wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 04:47 pm GMT

PDB ID	:	5NZU
EMDB ID	:	EMD-3723
Title	:	The structure of the COPI coat linkage II
Authors	:	Dodonova, S.O.; Aderhold, P.; Kopp, J.; Ganeva, I.; Roehling, S.; Hagen, W.J.H.; Sinning, I.; Wieland, F.; Briggs, J.A.G.
Deposited on	:	2017-05-15
Resolution	:	15.00 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:

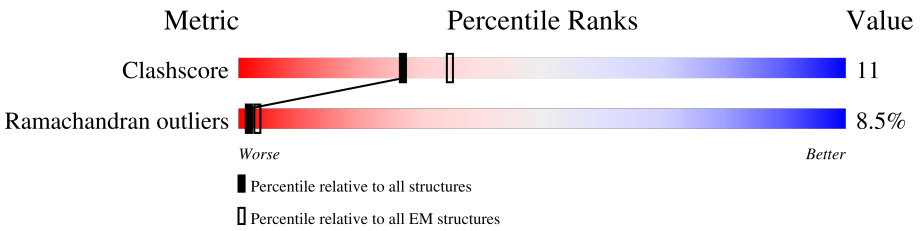
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 15.00 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

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	1-A	1262	7%; 48%; 14%; •; 36%
1	2-A	1262	48%; 14%; •; 36%
1	3-A	1262	48%; 14%; •; 36%
2	1-B	968	12%; 66%; 13%; •; 17%
2	2-B	968	66%; 13%; • •; 17%
2	3-B	968	67%; 13%; •; 17%
3	1-C	905	8%; 77%; 14%; •; 7%
3	2-C	905	77%; 14%; •; 7%
3	3-C	905	77%; 14%; •; 7%

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Mol	Chain	Length	Quality of chain
4	1-D	511	14% 78% 5% 16%
4	2-D	511	78% 5% 16%
4	3-D	511	78% 5% 16%
5	1-F	181	77% 8% 12%
5	1-M	181	8% 64% 20% 12%
5	1-R	181	22% 55% 27% 7% 12%
5	2-F	181	77% 8% 12%
5	2-M	181	64% 20% 12%
5	2-R	181	54% 27% 7% 12%
5	3-F	181	77% 8% 12%
5	3-M	181	64% 20% 12%
5	3-R	181	54% 27% 7% 12%
6	1-G	874	25% 75% 14% 9%
6	1-K	874	6% 52% 9% 36%
6	2-G	874	75% 13% 9%
6	2-K	874	52% 9% 36%
6	3-G	874	75% 14% 9%
6	3-K	874	52% 9% 36%
7	1-L	177	13% 66% 12% 21%
7	1-Z	177	13% 66% 12% 21%
7	2-L	177	66% 12% 21%
7	2-Z	177	66% 12% 21%
7	3-L	177	66% 12% 21%
7	3-Z	177	66% 12% 21%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 59913 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 Coatomer subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	1-A	813	3251	1626	813	812	0	0
1	2-A	813	3251	1626	813	812	0	0
1	3-A	813	3251	1626	813	812	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1225	LEU	-	expression tag	UNP Q8CIE6
A	1226	GLU	-	expression tag	UNP Q8CIE6
A	1227	VAL	-	expression tag	UNP Q8CIE6
A	1228	LEU	-	expression tag	UNP Q8CIE6
A	1229	PHE	-	expression tag	UNP Q8CIE6
A	1230	GLN	-	expression tag	UNP Q8CIE6
A	1231	GLY	-	expression tag	UNP Q8CIE6
A	1232	PRO	-	expression tag	UNP Q8CIE6
A	1233	SER	-	expression tag	UNP Q8CIE6
A	1234	ALA	-	expression tag	UNP Q8CIE6
A	1235	TRP	-	expression tag	UNP Q8CIE6
A	1236	SER	-	expression tag	UNP Q8CIE6
A	1237	HIS	-	expression tag	UNP Q8CIE6
A	1238	PRO	-	expression tag	UNP Q8CIE6
A	1239	GLN	-	expression tag	UNP Q8CIE6
A	1240	PHE	-	expression tag	UNP Q8CIE6
A	1241	GLU	-	expression tag	UNP Q8CIE6
A	1242	LYS	-	expression tag	UNP Q8CIE6
A	1243	GLY	-	expression tag	UNP Q8CIE6
A	1244	GLY	-	expression tag	UNP Q8CIE6
A	1245	GLY	-	expression tag	UNP Q8CIE6
A	1246	SER	-	expression tag	UNP Q8CIE6
A	1247	GLY	-	expression tag	UNP Q8CIE6
A	1248	GLY	-	expression tag	UNP Q8CIE6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1249	GLY	-	expression tag	UNP Q8CIE6
A	1250	SER	-	expression tag	UNP Q8CIE6
A	1251	GLY	-	expression tag	UNP Q8CIE6
A	1252	GLY	-	expression tag	UNP Q8CIE6
A	1253	SER	-	expression tag	UNP Q8CIE6
A	1254	ALA	-	expression tag	UNP Q8CIE6
A	1255	TRP	-	expression tag	UNP Q8CIE6
A	1256	SER	-	expression tag	UNP Q8CIE6
A	1257	HIS	-	expression tag	UNP Q8CIE6
A	1258	PRO	-	expression tag	UNP Q8CIE6
A	1259	GLN	-	expression tag	UNP Q8CIE6
A	1260	PHE	-	expression tag	UNP Q8CIE6
A	1261	GLU	-	expression tag	UNP Q8CIE6
A	1262	LYS	-	expression tag	UNP Q8CIE6

- Molecule 2 is a protein called Coatomer subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1-B	800	3198	1600	800	798	0	0
2	2-B	800	3198	1600	800	798	0	0
2	3-B	800	3198	1600	800	798	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP Q9JIF7
B	2	HIS	-	expression tag	UNP Q9JIF7
B	3	HIS	-	expression tag	UNP Q9JIF7
B	4	HIS	-	expression tag	UNP Q9JIF7
B	5	HIS	-	expression tag	UNP Q9JIF7
B	6	HIS	-	expression tag	UNP Q9JIF7
B	7	HIS	-	expression tag	UNP Q9JIF7
B	8	GLU	-	expression tag	UNP Q9JIF7
B	9	ASN	-	expression tag	UNP Q9JIF7
B	10	LEU	-	expression tag	UNP Q9JIF7
B	11	TYR	-	expression tag	UNP Q9JIF7
B	12	PHE	-	expression tag	UNP Q9JIF7
B	13	GLN	-	expression tag	UNP Q9JIF7
B	14	GLY	-	expression tag	UNP Q9JIF7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	15	HIS	-	expression tag	UNP Q9JIF7

- Molecule 3 is a protein called Coatomer subunit beta'.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	1-C	843	3371	1686	843	842	0	0
3	2-C	843	3371	1686	843	842	0	0
3	3-C	843	3371	1686	843	842	0	0

- Molecule 4 is a protein called Coatomer subunit delta.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	1-D	427	1707	854	427	426	0	0
4	2-D	427	1707	854	427	426	0	0
4	3-D	427	1707	854	427	426	0	0

- Molecule 5 is a protein called ADP-ribosylation factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	1-F	159	635	318	159	158	0	0
5	2-F	159	635	318	159	158	0	0
5	3-F	159	635	318	159	158	0	0
5	1-R	159	635	318	159	158	0	0
5	2-R	159	635	318	159	158	0	0
5	3-R	159	635	318	159	158	0	0
5	1-M	159	635	318	159	158	0	0
5	2-M	159	635	318	159	158	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	3-M	159	635	318	159	158	0	0

- Molecule 6 is a protein called Coatomer subunit gamma-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	1-G	798	3190	1596	798	796	0	0
6	2-G	798	3190	1596	798	796	0	0
6	3-G	798	3190	1596	798	796	0	0
6	1-K	560	2239	1120	560	559	0	0
6	2-K	560	2239	1120	560	559	0	0
6	3-K	560	2239	1120	560	559	0	0

- Molecule 7 is a protein called Coatomer subunit zeta-1.

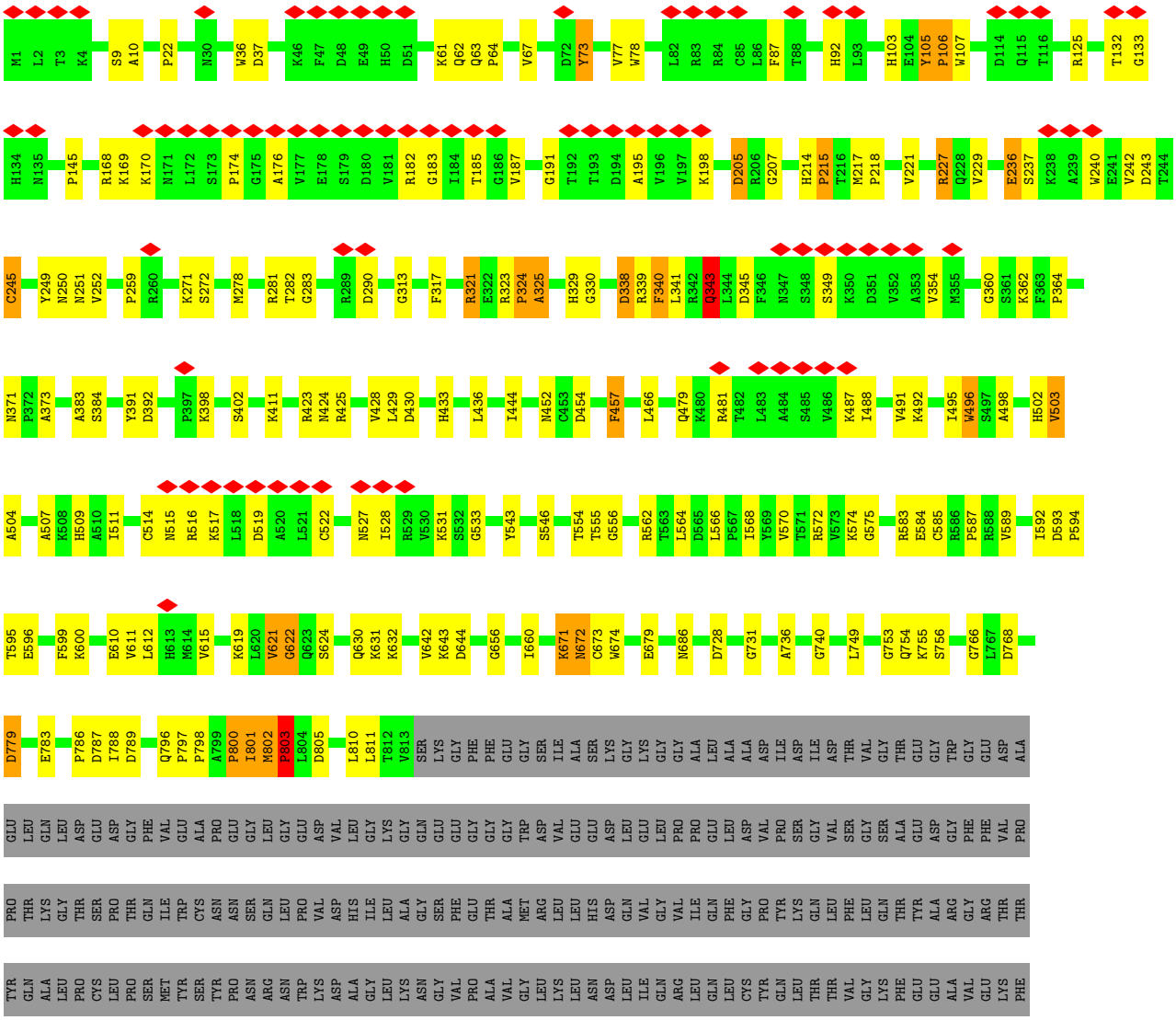
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	1-Z	139	555	278	139	138	0	0
7	2-Z	139	555	278	139	138	0	0
7	3-Z	139	555	278	139	138	0	0
7	1-L	139	555	278	139	138	0	0
7	2-L	139	555	278	139	138	0	0
7	3-L	139	555	278	139	138	0	0

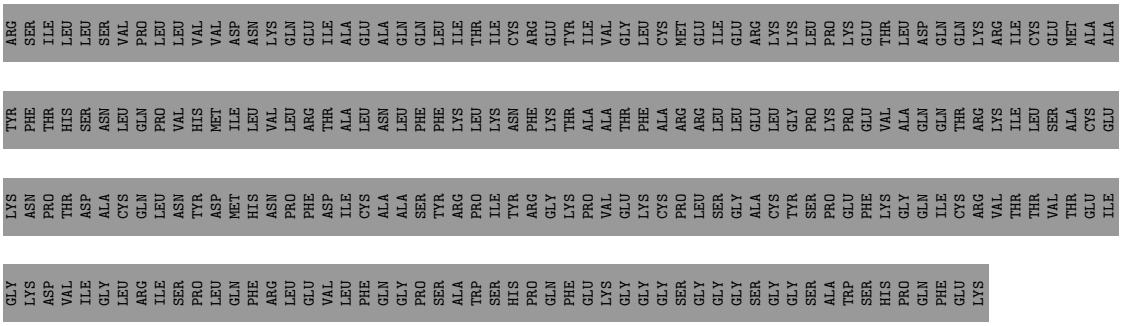
3 Residue-property plots (i)

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: Coatomer subunit alpha

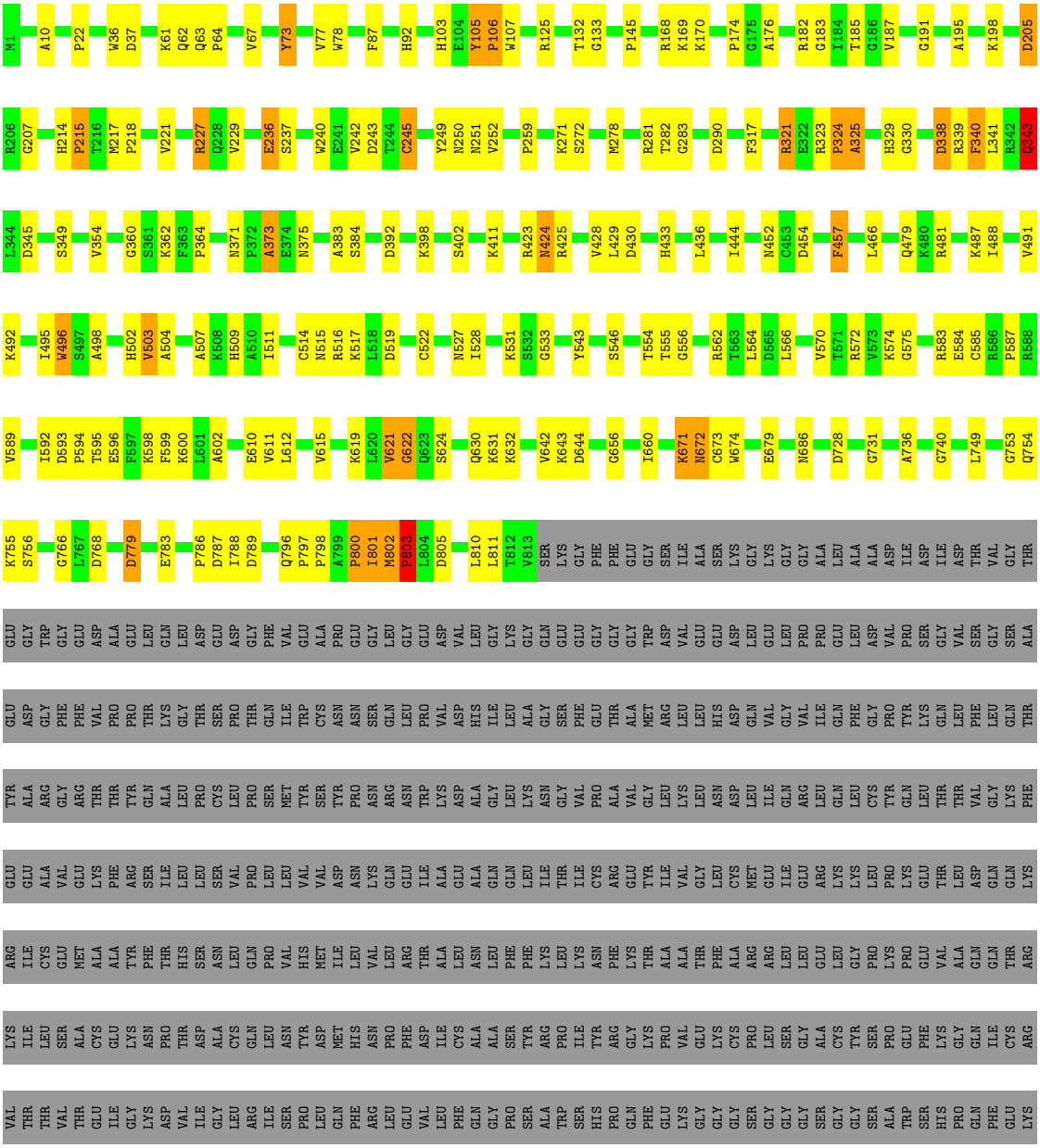
Chain 1-A: 7% 48% 14% 36%





- Molecule 1: Coatomer subunit alpha

Chain 2-A: 48% 14% • 36%



- Molecule 1: Coatomer subunit alpha

Chain 3-A: 48% 14% • 36%

M1 S9 A10 P22 W36 D37 K61 Q62 Q63 P64 V67 Y73 V77 W78 F87 H92 H103 E104 Y105 P106 W107 R125 T132 G133 P145 R168 K169 K170 P174 G175 A176 R182 G183 I184 T185 G186 V187 G191 A195 K198

D205 R206 G207 H214 P215 T216 M217 P218 V221 R227 Q228 V229 E236 S237 W240 E241 V242 D243 T244 C245 Y249 N250 N251 V252 P259 K271 S272 M278 R281 T282 G283 D290 G313 F317 R321 E322 R323 P324 A325 H329 G330 D338 R339 E340

L341 R342 Q343 L344 D345 S349 V354 G360 S361 K362 F363 P364 N371 P372 A373 A383 S384 D392 K398 S402 K411 R412 S413 R423 N424 R425 L429 D430 H433 L436 I444 N452 C453 D454 F457 L466 Q479 K480 R481 K487 I488

V491 K492 I495 W496 S497 A498 H502 V503 A504 A507 K508 H509 A510 I511 C514 N515 R516 K517 L518 D519 C522 N527 I528 K531 S532 G533 Y543 S546 T554 T555 G556 R562 T563 L564 D565 L566 V570 T571 R572 V573 K574 G575 R583 E584 C585 R586

P587 R588 V589 I592 D593 P594 T595 E596 F597 K598 F599 K600 L601 A602 E610 V611 L612 V615 K619 L620 V621 G622 Q623 S624 Q630 K631 K632 V642 K643 D644 G656 I660 K671 N672 C673 W674 E679 N686 D728 G731 A736 G740 L749

G753 Q754 K755 S756 G766 L767 D768 D779 E783 P786 D787 I788 D789 Q796 P797 P798 A799 P800 I801 M802 P803 L804 D805 L810 L811 T812 V813 SER LYS GLY PHE PHE GLU GLY SER ILE ALA SER LYS GLY LYS GLY GLY ALA LEU ALA ALA ASP ILE ASP ILE ASP THR VAL

GLY THR GLU GLY TRP GLY GLU ASP ALA GLU LEU GLN LEU ASP GLU ASP GLY PHE VAL GLU ALA PRO GLU GLY LEU GLY GLU ASP VAL LEU GLY LYS GLY GLN GLU GLU GLY GLY GLY TRP ASP VAL GLU GLU ASP LEU GLU LEU PRO PRO GLU LEU ASP VAL PRO SER GLY VAL SER GLY

SER ALA GLU ASP GLY PHE PHE VAL PRO PRO THR THR LYS GLY THR SER PRO THR GLN ILE TRP CYS ASN ASN SER GLN LEU PRO VAL ASP HIS ILE LEU ALA GLY SER PHE GLU THR ALA MET ARG LEU LEU HIS ASP GLN VAL GLY VAL ILE GLN PHE GLY PRO TYR LYS GLN LEU PHE LEU

GLN THR TYR ALA ARG GLY ARG THR THR TYR GLN ALA LEU PRO CYS LEU PRO SER MET TYR SER TYR PRO ASN ARG ASN TRP LYS ASP ALA GLY LEU LYS ASN GLY VAL PRO ALA VAL GLY LEU LYS LEU ASN ASP LEU ILE GLN ARG LEU GLN LEU CYS TYR GLN LEU THR THR VAL GLY

LYS PHE GLU GLU ALA VAL GLU LYS PHE ARG SER ILE LEU LEU SER VAL PRO LEU LEU VAL VAL ASP ASN LYS GLN GLU ILE ALA GLU ALA GLN GLN LEU ILE THR ILE CYS ARG GLU TYR ILE VAL GLY LEU CYS MET GLU ILE GLN ARG LEU GLU LYS LYS LEU PRO LYS GLU THR LEU ASP GLN

GLN LYS ARG ILE CYS GLU MET ALA ALA TYR PHE THR HIS SER ASN LEU GLN PRO VAL HIS MET ILE LEU VAL LEU ARG THR ALA LEU ASN LEU PHE PHE LYS LEU LYS ASN PHE LYS THR ALA ALA THR PHE ALA ARG ARG LEU LEU GLU LEU GLU LEU GLY PRO LYS PRO GLU VAL ALA GLN GLN

THR ARG LYS ILE LEU SER ALA CYS GLU LYS ASN PRO THR ASP ALA CYS GLN LEU ASN TYR ASP MET THR ASN PRO ILE CYS ALA ALA SER TYR ARG PRO ILE TYR ARG GLY LYS PRO VAL GLU LYS CYS PRO SER GLY ALA CYS TYR SER PRO GLU PHE LYS GLY GLN ILE

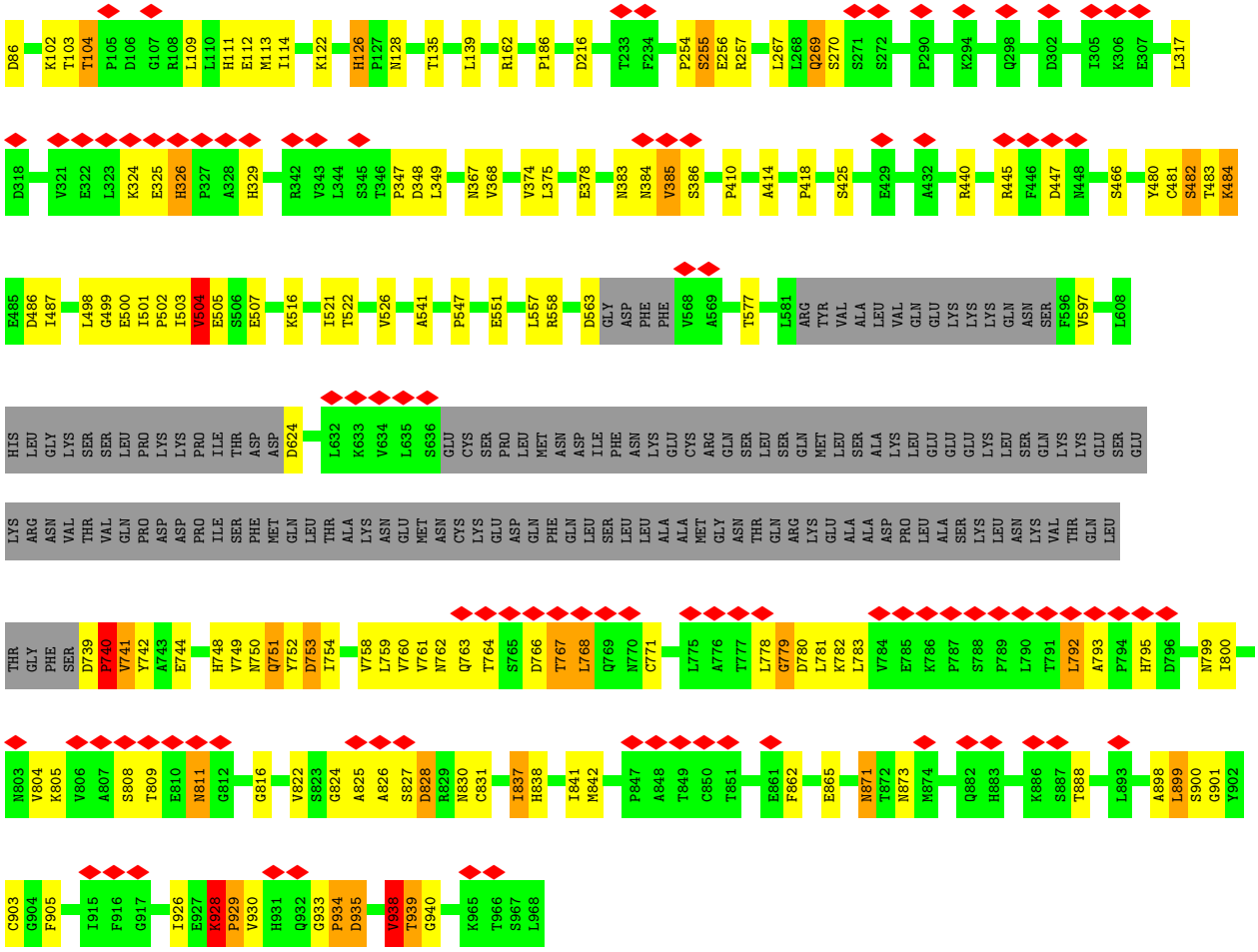
CYS ARG VAL THR THR VAL THR GLU ILE GLY LYS ASP VAL ILE ARG LEU ARG ILE SER PRO LEU GLN PHE ARG LEU GLU VAL LEU PHE GLN GLY PRO SER ALA TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY SER GLY GLY SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE

GLU LYS

• Molecule 2: Coatomer subunit beta

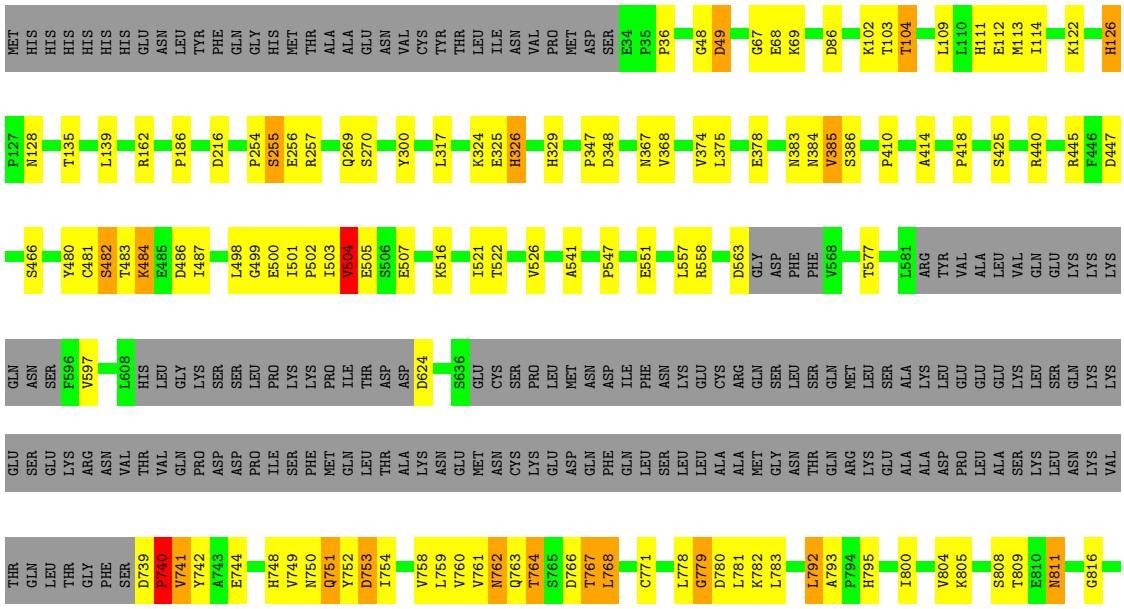
Chain 1-B: 12% 66% 13% • 17%

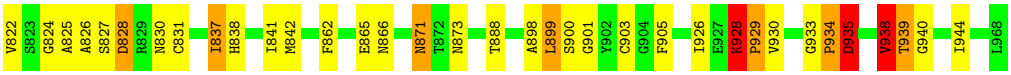
MET HIS HIS HIS HIS HIS GLU ASN LEU TYR PHE GLN GLY HIS MET THR ALA ALA GLU ASN VAL CYS TYR THR LEU ILE ASN VAL PRO MET ASP SER E34 P35 P36 S37 E38 I39 S40 L41 K42 N43 D44 L45 E46 K47 G48 D49 V50 K51 S52 N66 G67 E68 K69 L70 P71



• Molecule 2: Coatomer subunit beta

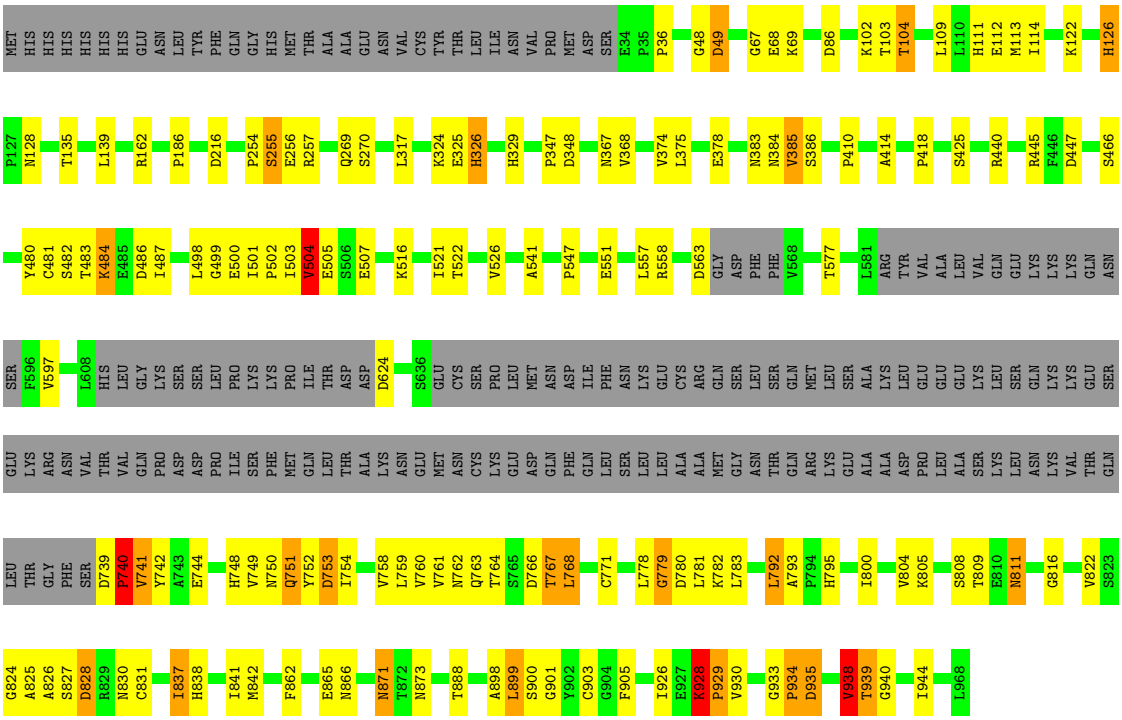
Chain 2-B: 66% 13% • • 17%





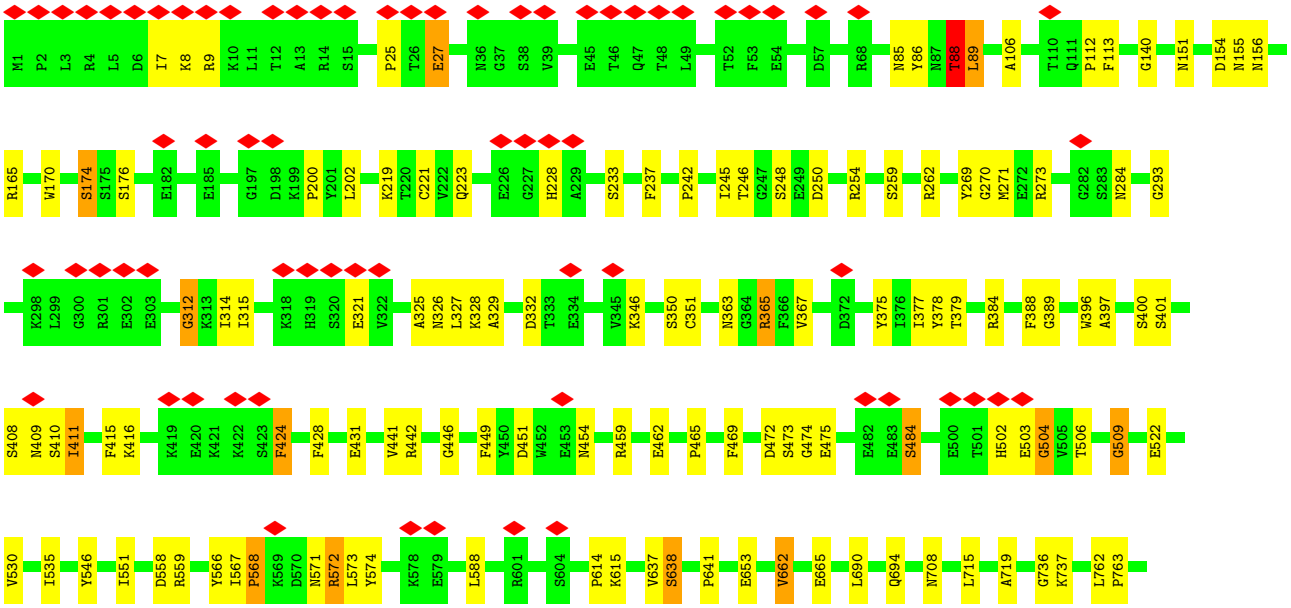
• Molecule 2: Coatomer subunit beta

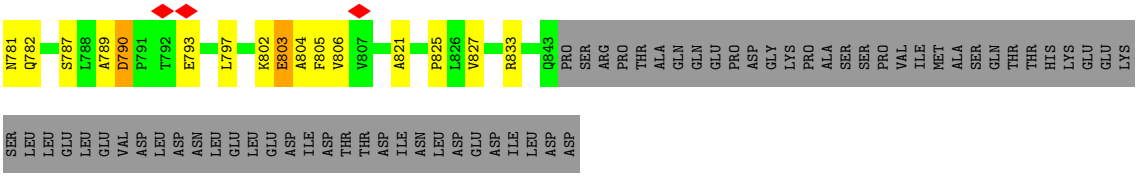
Chain 3-B:



• Molecule 3: Coatomer subunit beta'

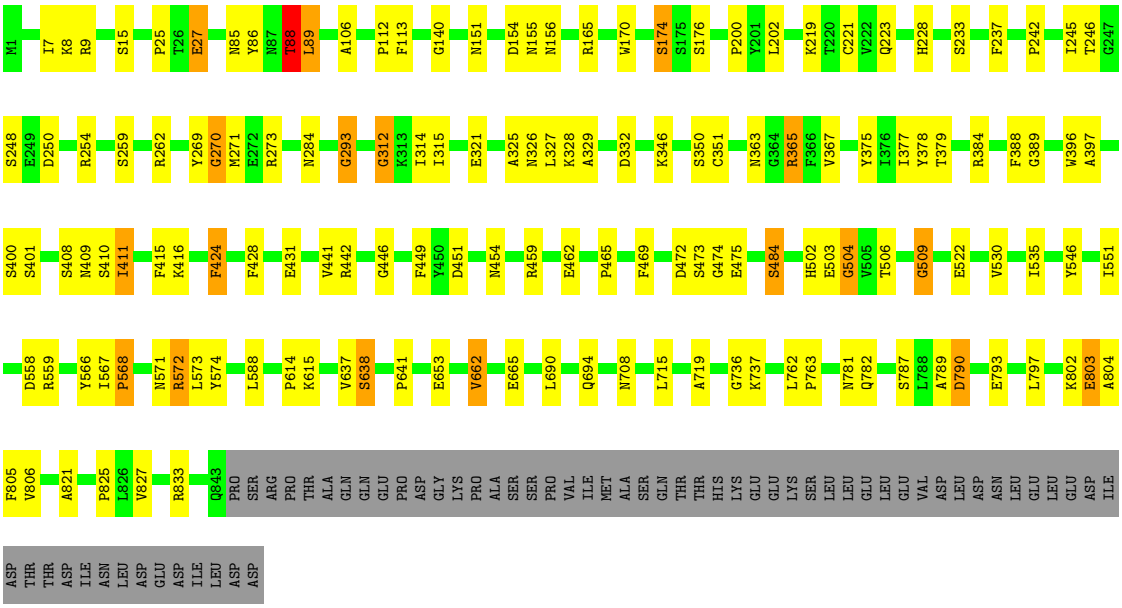
Chain 1-C:





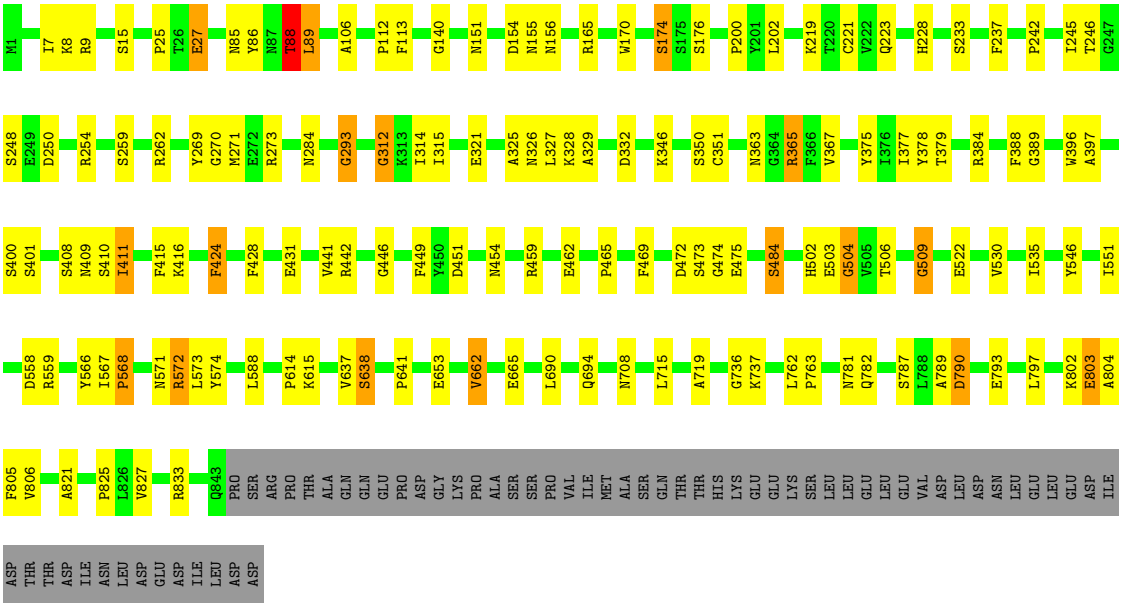
- Molecule 3: Coatomer subunit beta'

Chain 2-C:



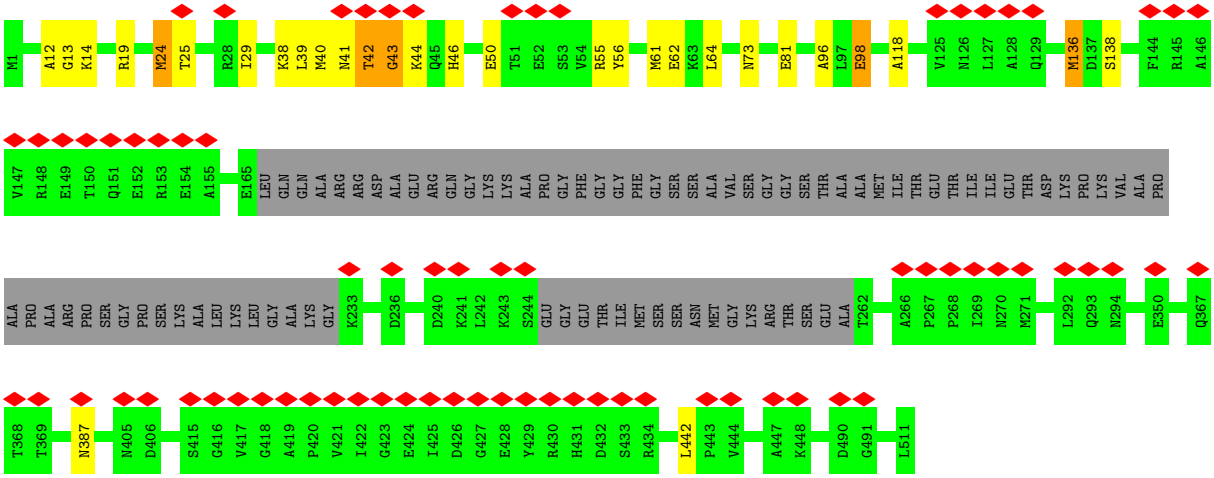
- Molecule 3: Coatomer subunit beta'

Chain 3-C:



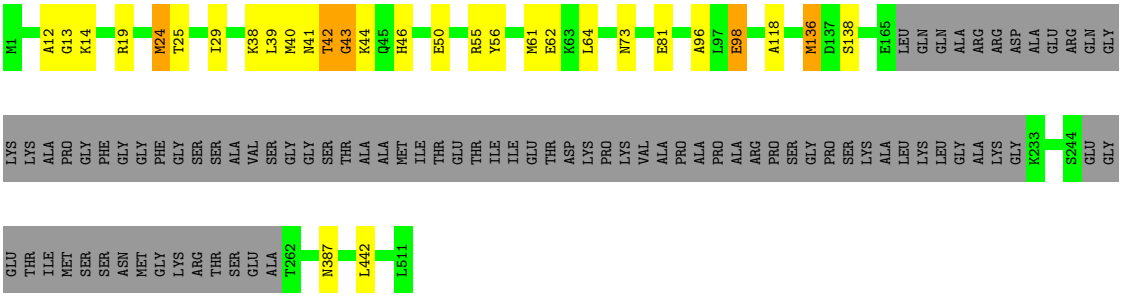
• Molecule 4: Coatomer subunit delta

Chain 1-D:



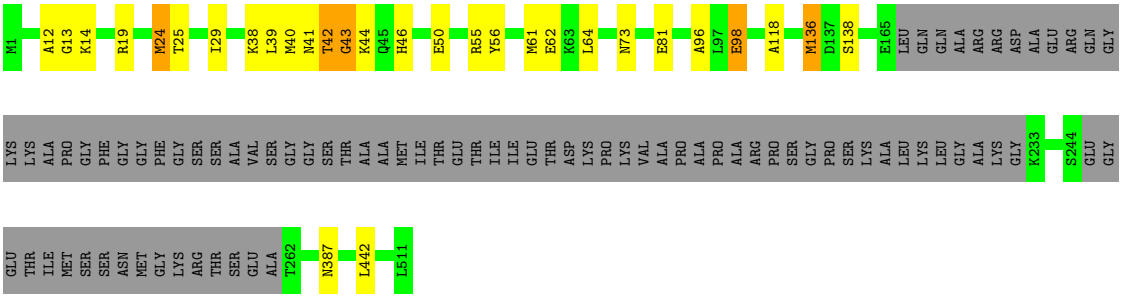
• Molecule 4: Coatomer subunit delta

Chain 2-D:



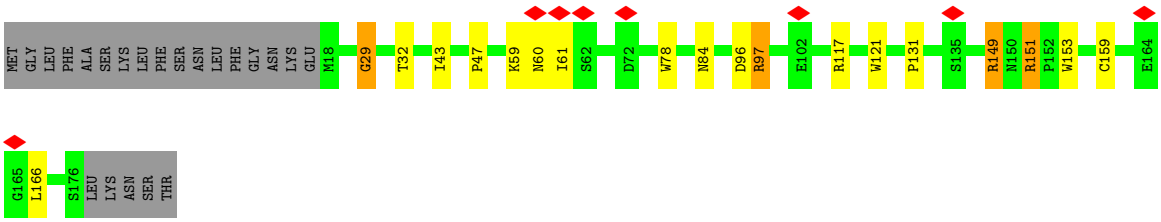
• Molecule 4: Coatomer subunit delta

Chain 3-D:



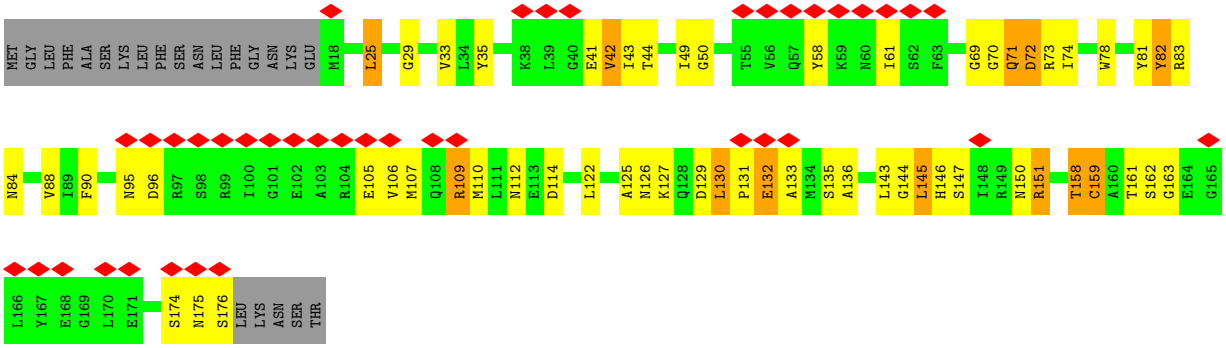
• Molecule 5: ADP-ribosylation factor 1

Chain 1-F:



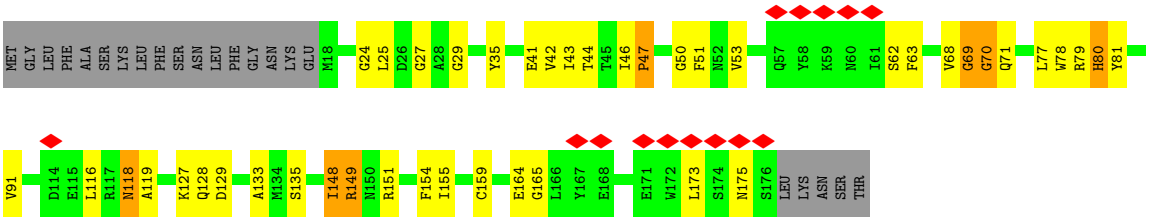
• Molecule 5: ADP-ribosylation factor 1

Chain 1-R:



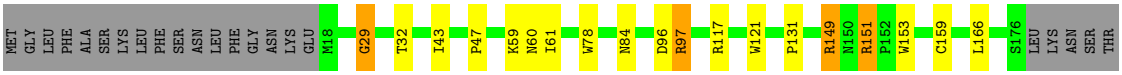
• Molecule 5: ADP-ribosylation factor 1

Chain 1-M:



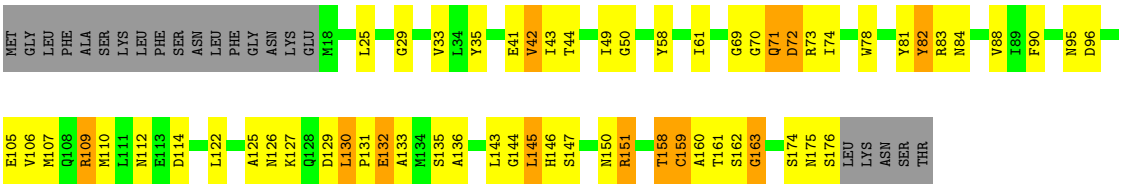
• Molecule 5: ADP-ribosylation factor 1

Chain 2-F:



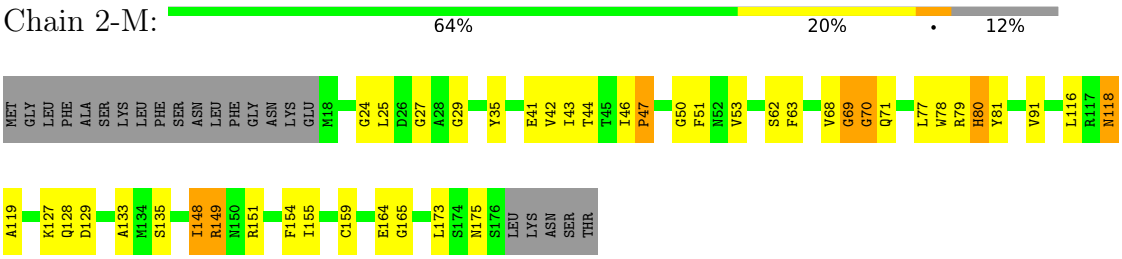
• Molecule 5: ADP-ribosylation factor 1

Chain 2-R:



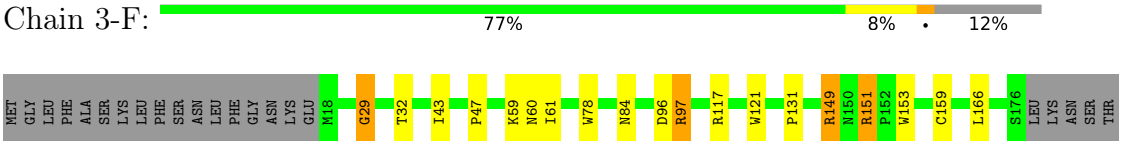
- Molecule 5: ADP-ribosylation factor 1

Chain 2-M:



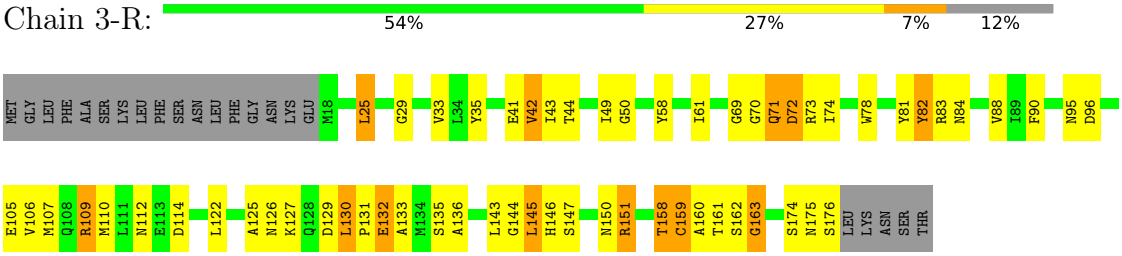
- Molecule 5: ADP-ribosylation factor 1

Chain 3-F:



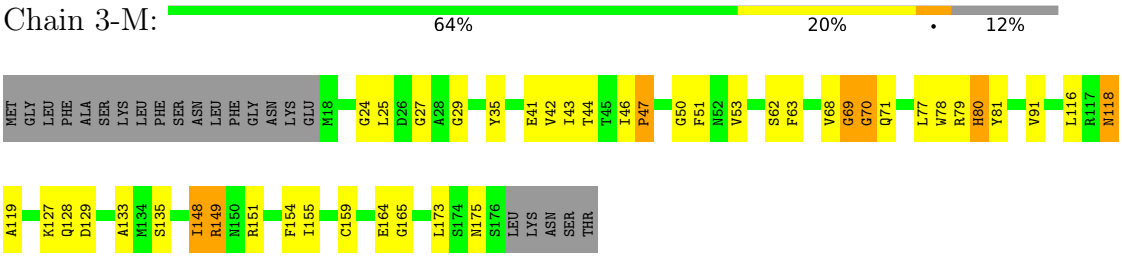
- Molecule 5: ADP-ribosylation factor 1

Chain 3-R:



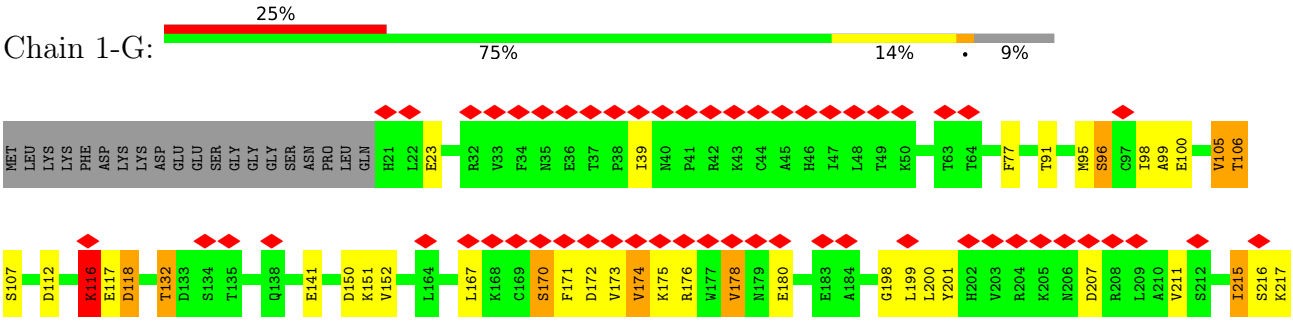
- Molecule 5: ADP-ribosylation factor 1

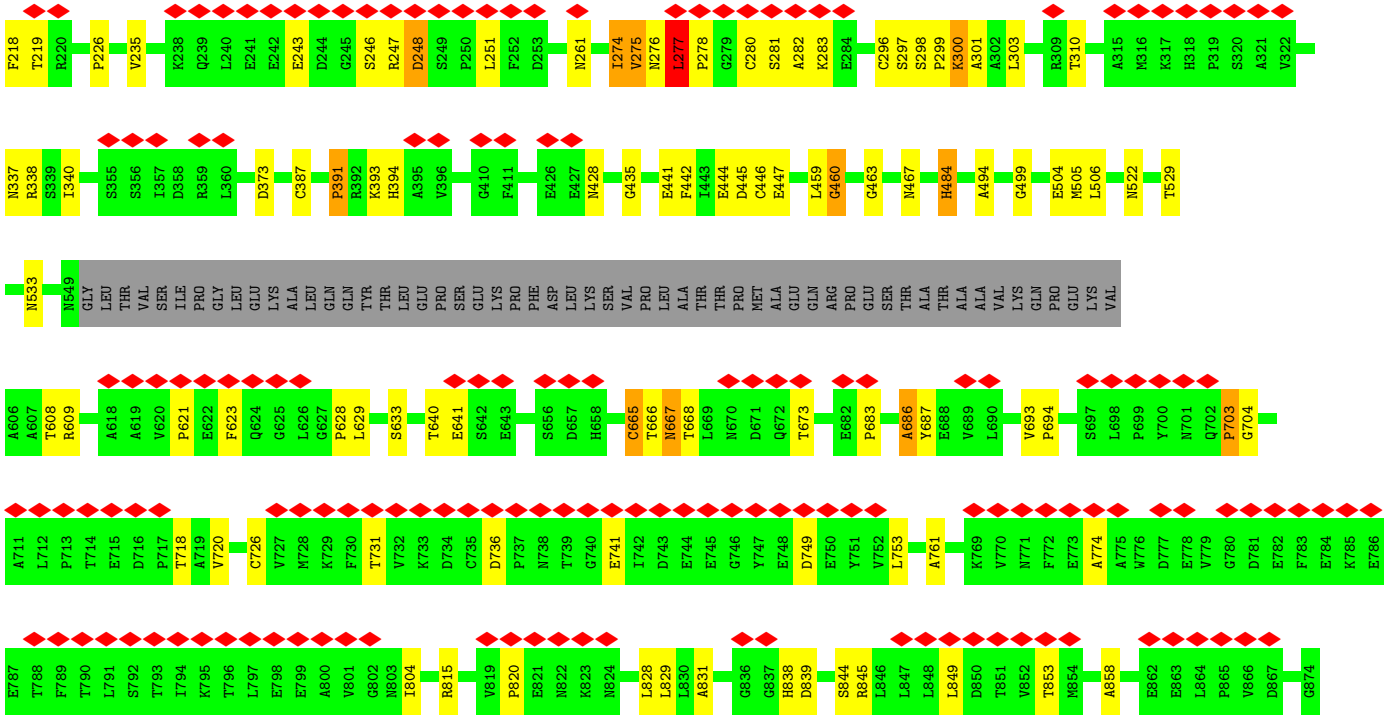
Chain 3-M:



- Molecule 6: Coatomer subunit gamma-1

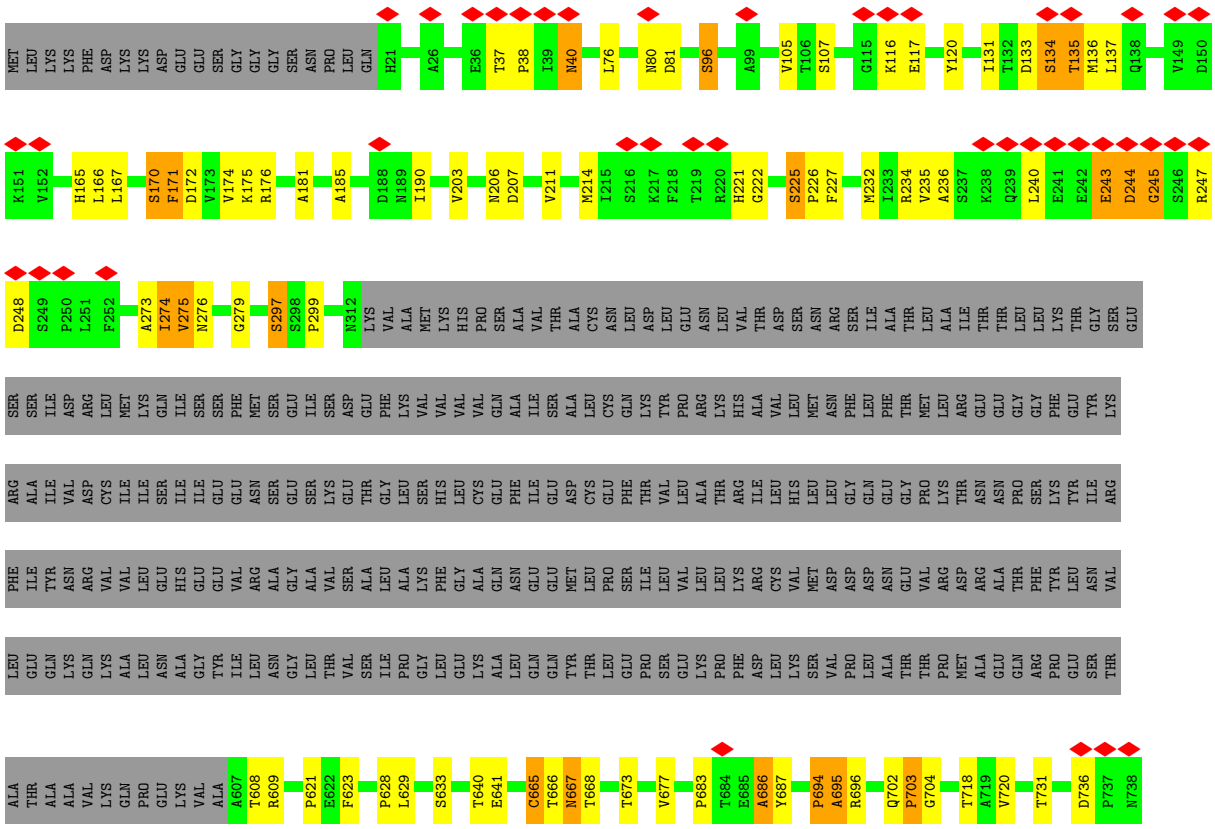
Chain 1-G:

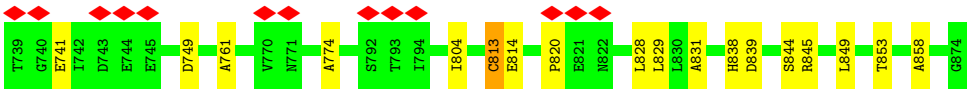




- Molecule 6: Coatomer subunit gamma-1

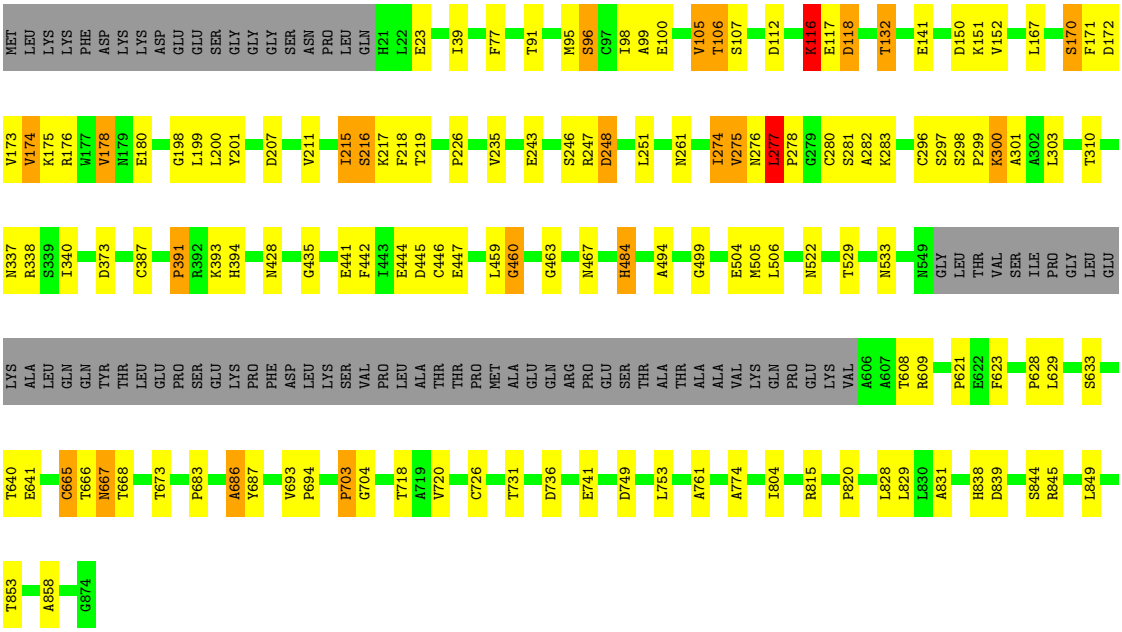
Chain 1-K:





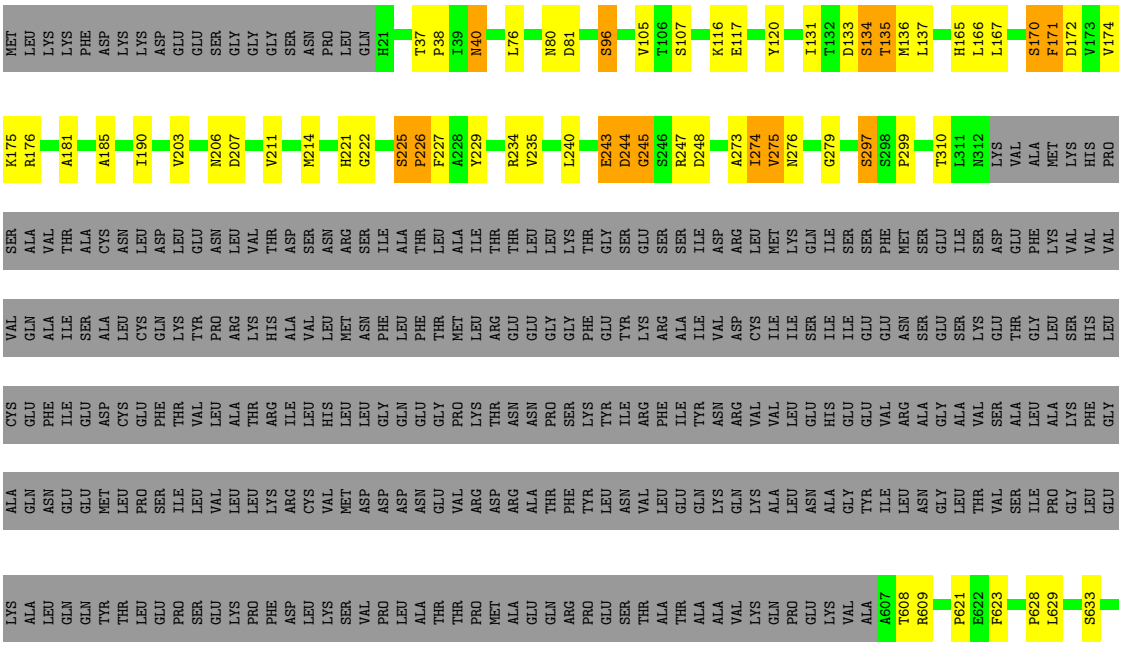
• Molecule 6: Coatomer subunit gamma-1

Chain 2-G: 75% 13% • 9%



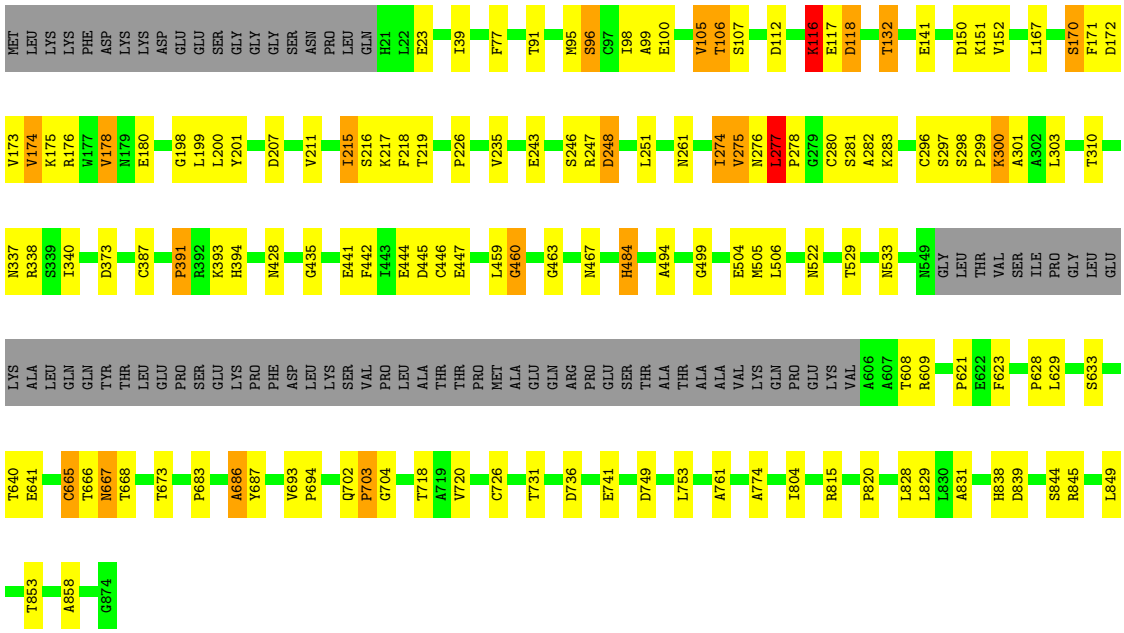
• Molecule 6: Coatomer subunit gamma-1

Chain 2-K: 52% 9% • 36%



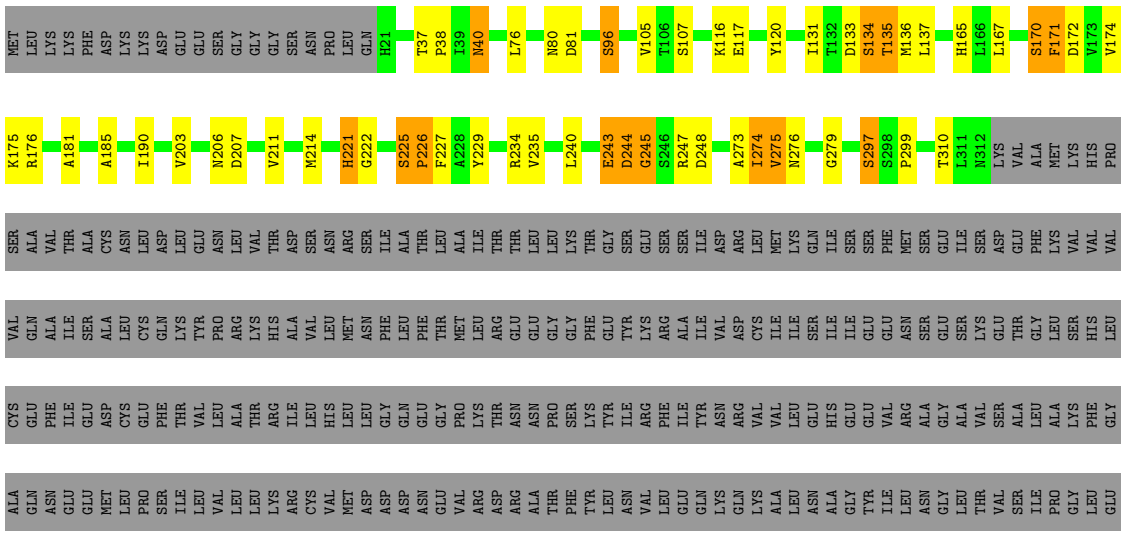
- Molecule 6: Coatomer subunit gamma-1

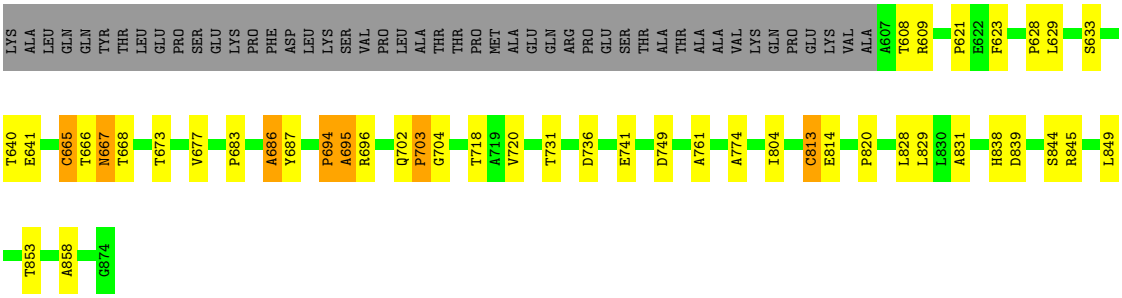
Chain 3-G:



- Molecule 6: Coatomer subunit gamma-1

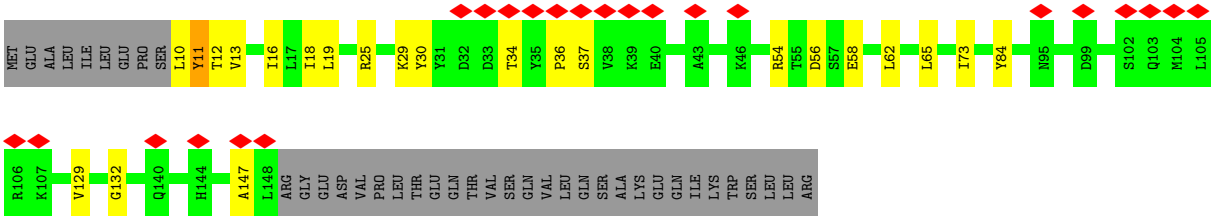
Chain 3-K:





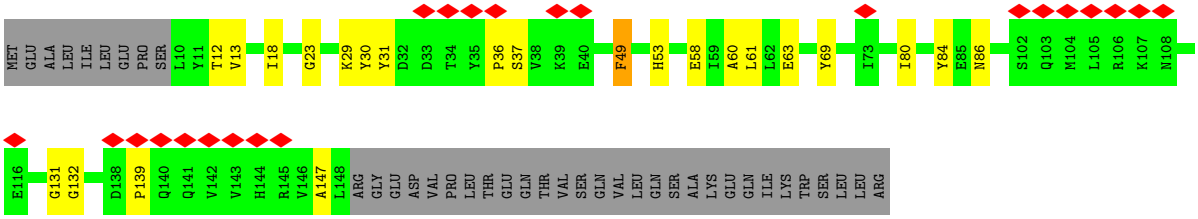
• Molecule 7: Coatomer subunit zeta-1

Chain 1-Z:



• Molecule 7: Coatomer subunit zeta-1

Chain 1-L:

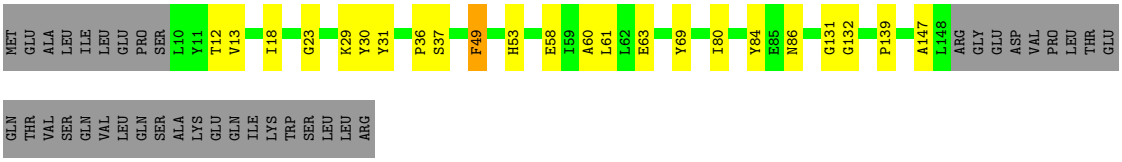


• Molecule 7: Coatomer subunit zeta-1

Chain 2-Z:

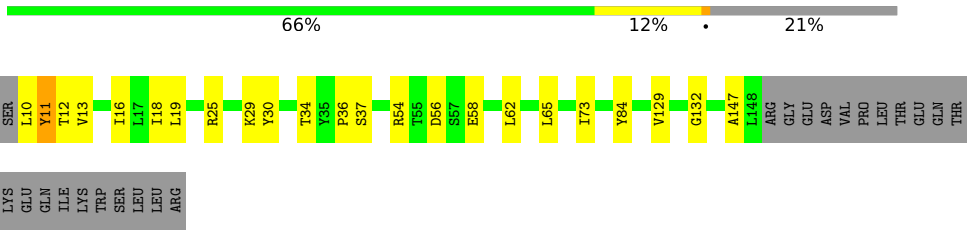
• Molecule 7: Coatomer subunit zeta-1

Chain 2-L:



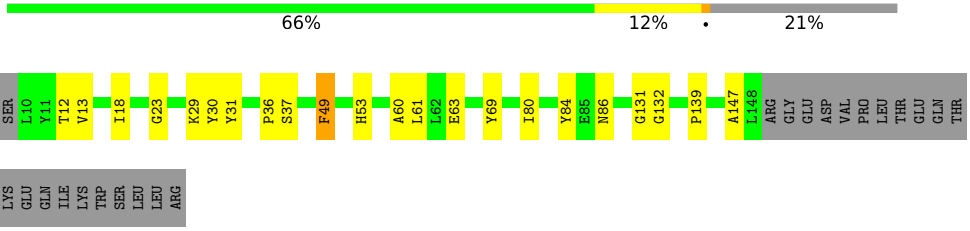
- Molecule 7: Coatomer subunit zeta-1

Chain 3-Z:



- Molecule 7: Coatomer subunit zeta-1

Chain 3-L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	3312	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; CTF-determination for each individual tilt image was performed using CTFFIND4. Strip-based CTF-correction and tomogram reconstruction was performed in Imod.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.200	Depositor
Minimum map value	-0.167	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	377.36, 377.36, 377.36	wwPDB
Map dimensions	212, 212, 212	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.78, 1.78, 1.78	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	1-A	1.56	15/3250 (0.5%)	1.81	76/4061 (1.9%)
1	2-A	1.56	15/3250 (0.5%)	1.81	75/4061 (1.8%)
1	3-A	1.56	15/3250 (0.5%)	1.81	74/4061 (1.8%)
2	1-B	1.71	20/3193 (0.6%)	1.55	45/3983 (1.1%)
2	2-B	1.71	19/3193 (0.6%)	1.55	46/3983 (1.2%)
2	3-B	1.71	18/3193 (0.6%)	1.55	45/3983 (1.1%)
3	1-C	1.76	22/3370 (0.7%)	1.70	60/4211 (1.4%)
3	2-C	1.76	23/3370 (0.7%)	1.70	60/4211 (1.4%)
3	3-C	1.76	23/3370 (0.7%)	1.70	60/4211 (1.4%)
4	1-D	1.29	3/1704 (0.2%)	1.24	10/2124 (0.5%)
4	2-D	1.29	3/1704 (0.2%)	1.24	10/2124 (0.5%)
4	3-D	1.29	3/1704 (0.2%)	1.24	10/2124 (0.5%)
5	1-F	1.56	1/634 (0.2%)	1.71	9/791 (1.1%)
5	1-M	1.60	4/634 (0.6%)	1.65	10/791 (1.3%)
5	1-R	1.88	10/634 (1.6%)	1.81	15/791 (1.9%)
5	2-F	1.56	1/634 (0.2%)	1.71	9/791 (1.1%)
5	2-M	1.60	4/634 (0.6%)	1.65	10/791 (1.3%)
5	2-R	1.88	10/634 (1.6%)	1.81	15/791 (1.9%)
5	3-F	1.56	1/634 (0.2%)	1.71	9/791 (1.1%)
5	3-M	1.60	4/634 (0.6%)	1.65	10/791 (1.3%)
5	3-R	1.88	10/634 (1.6%)	1.81	15/791 (1.9%)
6	1-G	1.62	11/3188 (0.3%)	1.59	45/3982 (1.1%)
6	1-K	1.72	9/2237 (0.4%)	1.69	43/2793 (1.5%)
6	2-G	1.62	11/3188 (0.3%)	1.59	45/3982 (1.1%)
6	2-K	1.72	9/2237 (0.4%)	1.69	43/2793 (1.5%)
6	3-G	1.62	11/3188 (0.3%)	1.59	45/3982 (1.1%)
6	3-K	1.72	9/2237 (0.4%)	1.69	44/2793 (1.6%)
7	1-L	2.05	3/554 (0.5%)	1.72	8/691 (1.2%)
7	1-Z	1.87	3/554 (0.5%)	1.69	10/691 (1.4%)
7	2-L	2.05	3/554 (0.5%)	1.72	8/691 (1.2%)
7	2-Z	1.87	3/554 (0.5%)	1.69	10/691 (1.4%)
7	3-L	2.05	3/554 (0.5%)	1.72	7/691 (1.0%)
7	3-Z	1.87	3/554 (0.5%)	1.69	10/691 (1.4%)
All	All	1.66	302/59856 (0.5%)	1.65	991/74727 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	1-B	0	3
2	2-B	0	3
2	3-B	0	3
All	All	0	9

The worst 5 of 302 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1-B	940	GLY	N-CA	-7.79	1.34	1.46
2	3-B	940	GLY	N-CA	-7.76	1.34	1.46
2	2-B	940	GLY	N-CA	-7.75	1.34	1.46
5	1-R	29	GLY	CA-C	-7.64	1.39	1.51
5	2-R	29	GLY	CA-C	-7.62	1.39	1.51

The worst 5 of 991 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2-A	343	GLN	N-CA-C	-9.88	84.32	111.00
1	1-A	343	GLN	N-CA-C	-9.86	84.38	111.00
1	3-A	343	GLN	N-CA-C	-9.86	84.38	111.00
6	3-K	117	GLU	C-N-CA	9.77	146.12	121.70
6	2-K	117	GLU	C-N-CA	9.76	146.10	121.70

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1-B	898	ALA	Peptide
2	1-B	903	CYS	Peptide
2	1-B	938	VAL	Mainchain
2	2-B	898	ALA	Peptide
2	2-B	903	CYS	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	1-A	3251	0	869	36	0
1	2-A	3251	0	869	37	0
1	3-A	3251	0	869	36	0
2	1-B	3198	0	810	56	0
2	2-B	3198	0	810	56	0
2	3-B	3198	0	810	54	0
3	1-C	3371	0	919	21	0
3	2-C	3371	0	919	23	0
3	3-C	3371	0	919	23	0
4	1-D	1707	0	450	9	0
4	2-D	1707	0	450	9	0
4	3-D	1707	0	450	9	0
5	1-F	635	0	181	3	0
5	1-M	635	0	181	19	0
5	1-R	635	0	181	38	0
5	2-F	635	0	181	3	0
5	2-M	635	0	181	20	0
5	2-R	635	0	181	38	0
5	3-F	635	0	181	3	0
5	3-M	635	0	181	19	0
5	3-R	635	0	181	35	0
6	1-G	3190	0	822	59	0
6	1-K	2239	0	572	37	0
6	2-G	3190	0	822	59	0
6	2-K	2239	0	572	38	0
6	3-G	3190	0	822	57	0
6	3-K	2239	0	572	36	0
7	1-L	555	0	148	2	0
7	1-Z	555	0	147	14	0
7	2-L	555	0	148	2	0
7	2-Z	555	0	147	14	0
7	3-L	555	0	148	2	0
7	3-Z	555	0	147	14	0
All	All	59913	0	15840	824	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 11.

The worst 5 of 824 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)
6:G:107:SER:N	5:R:50:GLY:HA3	1.16	1.47
6:K:107:SER:N	5:M:50:GLY:HA3	1.28	1.47
6:G:107:SER:N	5:R:50:GLY:HA3	1.16	1.47
6:G:107:SER:N	5:R:50:GLY:HA3	1.16	1.45
6:G:107:SER:H	5:R:50:GLY:CA	1.31	1.44

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	1-A	811/1262 (64%)	590 (73%)	112 (14%)	109 (13%)	0 5
1	2-A	811/1262 (64%)	590 (73%)	112 (14%)	109 (13%)	0 5
1	3-A	811/1262 (64%)	590 (73%)	112 (14%)	109 (13%)	0 5
2	1-B	790/968 (82%)	648 (82%)	68 (9%)	74 (9%)	0 10
2	2-B	790/968 (82%)	648 (82%)	68 (9%)	74 (9%)	0 10
2	3-B	790/968 (82%)	648 (82%)	68 (9%)	74 (9%)	0 10
3	1-C	841/905 (93%)	681 (81%)	91 (11%)	69 (8%)	1 12
3	2-C	841/905 (93%)	682 (81%)	90 (11%)	69 (8%)	1 12
3	3-C	841/905 (93%)	681 (81%)	91 (11%)	69 (8%)	1 12
4	1-D	421/511 (82%)	386 (92%)	20 (5%)	15 (4%)	3 25
4	2-D	421/511 (82%)	386 (92%)	20 (5%)	15 (4%)	3 25
4	3-D	421/511 (82%)	386 (92%)	20 (5%)	15 (4%)	3 25
5	1-F	157/181 (87%)	134 (85%)	14 (9%)	9 (6%)	1 18
5	1-M	157/181 (87%)	126 (80%)	13 (8%)	18 (12%)	0 6
5	1-R	157/181 (87%)	120 (76%)	17 (11%)	20 (13%)	0 5
5	2-F	157/181 (87%)	134 (85%)	14 (9%)	9 (6%)	1 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	2-M	157/181 (87%)	126 (80%)	13 (8%)	18 (12%)	0	6
5	2-R	157/181 (87%)	120 (76%)	17 (11%)	20 (13%)	0	5
5	3-F	157/181 (87%)	134 (85%)	14 (9%)	9 (6%)	1	18
5	3-M	157/181 (87%)	126 (80%)	13 (8%)	18 (12%)	0	6
5	3-R	157/181 (87%)	120 (76%)	17 (11%)	20 (13%)	0	5
6	1-G	794/874 (91%)	678 (85%)	61 (8%)	55 (7%)	1	15
6	1-K	556/874 (64%)	475 (85%)	43 (8%)	38 (7%)	1	15
6	2-G	794/874 (91%)	678 (85%)	61 (8%)	55 (7%)	1	15
6	2-K	556/874 (64%)	475 (85%)	42 (8%)	39 (7%)	1	14
6	3-G	794/874 (91%)	679 (86%)	60 (8%)	55 (7%)	1	15
6	3-K	556/874 (64%)	475 (85%)	42 (8%)	39 (7%)	1	14
7	1-L	137/177 (77%)	117 (85%)	11 (8%)	9 (7%)	1	16
7	1-Z	137/177 (77%)	119 (87%)	11 (8%)	7 (5%)	2	19
7	2-L	137/177 (77%)	117 (85%)	11 (8%)	9 (7%)	1	16
7	2-Z	137/177 (77%)	119 (87%)	11 (8%)	7 (5%)	2	19
7	3-L	137/177 (77%)	117 (85%)	11 (8%)	9 (7%)	1	16
7	3-Z	137/177 (77%)	119 (87%)	11 (8%)	7 (5%)	2	19
All	All	14874/18873 (79%)	12224 (82%)	1379 (9%)	1271 (8%)	2	12

5 of 1271 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	63	GLN
1	1-A	64	PRO
1	1-A	92	HIS
1	1-A	106	PRO
1	1-A	125	ARG

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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.

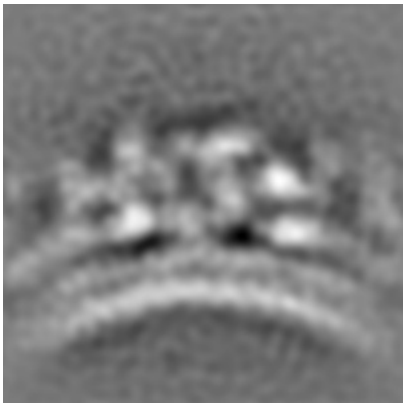
6 Map visualisation (i)

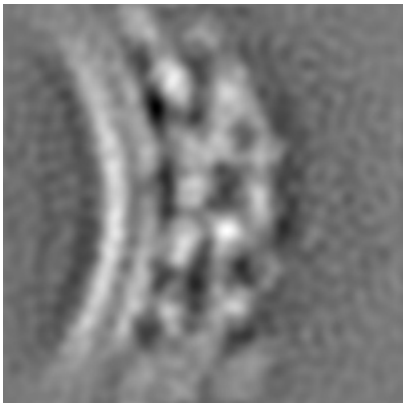
This section contains visualisations of the EMDB entry EMD-3723. These allow visual inspection of the internal detail of the map and identification of artifacts.

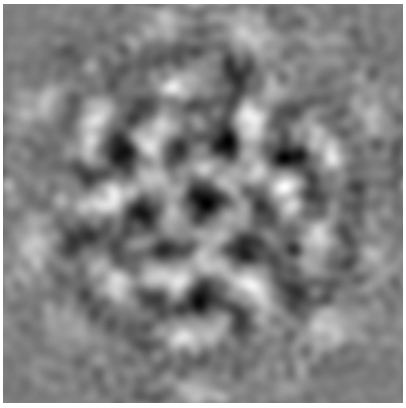
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

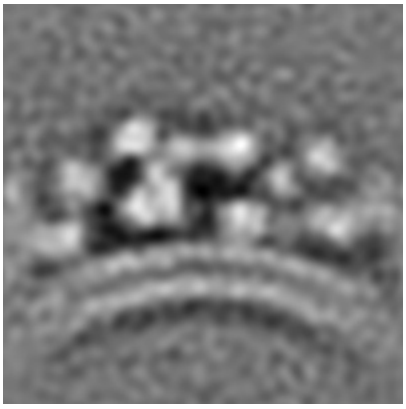

Y

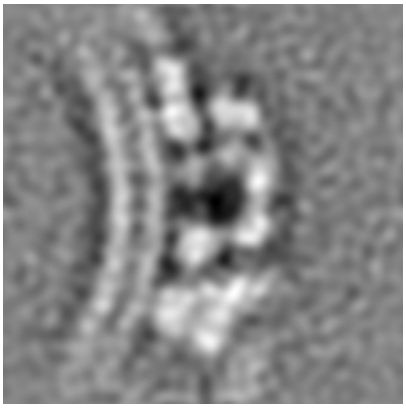

Z

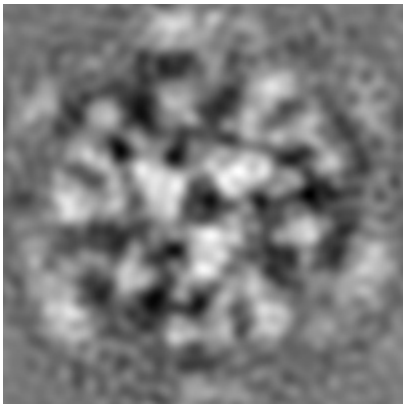
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 106

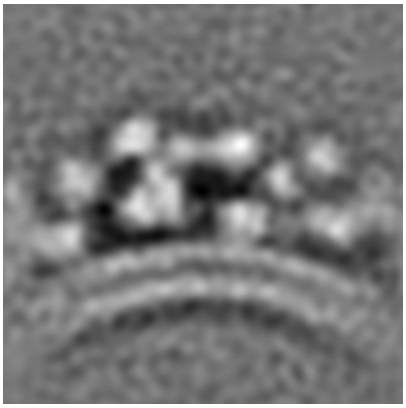

Y Index: 106


Z Index: 106

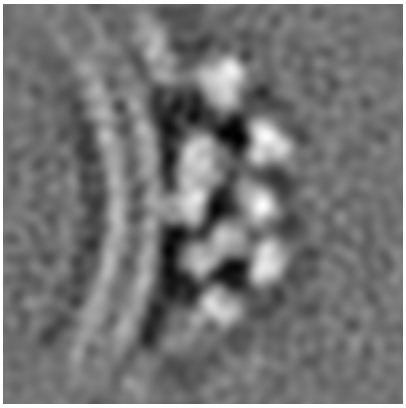
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

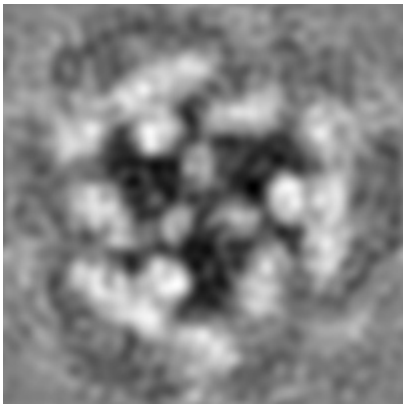
6.3.1 Primary map



X Index: 105



Y Index: 127



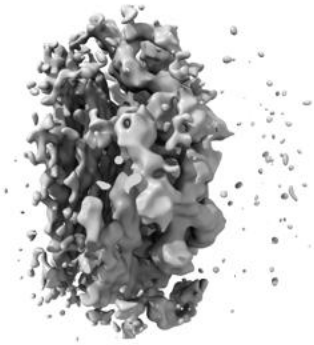
Z Index: 89

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

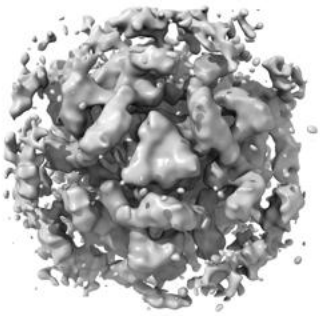
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

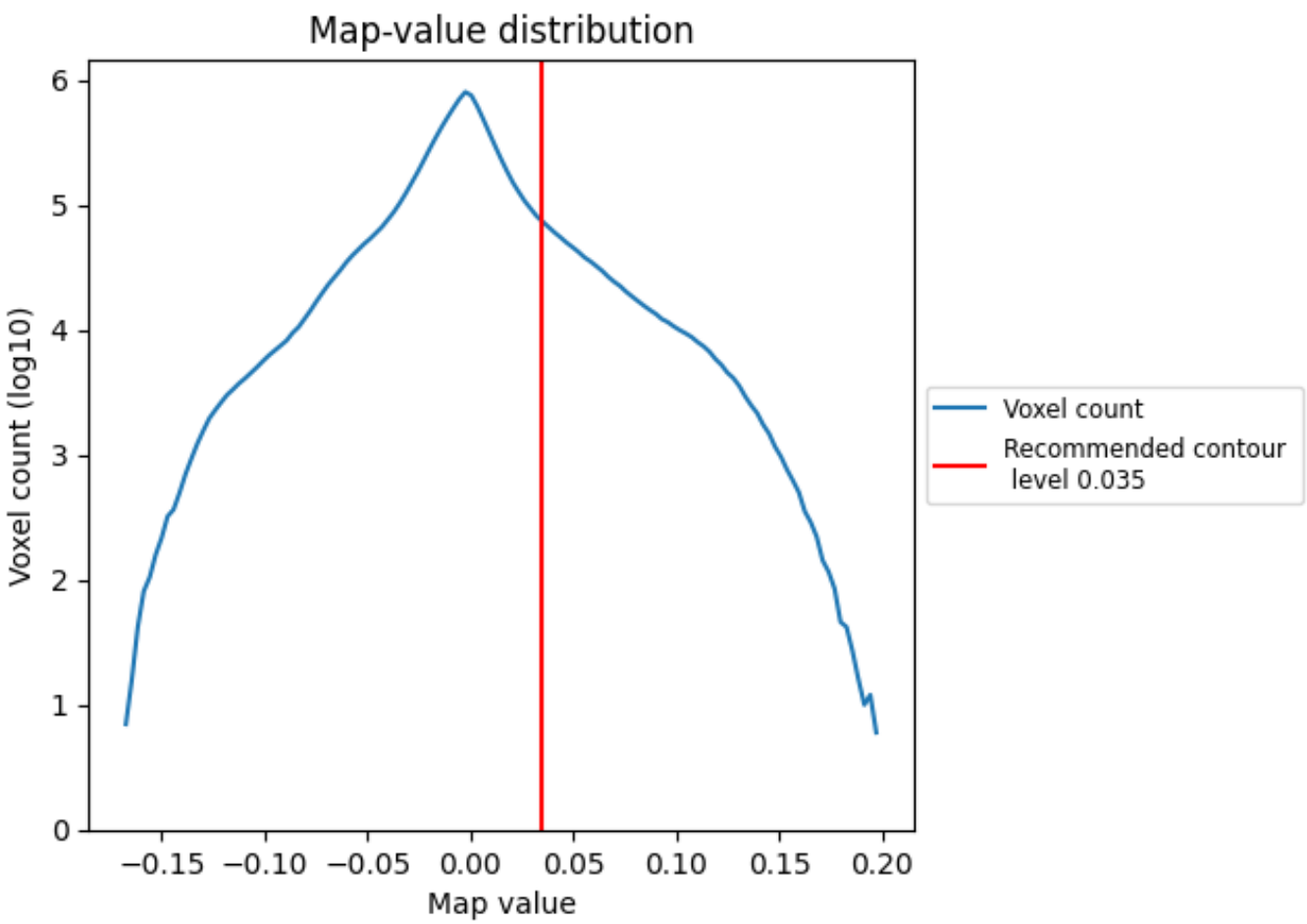
6.5 Mask visualisation (i)

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

7 Map analysis (i)

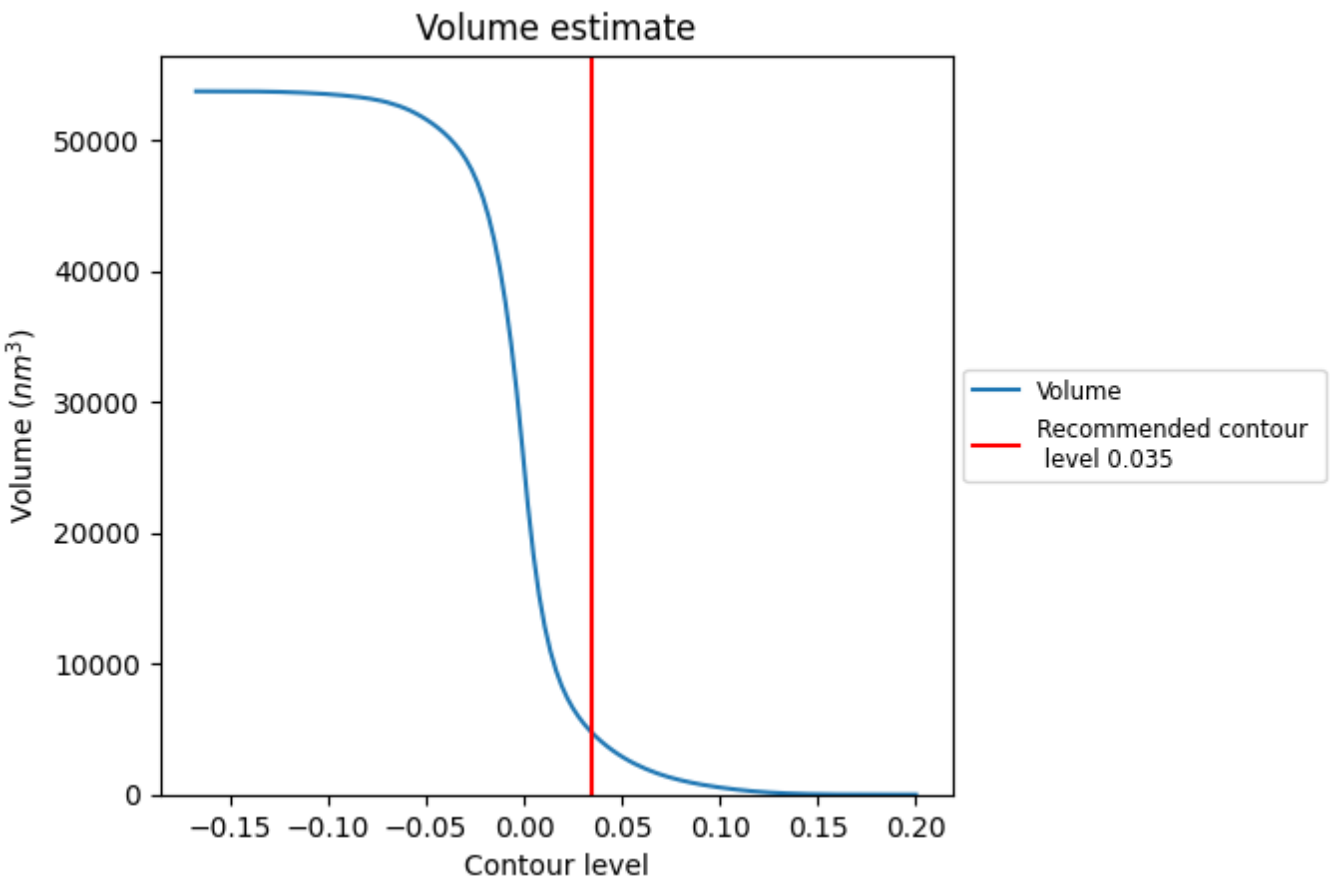
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

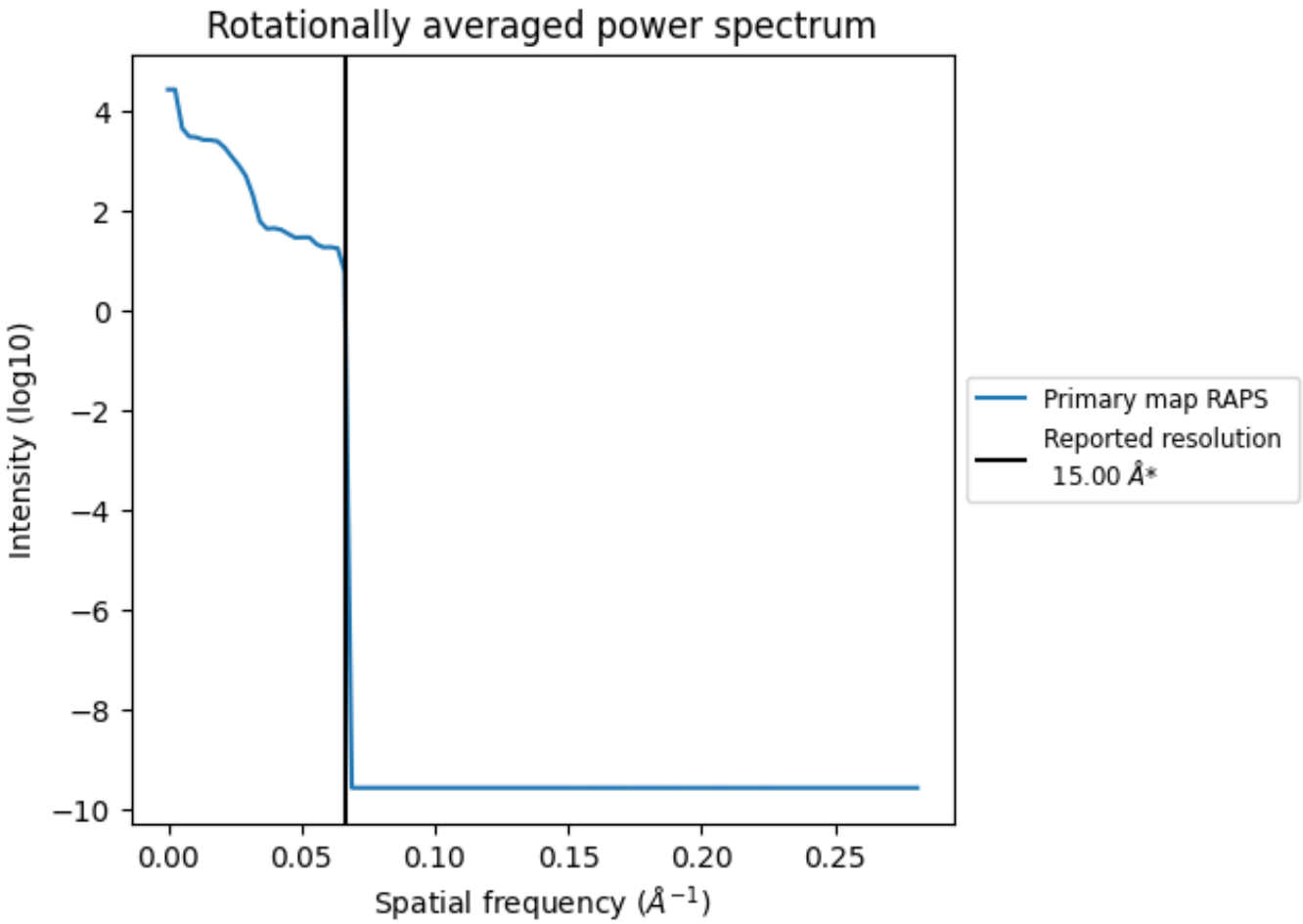
7.2 Volume estimate (i)



The volume at the recommended contour level is 4694 nm^3; this corresponds to an approximate mass of 4240 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)

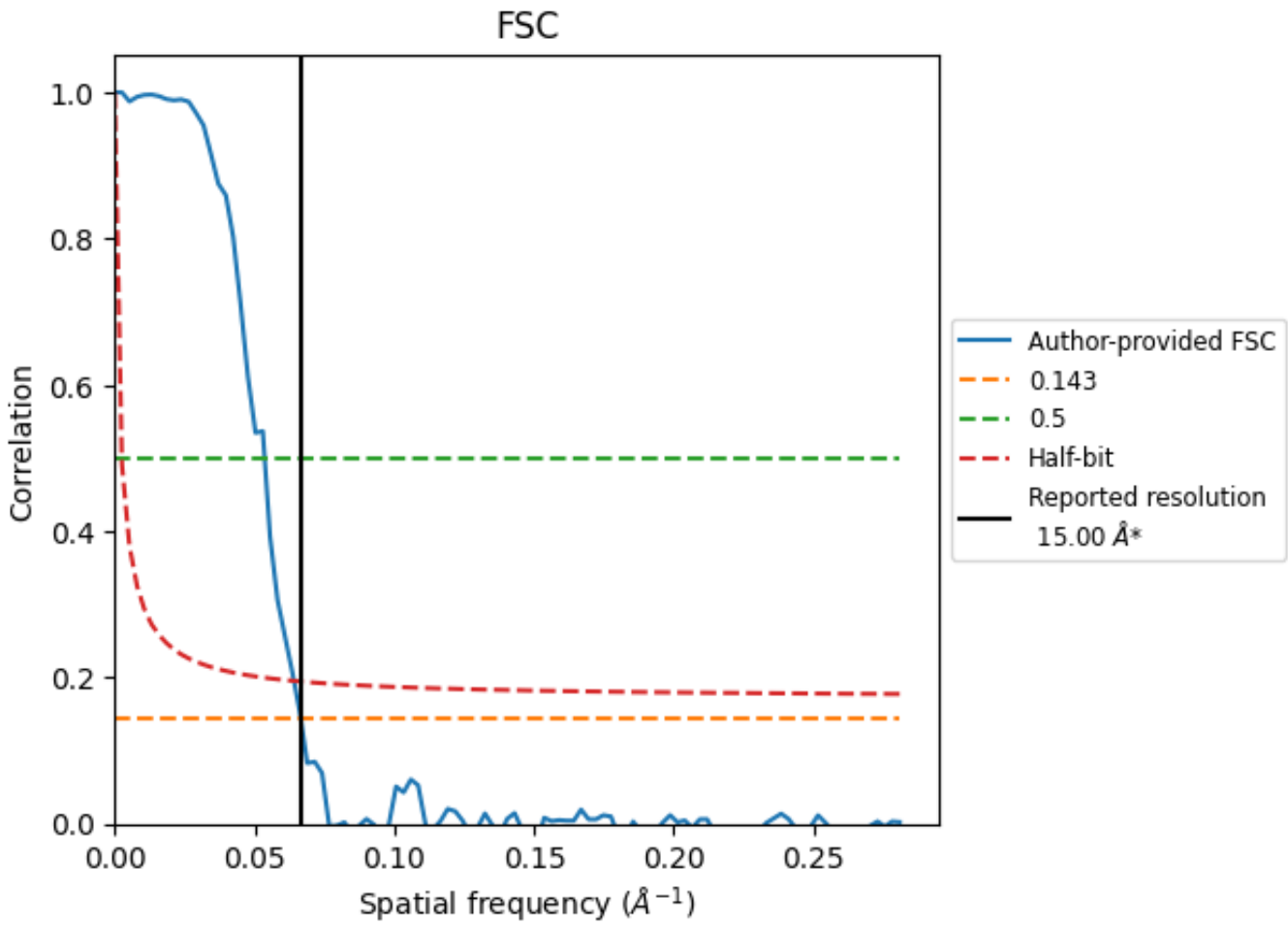


*Reported resolution corresponds to spatial frequency of 0.067 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.067 Å^{-1}

8.2 Resolution estimates (i)

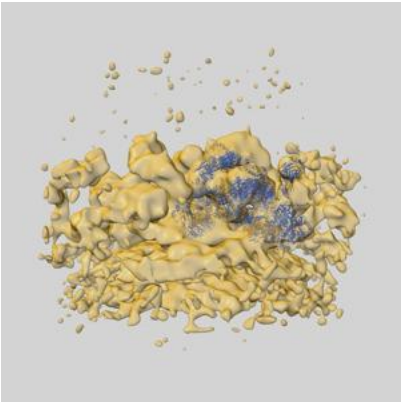
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	15.00	-	-
Author-provided FSC curve	15.02	18.62	15.58
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

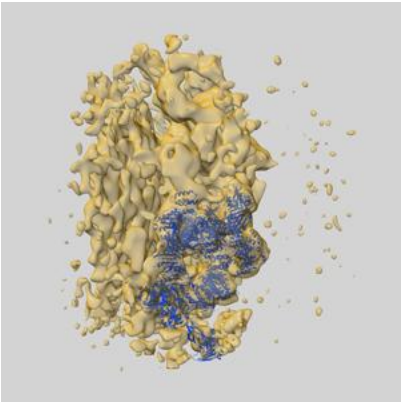
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3723 and PDB model 5NZU. Per-residue inclusion information can be found in section 3 on page 8.

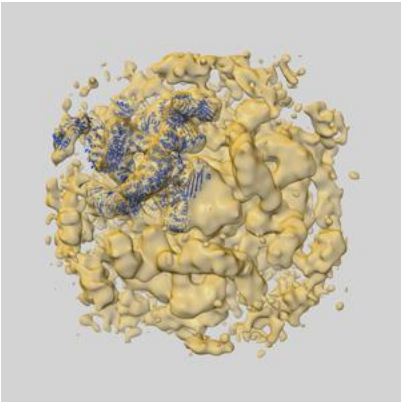
9.1 Map-model overlay (i)



X



Y



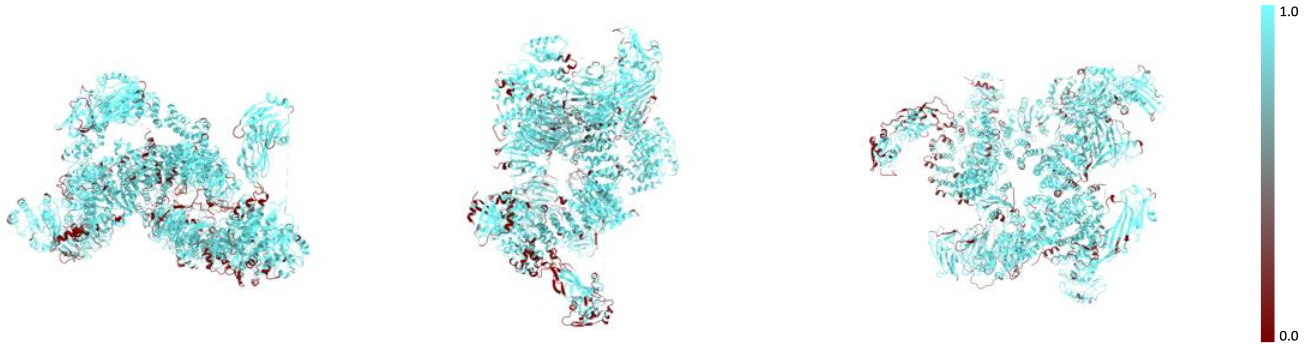
Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 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)

This section was not generated.

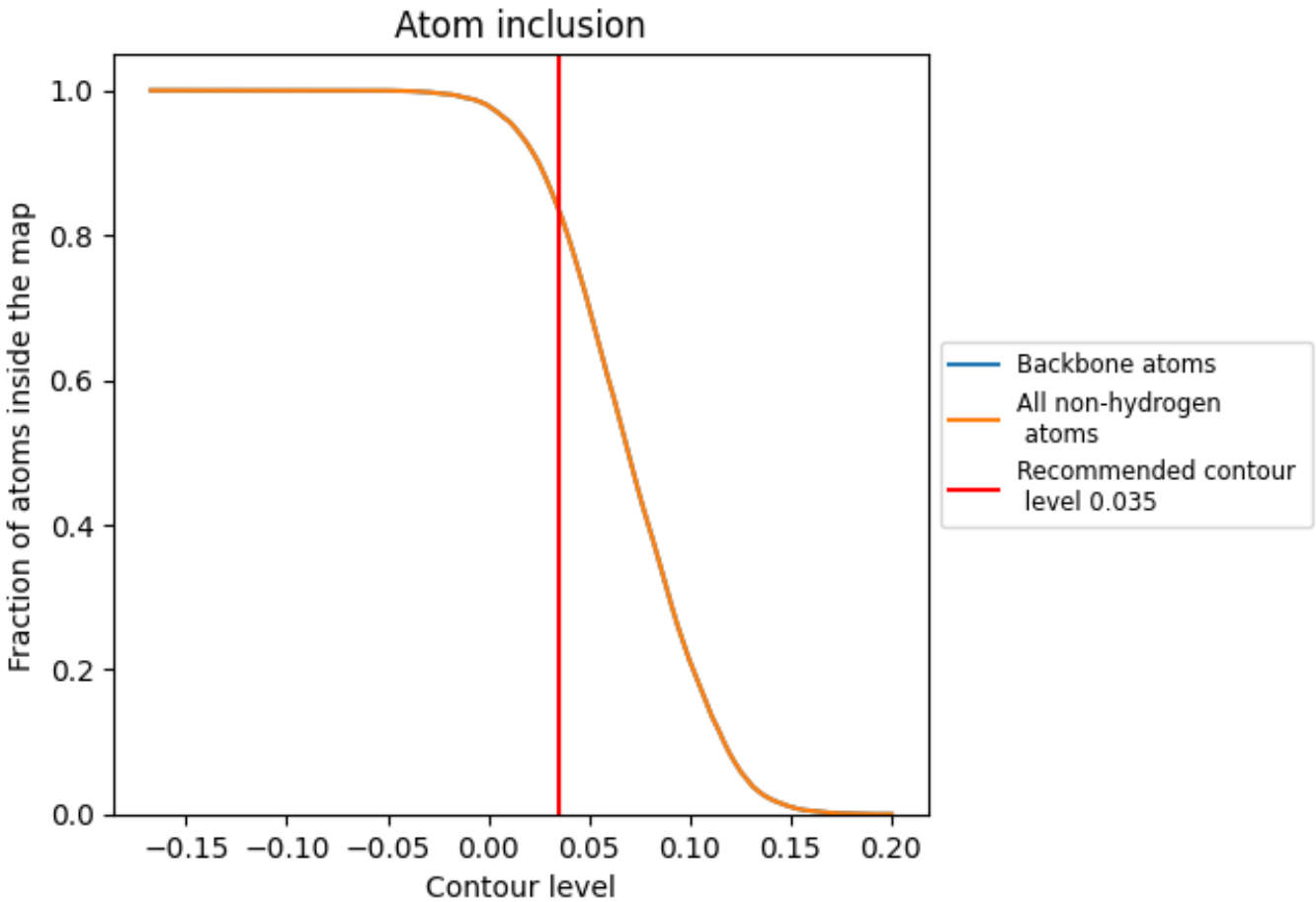
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.8354
A	0.8868
B	0.8324
C	0.8959
D	0.8120
F	0.9181
G	0.7044
K	0.8781
L	0.8108
M	0.8945
R	0.7370
Z	0.8126