	0	4401	72	0
8	G	271	0	129	10	0
9	J	482	0	455	19	0
10	K	3131	0	3132	108	0
11	L	3167	0	3149	87	0
All	All	29757	0	29801	613	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 613 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)
7:I:1051:LYS:HB3	7:I:1052:PRO:CD	1.70	1.19
11:L:403:CYS:SG	11:L:404:PRO:HD3	1.89	1.11
7:I:1051:LYS:HE2	7:I:1051:LYS:HA	1.17	1.08
10:K:216:ARG:HG2	10:K:216:ARG:HH11	1.17	1.07
11:L:359:ILE:HD11	11:L:404:PRO:HG2	1.34	1.07

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	360/566 (64%)	344 (96%)	15 (4%)	1 (0%)	41 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	385/825 (47%)	361 (94%)	21 (6%)	3 (1%)	19 51
2	D	413/825 (50%)	383 (93%)	27 (6%)	3 (1%)	22 54
3	C	146/332 (44%)	134 (92%)	10 (7%)	2 (1%)	11 36
4	E	272/623 (44%)	245 (90%)	24 (9%)	3 (1%)	14 42
5	F	379/905 (42%)	333 (88%)	43 (11%)	3 (1%)	19 51
6	H	240/1703 (14%)	230 (96%)	9 (4%)	1 (0%)	34 66
7	I	506/1314 (38%)	486 (96%)	15 (3%)	5 (1%)	15 45
8	G	13/82 (16%)	12 (92%)	1 (8%)	0	100 100
9	J	45/157 (29%)	42 (93%)	2 (4%)	1 (2%)	6 24
10	K	360/477 (76%)	340 (94%)	17 (5%)	3 (1%)	19 51
11	L	381/467 (82%)	360 (94%)	19 (5%)	2 (0%)	29 61
All	All	3500/8276 (42%)	3270 (93%)	203 (6%)	27 (1%)	24 51

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	431	SER
2	B	432	VAL
4	E	208	ASP
5	F	358	ASN
7	I	867	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	345/517 (67%)	325 (94%)	20 (6%)	20 50
2	B	368/751 (49%)	346 (94%)	22 (6%)	19 49
2	D	392/751 (52%)	367 (94%)	25 (6%)	17 45
3	C	141/288 (49%)	133 (94%)	8 (6%)	20 51
4	E	257/558 (46%)	233 (91%)	24 (9%)	9 27

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	F	351/823 (43%)	334 (95%)	17 (5%)	25 58
6	H	222/1520 (15%)	206 (93%)	16 (7%)	14 39
7	I	500/1218 (41%)	479 (96%)	21 (4%)	30 63
8	G	7/15 (47%)	6 (86%)	1 (14%)	3 10
9	J	52/140 (37%)	51 (98%)	1 (2%)	57 84
10	K	345/420 (82%)	326 (94%)	19 (6%)	21 53
11	L	359/423 (85%)	337 (94%)	22 (6%)	18 48
All	All	3339/7424 (45%)	3143 (94%)	196 (6%)	23 49

5 of 196 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	743	VAL
7	I	1051	LYS
6	H	447	ASP
6	H	651	LYS
7	I	1207	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	690	GLN
11	L	304	ASN
5	F	434	ASN
11	L	303	ASN
7	I	1006	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

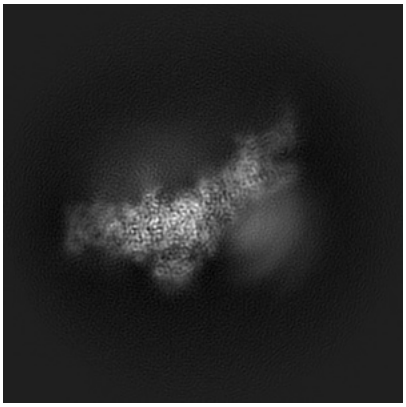
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30285. These allow visual inspection of the internal detail of the map and identification of artifacts.

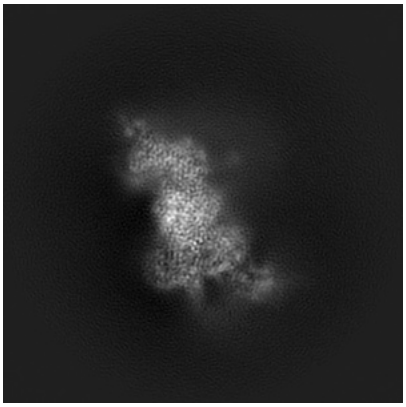
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

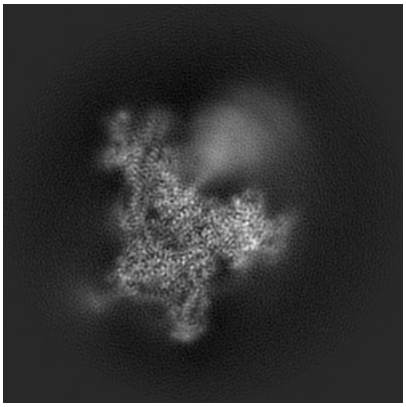
6.1.1 Primary map



X



Y

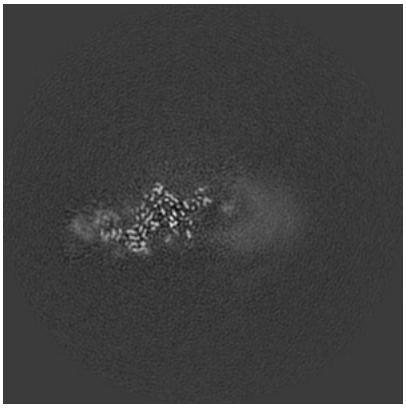


Z

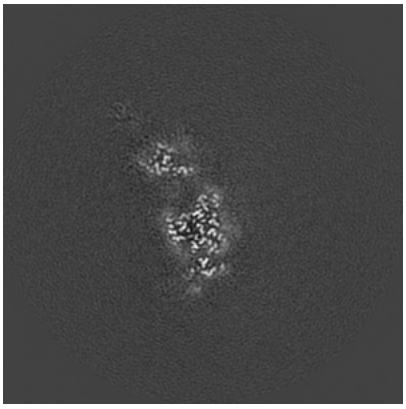
The images above show the map projected in three orthogonal directions.

6.2 Central slices

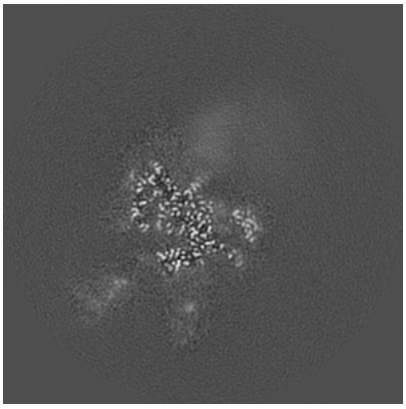
6.2.1 Primary map



X Index: 160



Y Index: 160

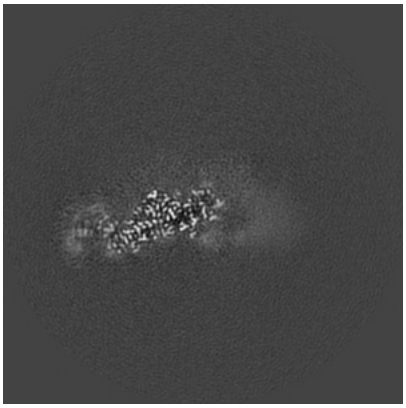


Z Index: 160

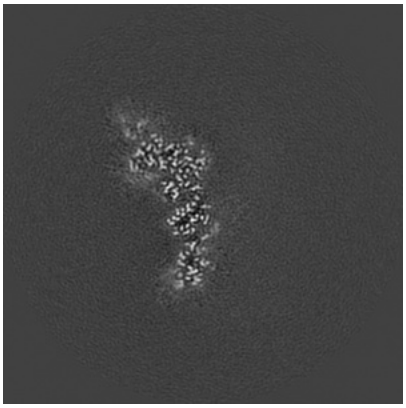
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

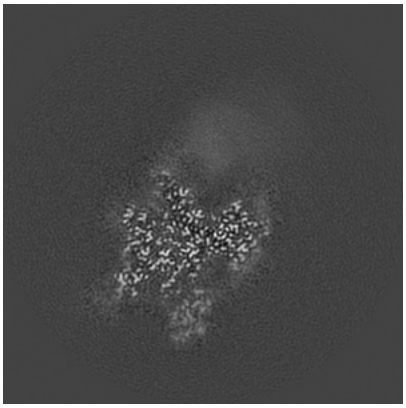
6.3.1 Primary map



X Index: 152



Y Index: 143

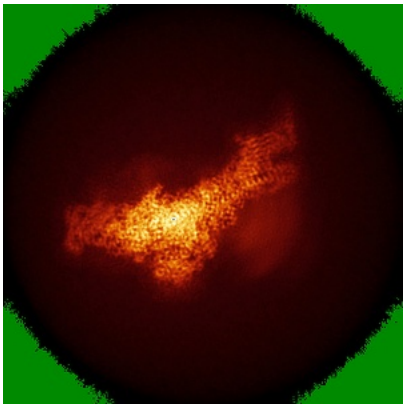


Z Index: 146

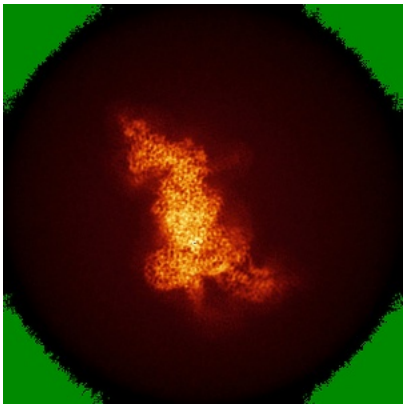
The images above show the largest variance slices of the map in three orthogonal directions.

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

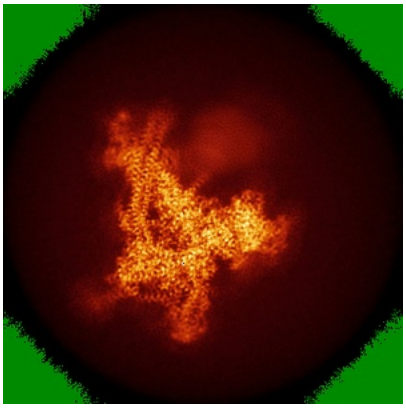
6.4.1 Primary map



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

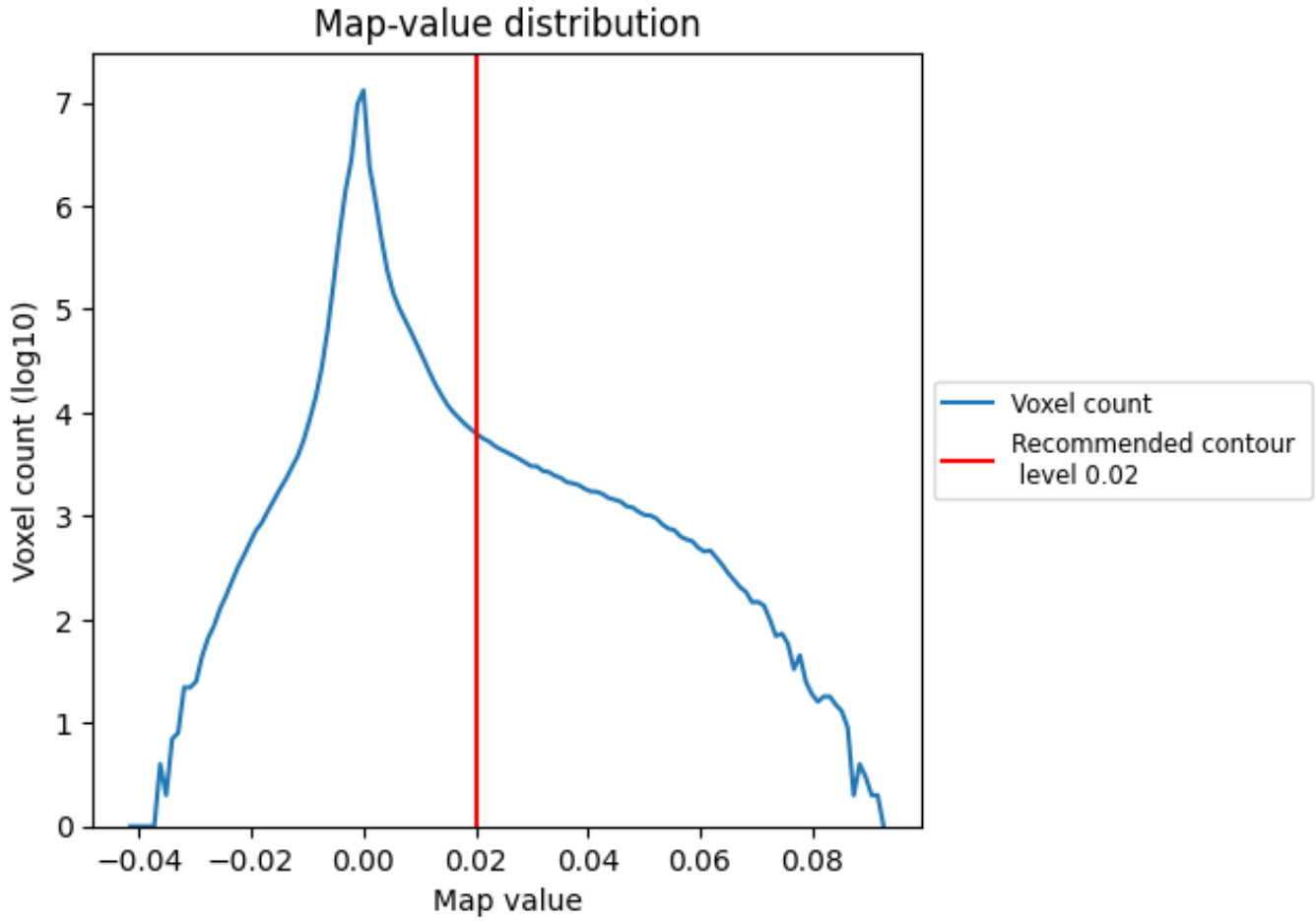
6.6 Mask visualisation (i)

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

7 Map analysis

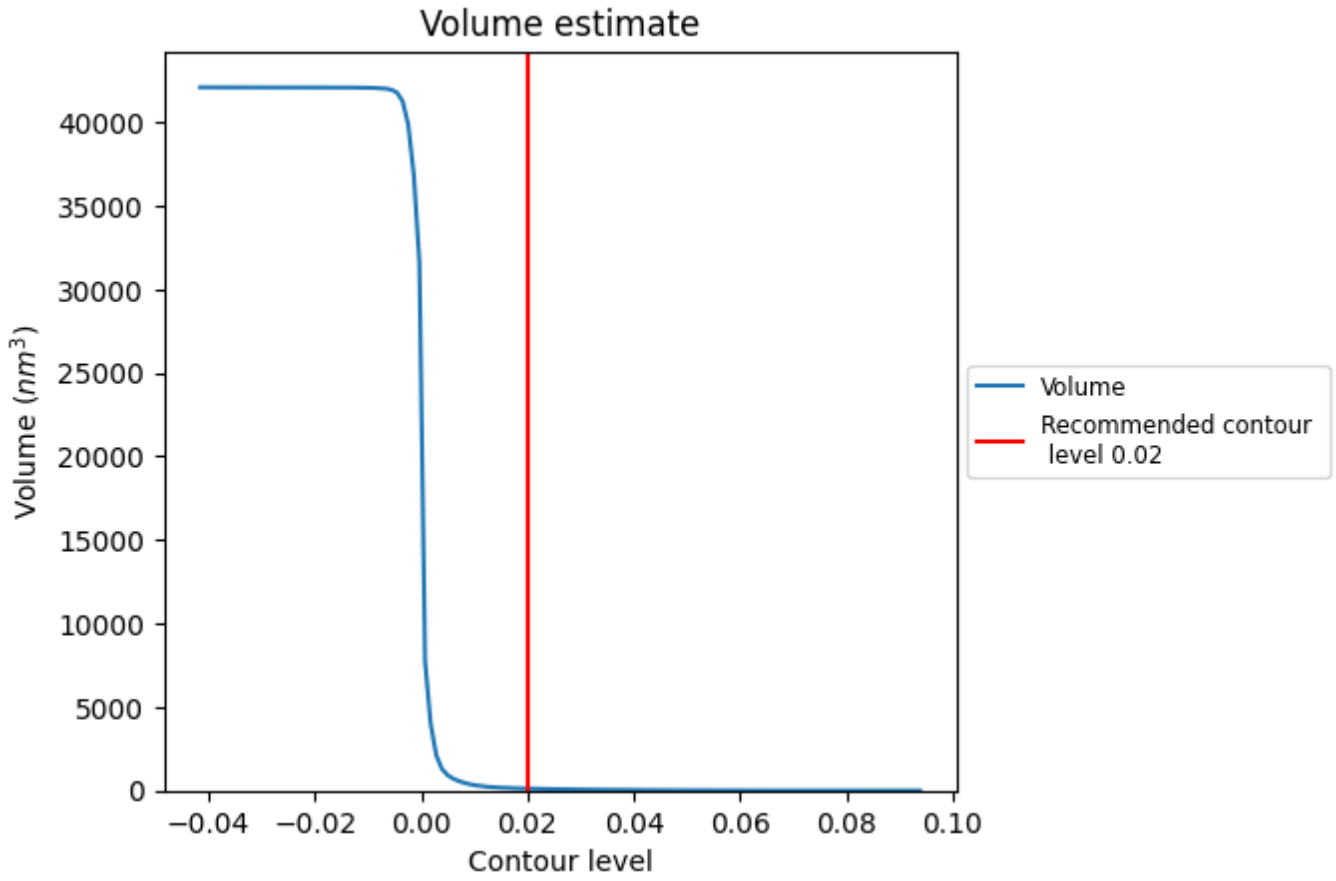
This section contains the results of statistical analysis of the map.

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.

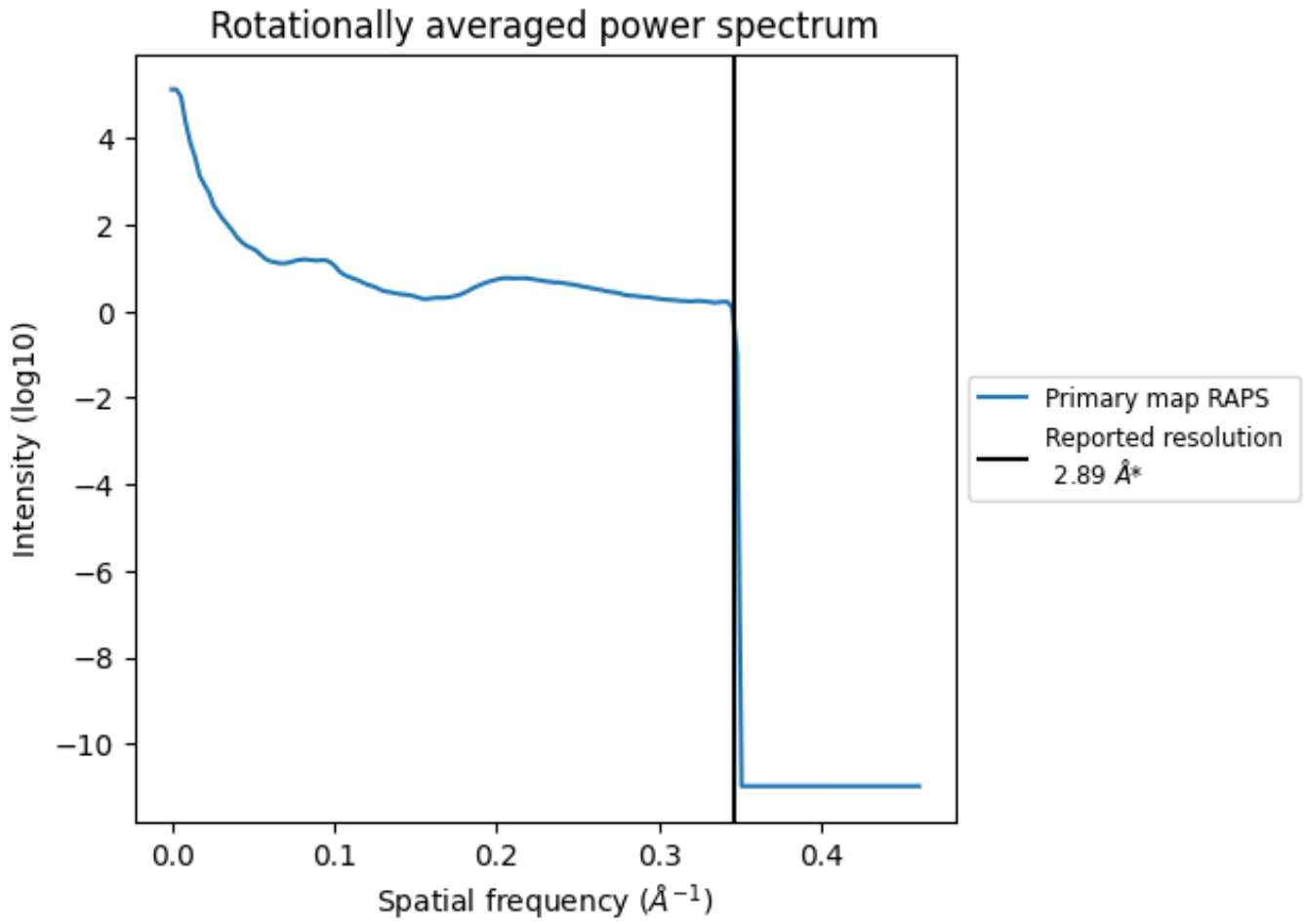
7.2 Volume estimate (i)



The volume at the recommended contour level is 117 nm^3; this corresponds to an approximate mass of 106 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 0.346 Å^{-1}

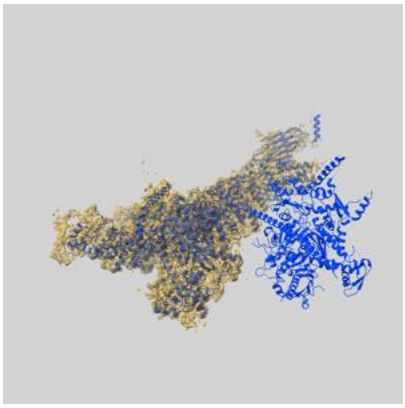
8 Fourier-Shell correlation (i)

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

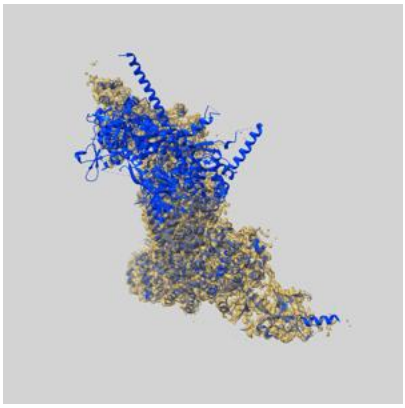
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30285 and PDB model 7C4J. Per-residue inclusion information can be found in section 3 on page 6.

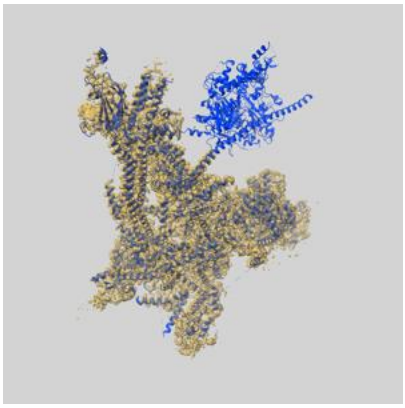
9.1 Map-model overlay



X



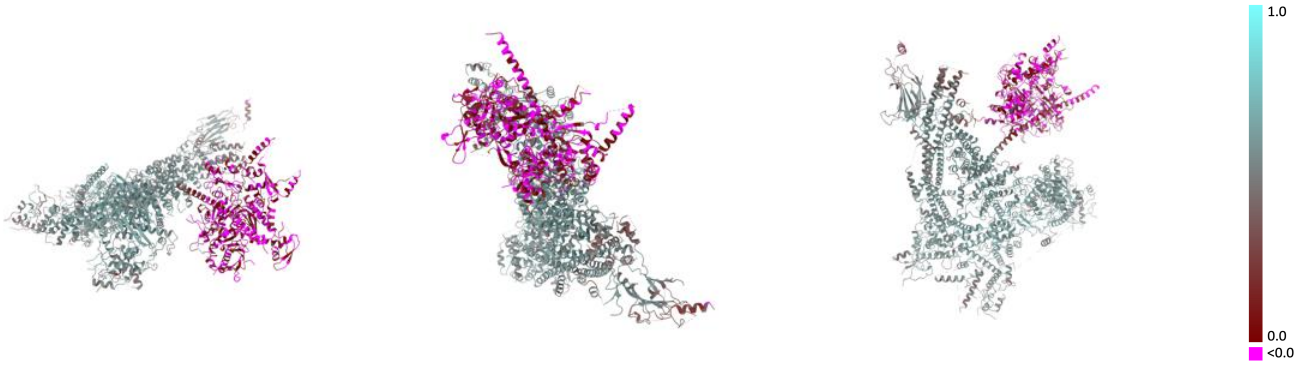
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

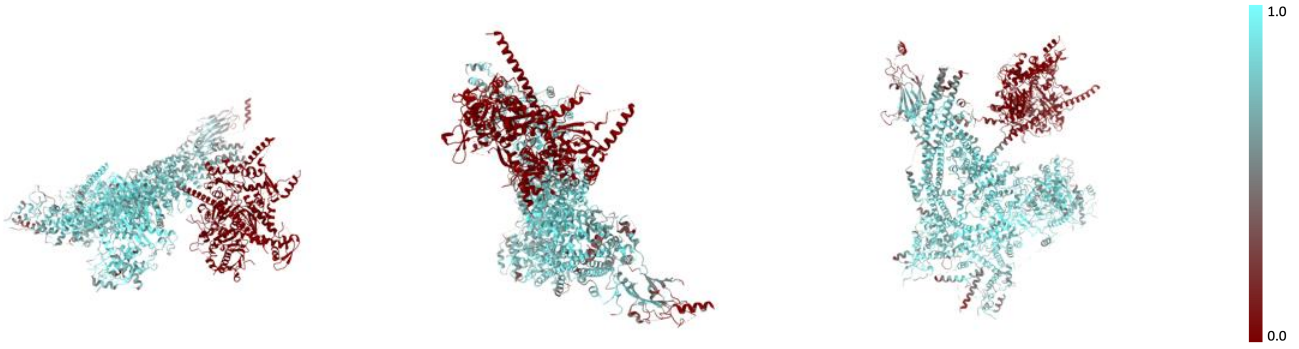
9.2 Q-score mapped to coordinate model



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.

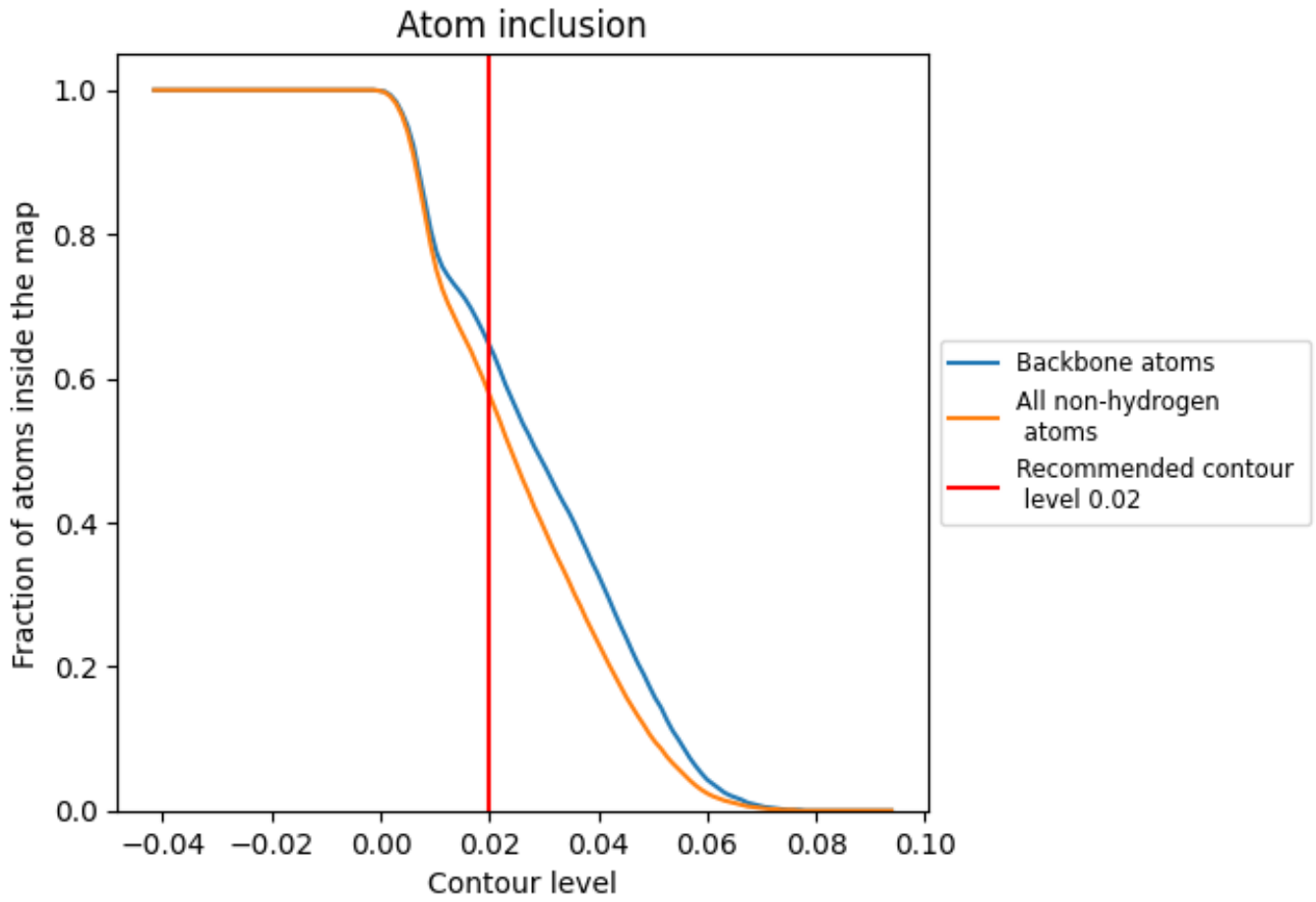
9.3 Atom inclusion mapped to coordinate model



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 58% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5770	0.4210
A	0.6750	0.5210
B	0.7750	0.5570
C	0.6390	0.5020
D	0.7580	0.5560
E	0.7080	0.5270
F	0.8220	0.5720
G	0.7980	0.5180
H	0.5780	0.4090
I	0.8420	0.5850
J	0.0000	0.0470
K	0.0000	0.0130
L	0.0000	0.0160