wwPDB EM Validation Summary Report

Dec 12, 2022 – 03:07 am GMT

PDB ID	:	5A1Y
EMDB ID	:	EMD-2989
Title	:	The structure of the COPI coat linkage IV
Authors	:	Dodonova, S.O.; Diestelkoetter-Bachert, P.; von Appen, A.; Hagen, W.J.H.; Beck, R.; Beck, M.; Wieland, F.; Briggs, J.A.G.
Deposited on	:	2015-05-06
Resolution	:	21.00 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 ⓘ symbol.

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

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

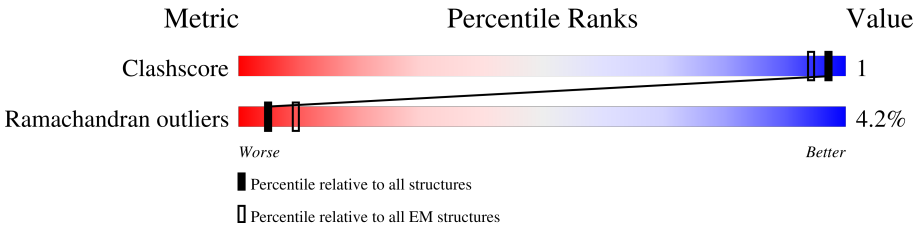
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 21.00 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	A	181	23% 88% 12%
1	B	181	8% 88% 12%
1	I	181	66% 88% 12%
1	J	181	43% 87% · 12%
1	R	181	26% 88% 12%
2	C	1262	9% 84% 5% 11%
2	K	1262	26% 84% 5% 11%
3	D	905	10% 80% 9% 11%
3	L	905	14% 80% 9% 11%

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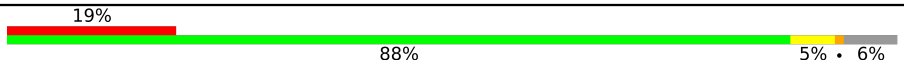
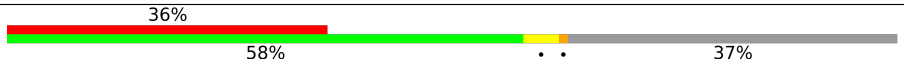
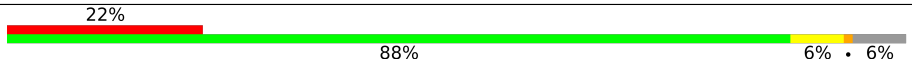
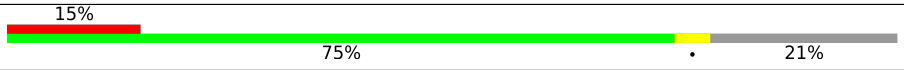
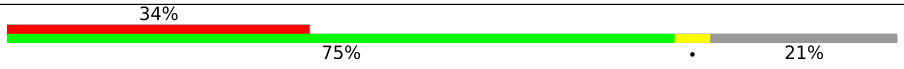
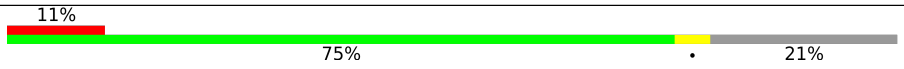
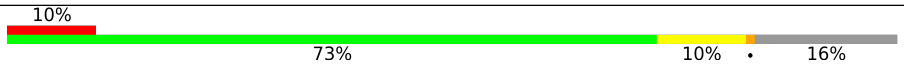
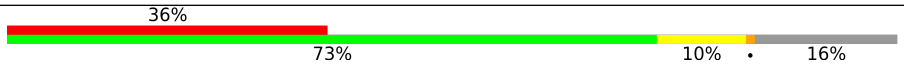
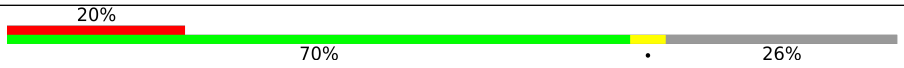
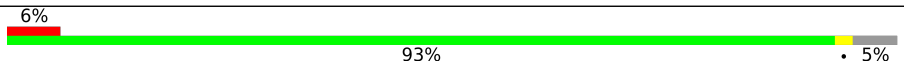
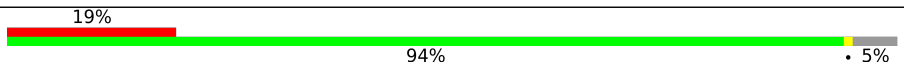
Mol	Chain	Length	Quality of chain
4	E	874	
4	M	874	
4	V	874	
5	F	177	
5	N	177	
5	W	177	
6	G	968	
6	O	968	
7	H	511	
7	P	511	
8	X	308	
8	Z	308	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 39957 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 ADP-RIBOSYLATION FACTOR 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	159	Total 636	C 318	N 159	O 159	0	0
1	B	159	Total 636	C 318	N 159	O 159	0	0
1	I	159	Total 636	C 318	N 159	O 159	0	0
1	J	159	Total 636	C 318	N 159	O 159	0	0
1	R	159	Total 636	C 318	N 159	O 159	0	0

- Molecule 2 is a protein called COATOMER SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	1126	Total 4503	C 2252	N 1126	O 1125	0	0
2	K	1126	Total 4503	C 2252	N 1126	O 1125	0	0

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1225	LEU	-	expression tag	UNP Q8CIE6
C	1226	GLU	-	expression tag	UNP Q8CIE6
C	1227	VAL	-	expression tag	UNP Q8CIE6
C	1228	LEU	-	expression tag	UNP Q8CIE6
C	1229	PHE	-	expression tag	UNP Q8CIE6
C	1230	GLN	-	expression tag	UNP Q8CIE6
C	1231	GLY	-	expression tag	UNP Q8CIE6
C	1232	PRO	-	expression tag	UNP Q8CIE6
C	1233	SER	-	expression tag	UNP Q8CIE6
C	1234	ALA	-	expression tag	UNP Q8CIE6
C	1235	TRP	-	expression tag	UNP Q8CIE6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1236	SER	-	expression tag	UNP Q8CIE6
C	1237	HIS	-	expression tag	UNP Q8CIE6
C	1238	PRO	-	expression tag	UNP Q8CIE6
C	1239	GLN	-	expression tag	UNP Q8CIE6
C	1240	PHE	-	expression tag	UNP Q8CIE6
C	1241	GLU	-	expression tag	UNP Q8CIE6
C	1242	LYS	-	expression tag	UNP Q8CIE6
C	1243	GLY	-	expression tag	UNP Q8CIE6
C	1244	GLY	-	expression tag	UNP Q8CIE6
C	1245	GLY	-	expression tag	UNP Q8CIE6
C	1246	SER	-	expression tag	UNP Q8CIE6
C	1247	GLY	-	expression tag	UNP Q8CIE6
C	1248	GLY	-	expression tag	UNP Q8CIE6
C	1249	GLY	-	expression tag	UNP Q8CIE6
C	1250	SER	-	expression tag	UNP Q8CIE6
C	1251	GLY	-	expression tag	UNP Q8CIE6
C	1252	GLY	-	expression tag	UNP Q8CIE6
C	1253	SER	-	expression tag	UNP Q8CIE6
C	1254	ALA	-	expression tag	UNP Q8CIE6
C	1255	TRP	-	expression tag	UNP Q8CIE6
C	1256	SER	-	expression tag	UNP Q8CIE6
C	1257	HIS	-	expression tag	UNP Q8CIE6
C	1258	PRO	-	expression tag	UNP Q8CIE6
C	1259	GLN	-	expression tag	UNP Q8CIE6
C	1260	PHE	-	expression tag	UNP Q8CIE6
C	1261	GLU	-	expression tag	UNP Q8CIE6
C	1262	LYS	-	expression tag	UNP Q8CIE6
K	1225	LEU	-	expression tag	UNP Q8CIE6
K	1226	GLU	-	expression tag	UNP Q8CIE6
K	1227	VAL	-	expression tag	UNP Q8CIE6
K	1228	LEU	-	expression tag	UNP Q8CIE6
K	1229	PHE	-	expression tag	UNP Q8CIE6
K	1230	GLN	-	expression tag	UNP Q8CIE6
K	1231	GLY	-	expression tag	UNP Q8CIE6
K	1232	PRO	-	expression tag	UNP Q8CIE6
K	1233	SER	-	expression tag	UNP Q8CIE6
K	1234	ALA	-	expression tag	UNP Q8CIE6
K	1235	TRP	-	expression tag	UNP Q8CIE6
K	1236	SER	-	expression tag	UNP Q8CIE6
K	1237	HIS	-	expression tag	UNP Q8CIE6
K	1238	PRO	-	expression tag	UNP Q8CIE6
K	1239	GLN	-	expression tag	UNP Q8CIE6

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1240	PHE	-	expression tag	UNP Q8CIE6
K	1241	GLU	-	expression tag	UNP Q8CIE6
K	1242	LYS	-	expression tag	UNP Q8CIE6
K	1243	GLY	-	expression tag	UNP Q8CIE6
K	1244	GLY	-	expression tag	UNP Q8CIE6
K	1245	GLY	-	expression tag	UNP Q8CIE6
K	1246	SER	-	expression tag	UNP Q8CIE6
K	1247	GLY	-	expression tag	UNP Q8CIE6
K	1248	GLY	-	expression tag	UNP Q8CIE6
K	1249	GLY	-	expression tag	UNP Q8CIE6
K	1250	SER	-	expression tag	UNP Q8CIE6
K	1251	GLY	-	expression tag	UNP Q8CIE6
K	1252	GLY	-	expression tag	UNP Q8CIE6
K	1253	SER	-	expression tag	UNP Q8CIE6
K	1254	ALA	-	expression tag	UNP Q8CIE6
K	1255	TRP	-	expression tag	UNP Q8CIE6
K	1256	SER	-	expression tag	UNP Q8CIE6
K	1257	HIS	-	expression tag	UNP Q8CIE6
K	1258	PRO	-	expression tag	UNP Q8CIE6
K	1259	GLN	-	expression tag	UNP Q8CIE6
K	1260	PHE	-	expression tag	UNP Q8CIE6
K	1261	GLU	-	expression tag	UNP Q8CIE6
K	1262	LYS	-	expression tag	UNP Q8CIE6

- Molecule 3 is a protein called COATOMER SUBUNIT BETA'.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	803	Total	C	N	O	0	0
			3211	1606	803	802		
3	L	803	Total	C	N	O	0	0
			3211	1606	803	802		

- Molecule 4 is a protein called COATOMER SUBUNIT GAMMA-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	824	Total	C	N	O	0	0
			3294	1648	824	822		
4	M	550	Total	C	N	O	0	0
			2199	1100	550	549		
4	V	824	Total	C	N	O	0	0
			3294	1648	824	822		

- Molecule 5 is a protein called COATOMER SUBUNIT ZETA-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	F	139	Total 555	C 278	N 139	O 138	0	0
5	N	139	Total 555	C 278	N 139	O 138	0	0
5	W	139	Total 555	C 278	N 139	O 138	0	0

- Molecule 6 is a protein called COATOMER SUBUNIT BETA.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	G	813	Total 3250	C 1626	N 813	O 811	0	0
6	O	813	Total 3250	C 1626	N 813	O 811	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-14	MET	-	expression tag	UNP Q9JIF7
G	-13	HIS	-	expression tag	UNP Q9JIF7
G	-12	HIS	-	expression tag	UNP Q9JIF7
G	-11	HIS	-	expression tag	UNP Q9JIF7
G	-10	HIS	-	expression tag	UNP Q9JIF7
G	-9	HIS	-	expression tag	UNP Q9JIF7
G	-8	HIS	-	expression tag	UNP Q9JIF7
G	-7	GLU	-	expression tag	UNP Q9JIF7
G	-6	ASN	-	expression tag	UNP Q9JIF7
G	-5	LEU	-	expression tag	UNP Q9JIF7
G	-4	TYR	-	expression tag	UNP Q9JIF7
G	-3	PHE	-	expression tag	UNP Q9JIF7
G	-2	GLN	-	expression tag	UNP Q9JIF7
G	-1	GLY	-	expression tag	UNP Q9JIF7
G	0	HIS	-	expression tag	UNP Q9JIF7
O	-14	MET	-	expression tag	UNP Q9JIF7
O	-13	HIS	-	expression tag	UNP Q9JIF7
O	-12	HIS	-	expression tag	UNP Q9JIF7
O	-11	HIS	-	expression tag	UNP Q9JIF7
O	-10	HIS	-	expression tag	UNP Q9JIF7
O	-9	HIS	-	expression tag	UNP Q9JIF7
O	-8	HIS	-	expression tag	UNP Q9JIF7
O	-7	GLU	-	expression tag	UNP Q9JIF7

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-6	ASN	-	expression tag	UNP Q9JIF7
O	-5	LEU	-	expression tag	UNP Q9JIF7
O	-4	TYR	-	expression tag	UNP Q9JIF7
O	-3	PHE	-	expression tag	UNP Q9JIF7
O	-2	GLN	-	expression tag	UNP Q9JIF7
O	-1	GLY	-	expression tag	UNP Q9JIF7
O	0	HIS	-	expression tag	UNP Q9JIF7

- Molecule 7 is a protein called COATOMER SUBUNIT DELTA.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	380	Total	C	N	O	0	0
			1520	760	380	380		
7	P	135	Total	C	N	O	0	0
			539	270	135	134		

- Molecule 8 is a protein called COATOMER SUBUNIT EPSILON.

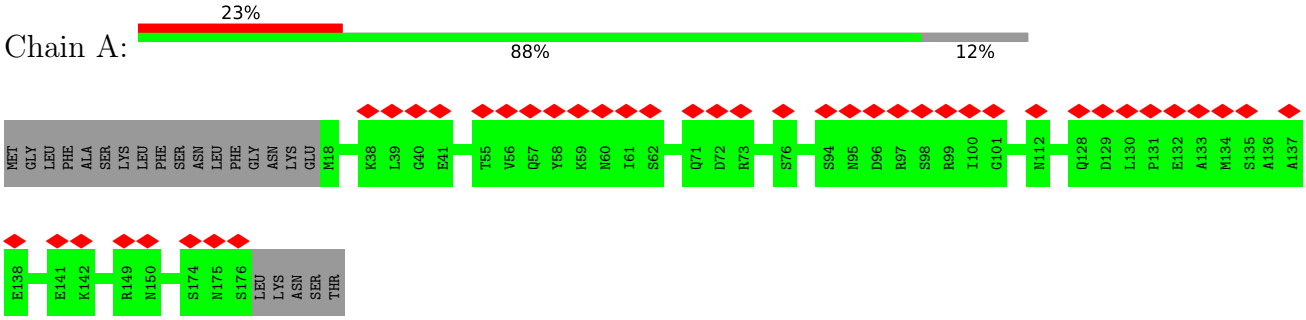
Mol	Chain	Residues	Atoms				AltConf	Trace
8	X	292	Total	C	N	O	0	0
			1169	584	292	293		
8	Z	292	Total	C	N	O	0	0
			1169	584	292	293		

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.

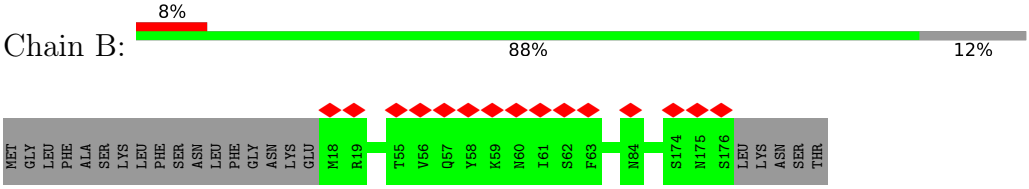
• Molecule 1: ADP-RIBOSYLATION FACTOR 1

Chain A:



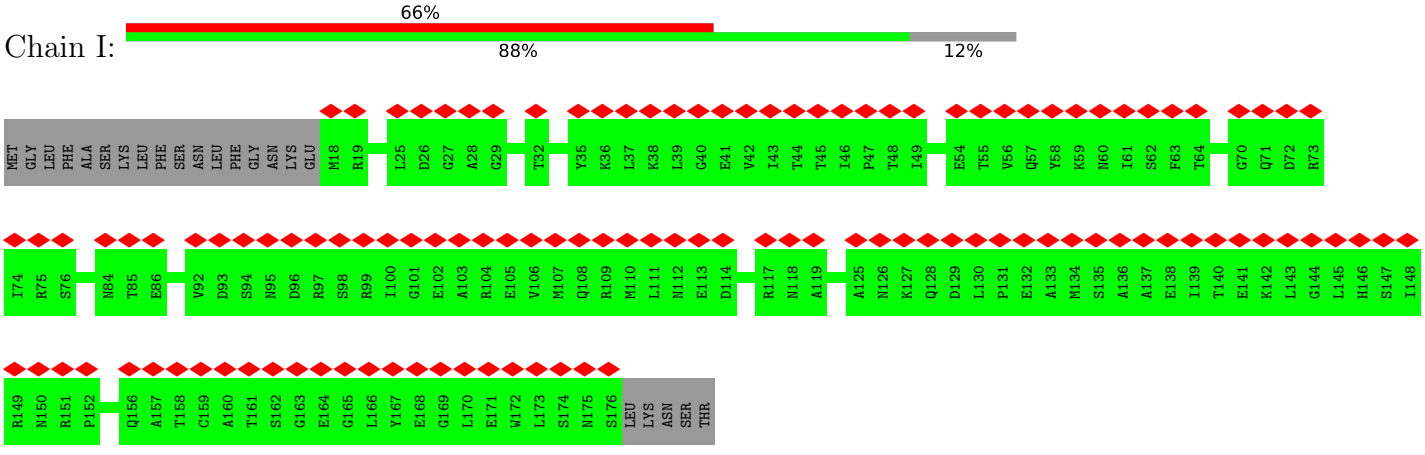
• Molecule 1: ADP-RIBOSYLATION FACTOR 1

Chain B:



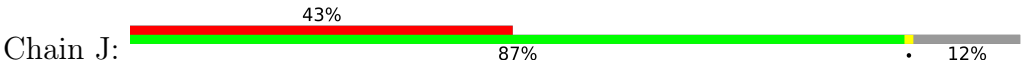
• Molecule 1: ADP-RIBOSYLATION FACTOR 1

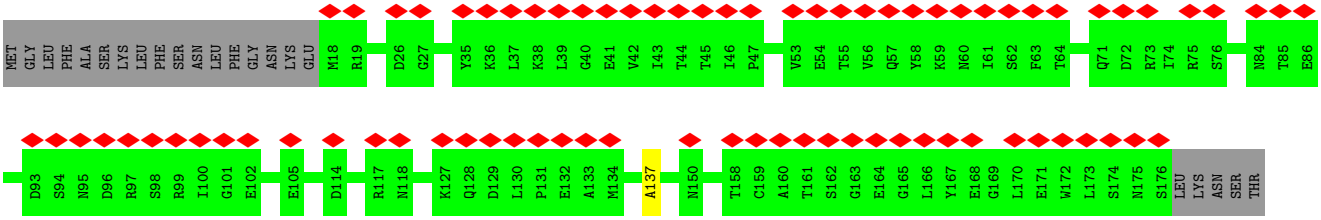
Chain I:



• Molecule 1: ADP-RIBOSYLATION FACTOR 1

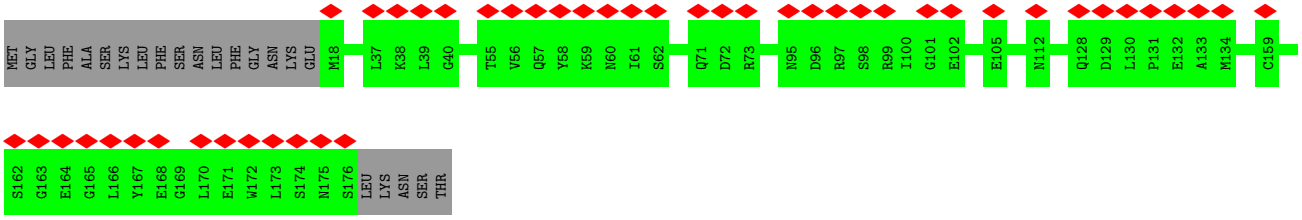
Chain J:





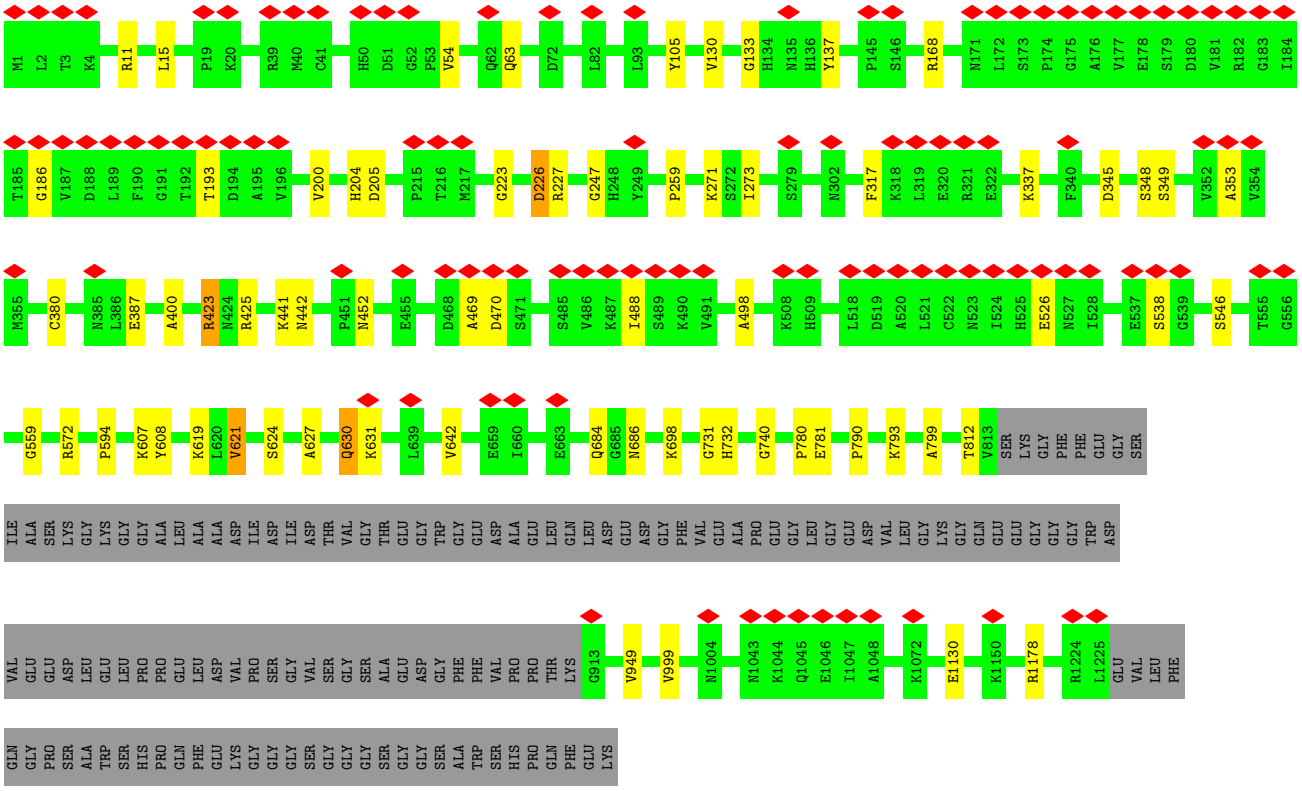
• Molecule 1: ADP-RIBOSYLATION FACTOR 1

Chain R:



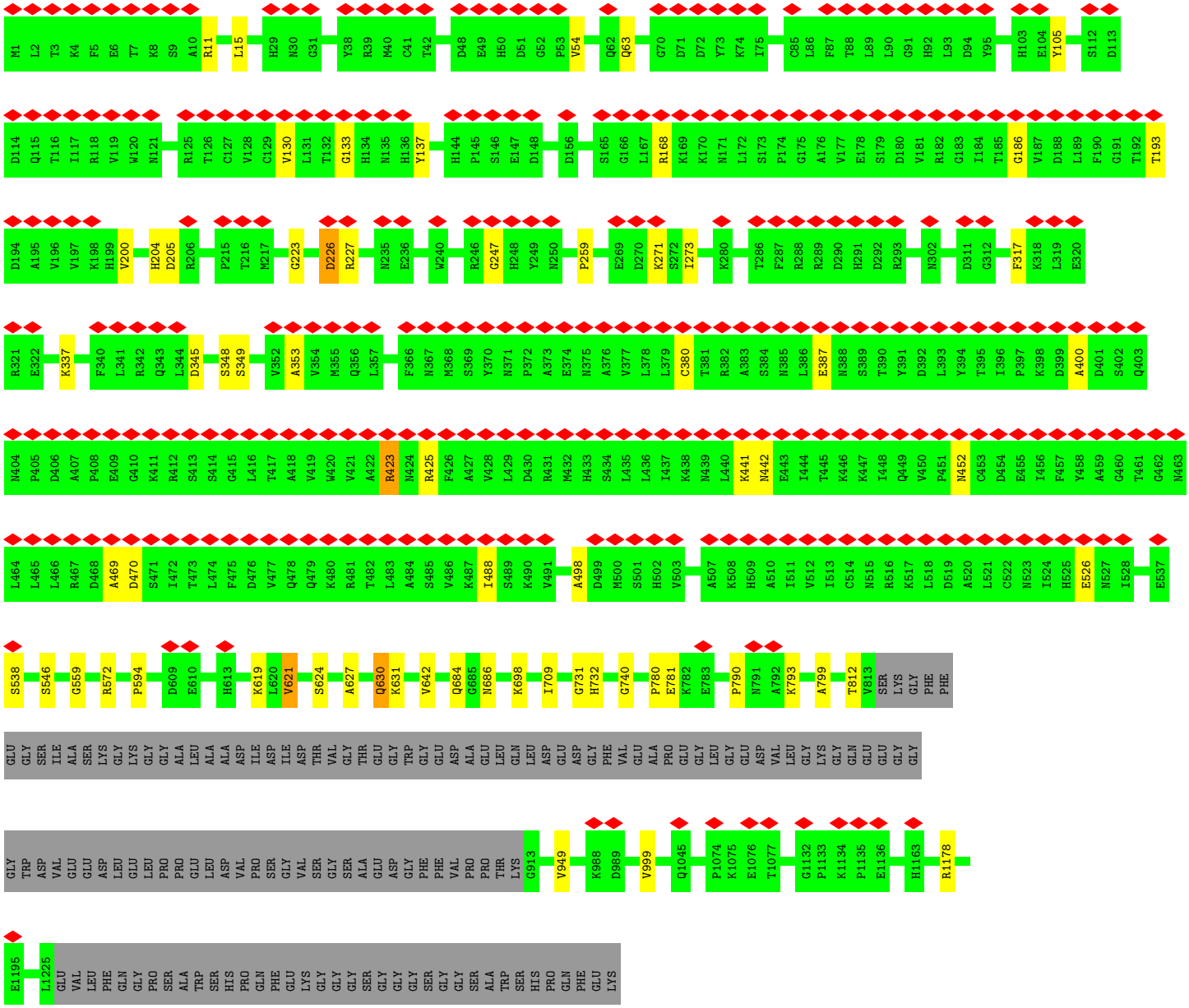
• Molecule 2: COATOMER SUBUNIT ALPHA

Chain C:



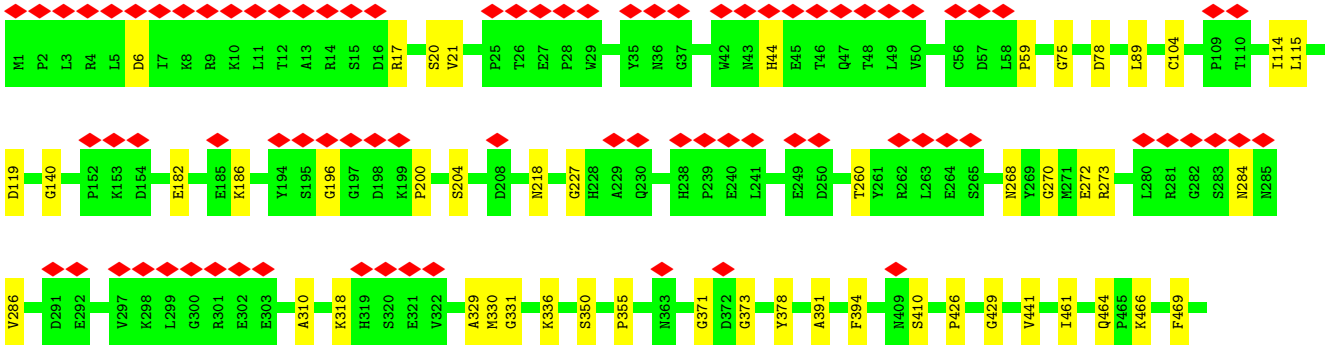
• Molecule 2: COATOMER SUBUNIT ALPHA

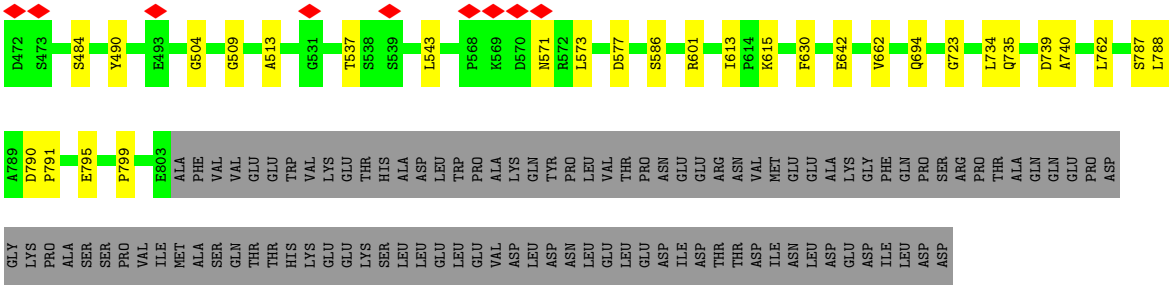
Chain K:



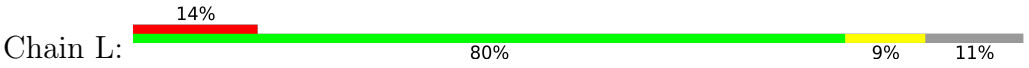
• Molecule 3: COATOMER SUBUNIT BETA'

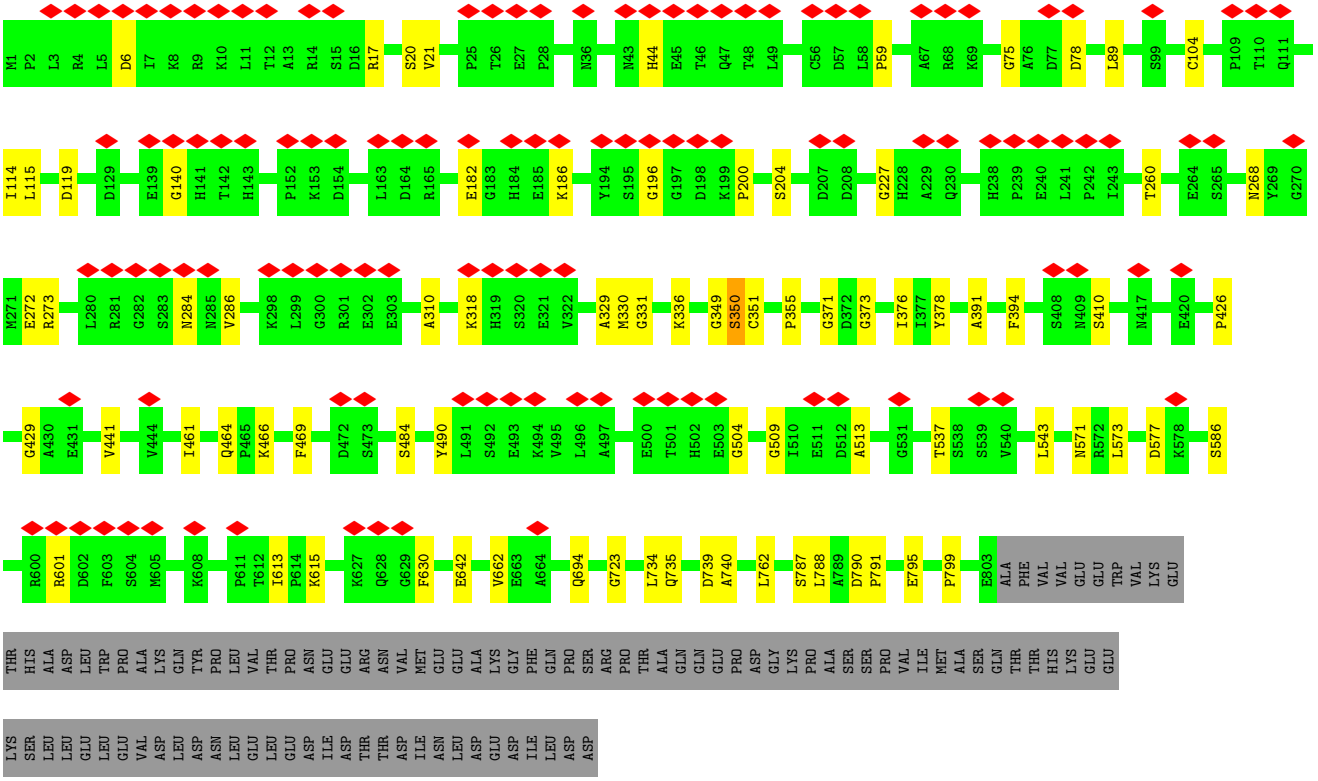
Chain D:



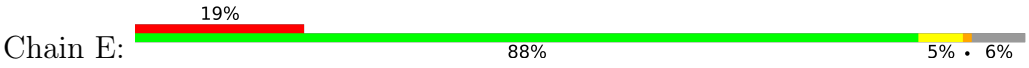


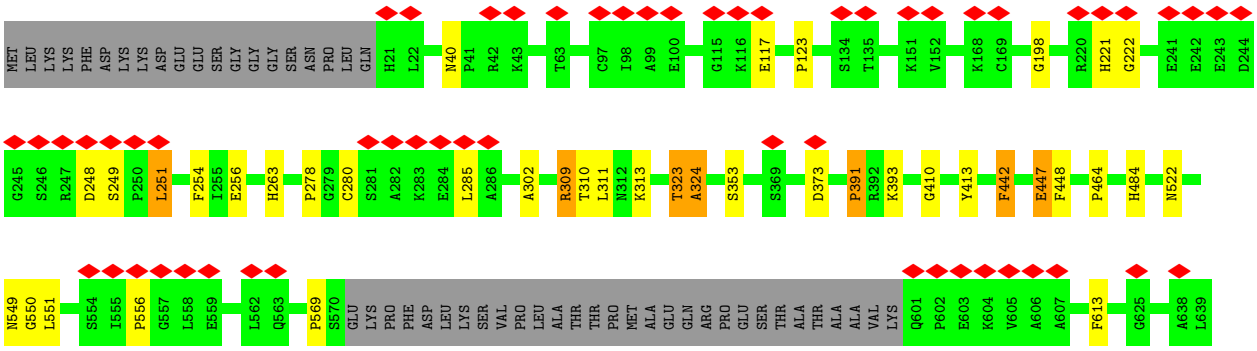
• Molecule 3: COATOMER SUBUNIT BETA'

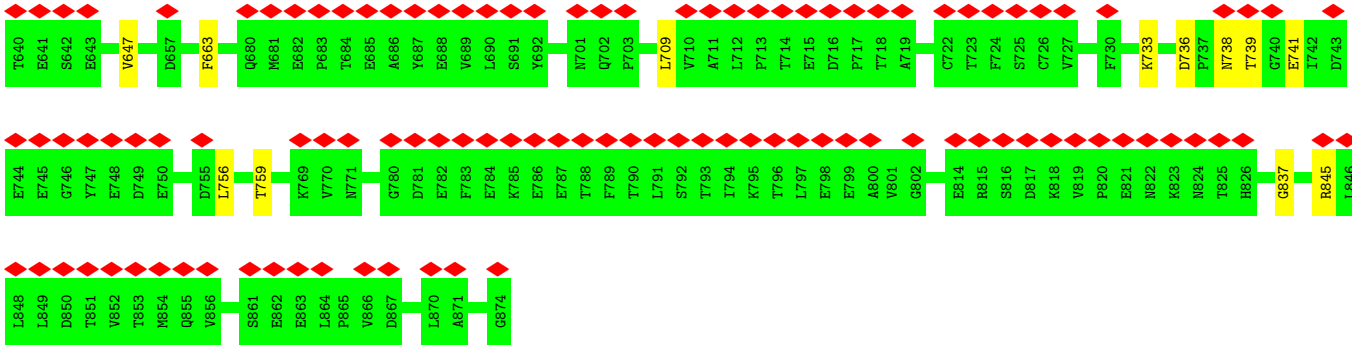




• Molecule 4: COATOMER SUBUNIT GAMMA-1

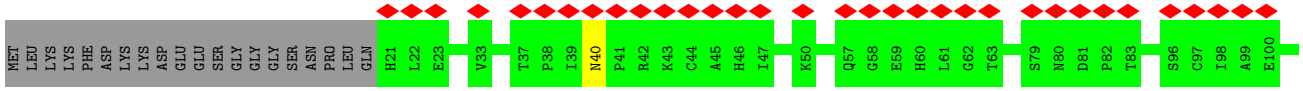


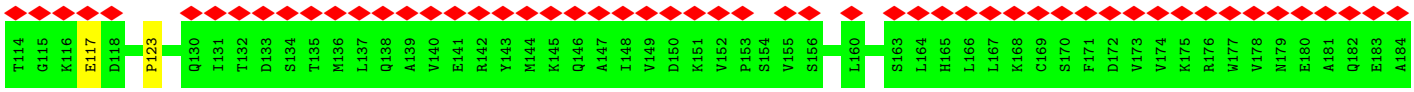


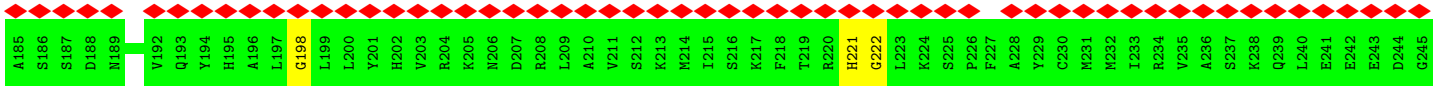


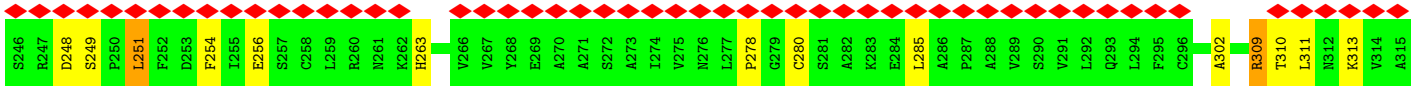
• Molecule 4: COATOMER SUBUNIT GAMMA-1

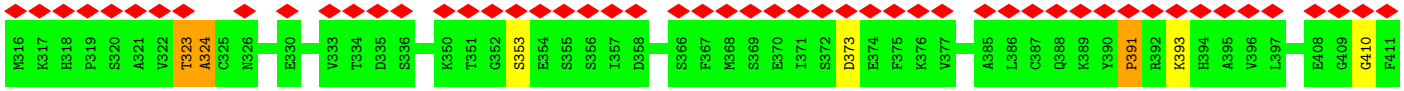
Chain M:

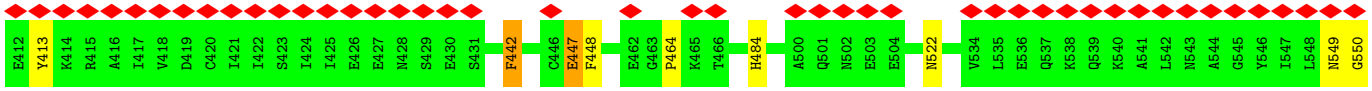


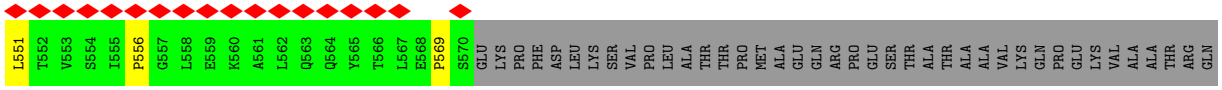


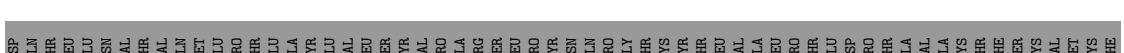


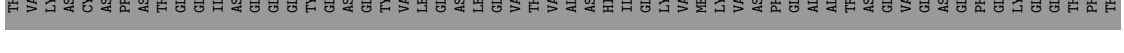






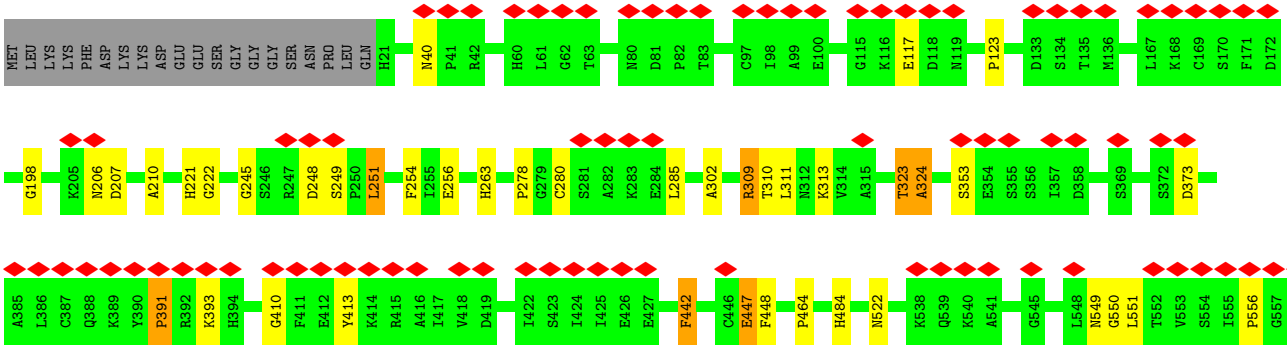


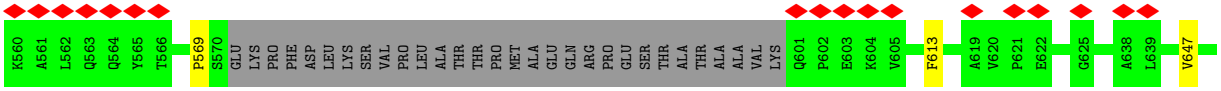


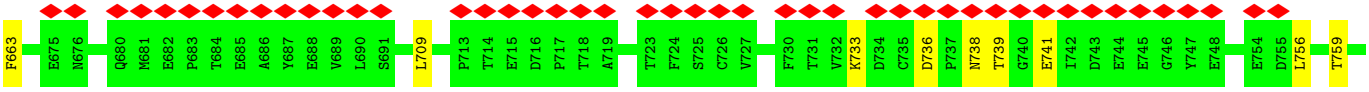


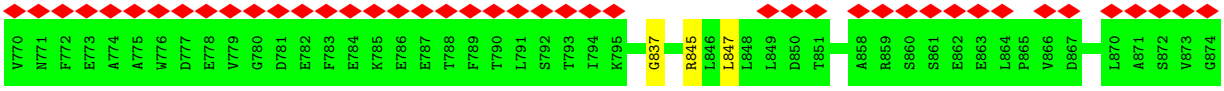
• Molecule 4: COATOMER SUBUNIT GAMMA-1

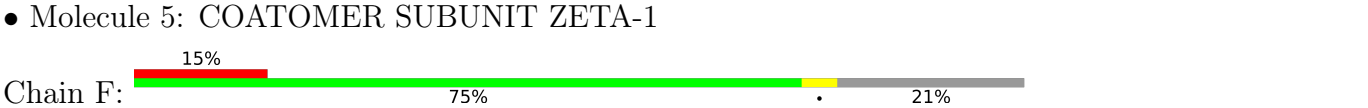
Chain V:

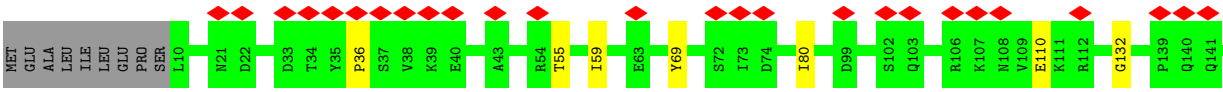






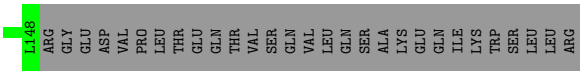






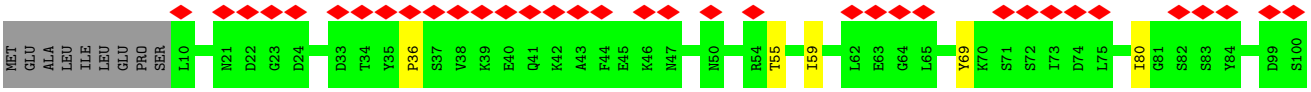
• Molecule 5: COATOMER SUBUNIT ZETA-1

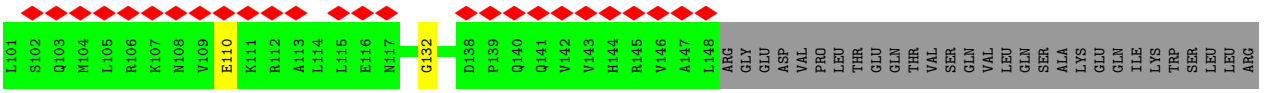
Chain F:



• Molecule 5: COATOMER SUBUNIT ZETA-1

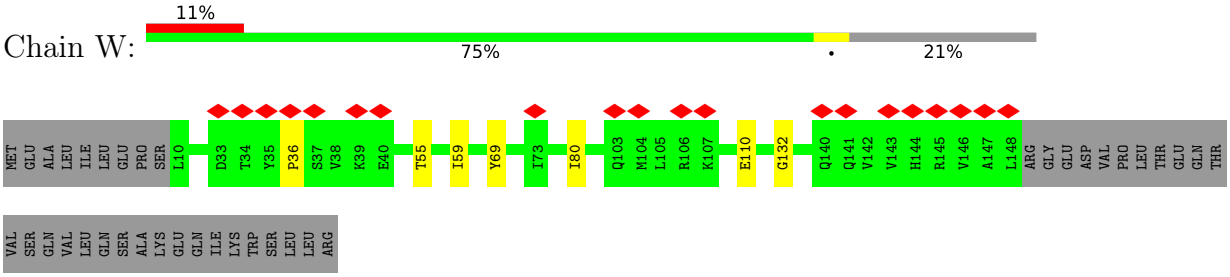
Chain N:





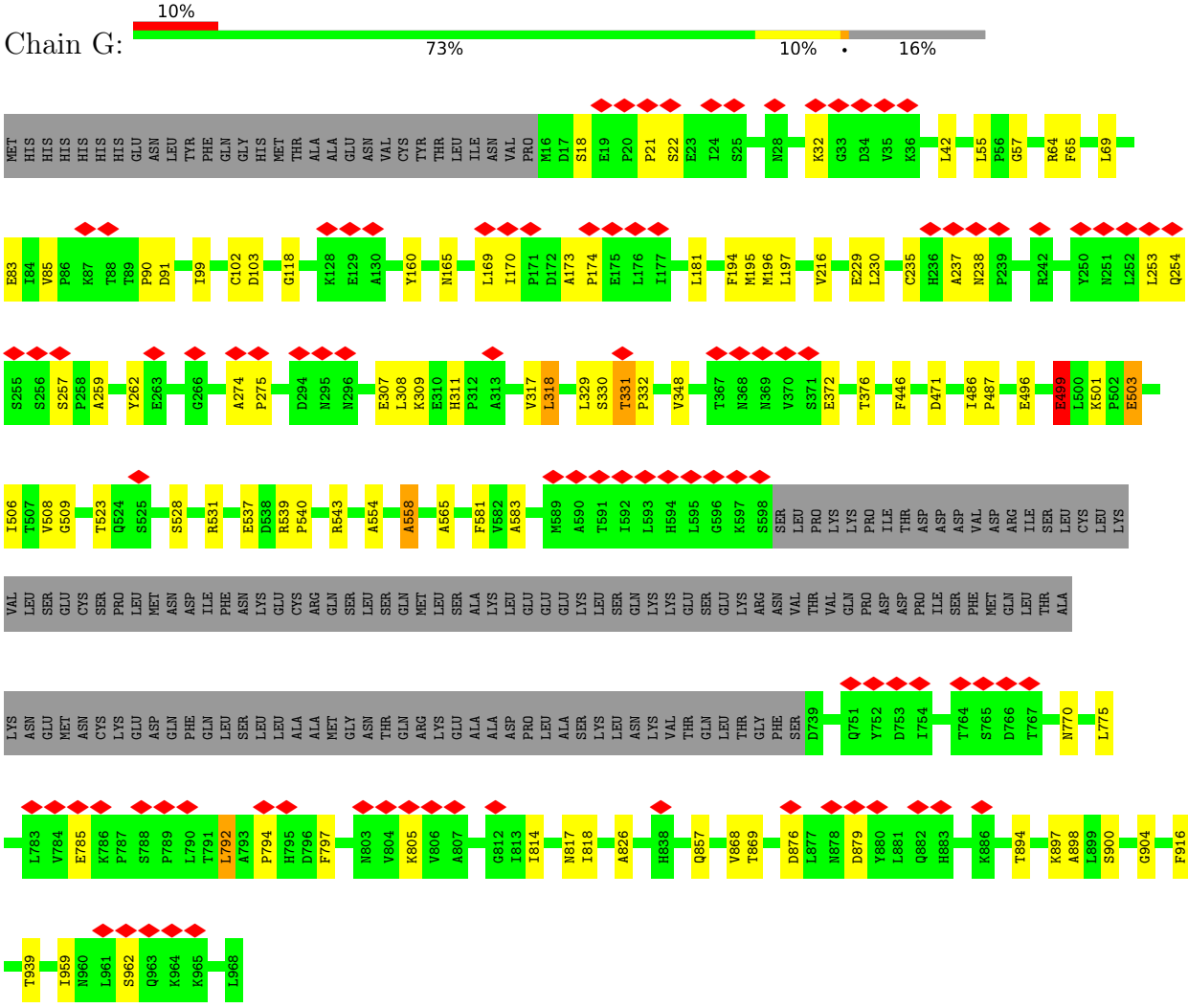
• Molecule 5: COATOMER SUBUNIT ZETA-1

Chain W:



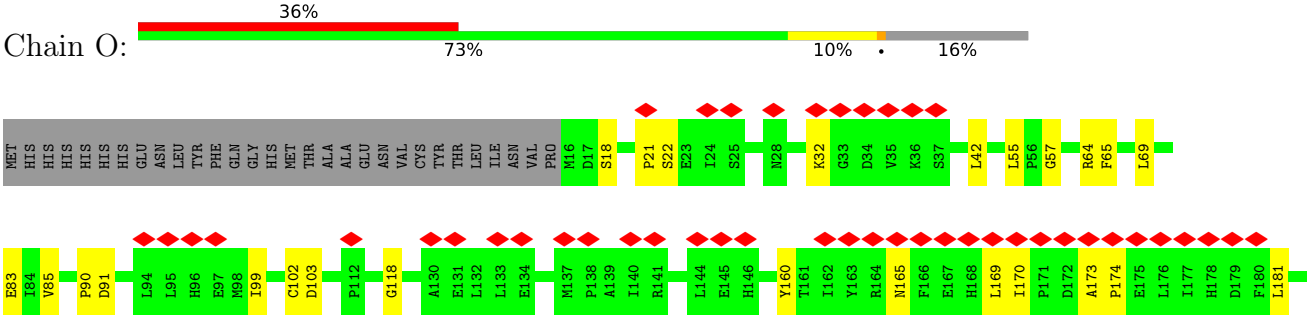
• Molecule 6: COATOMER SUBUNIT BETA

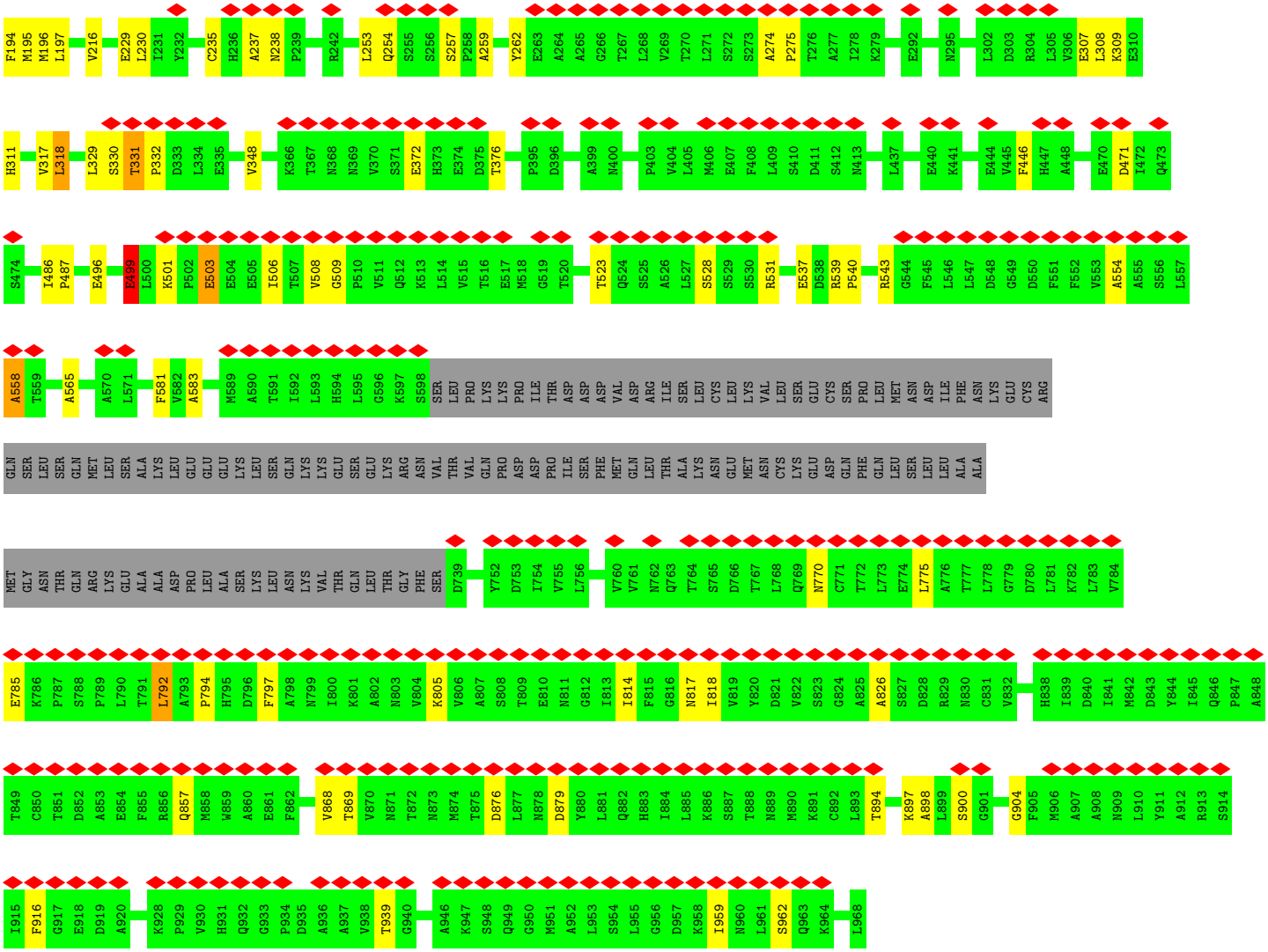
Chain G:

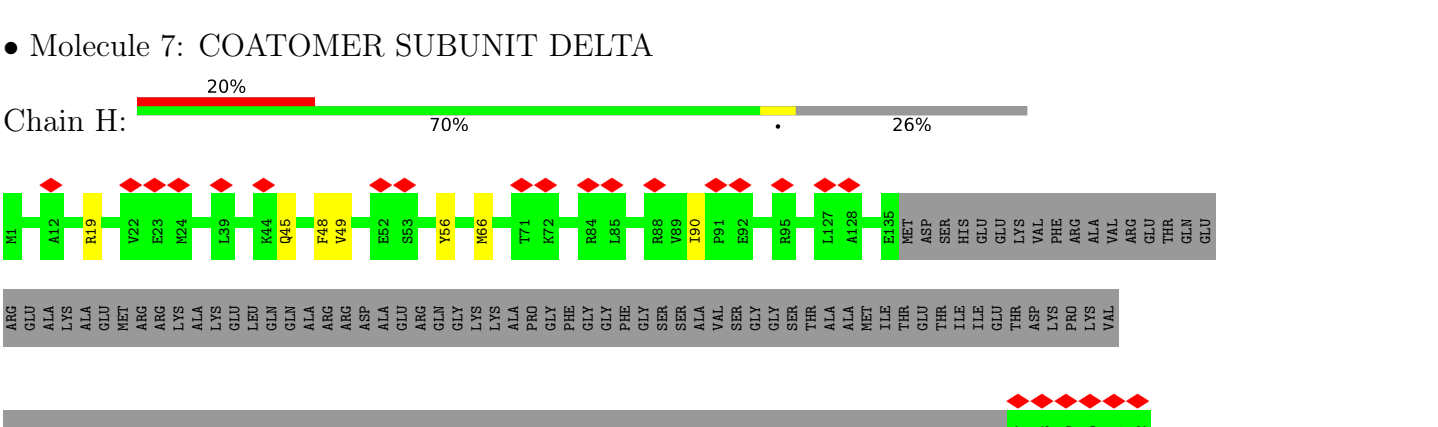


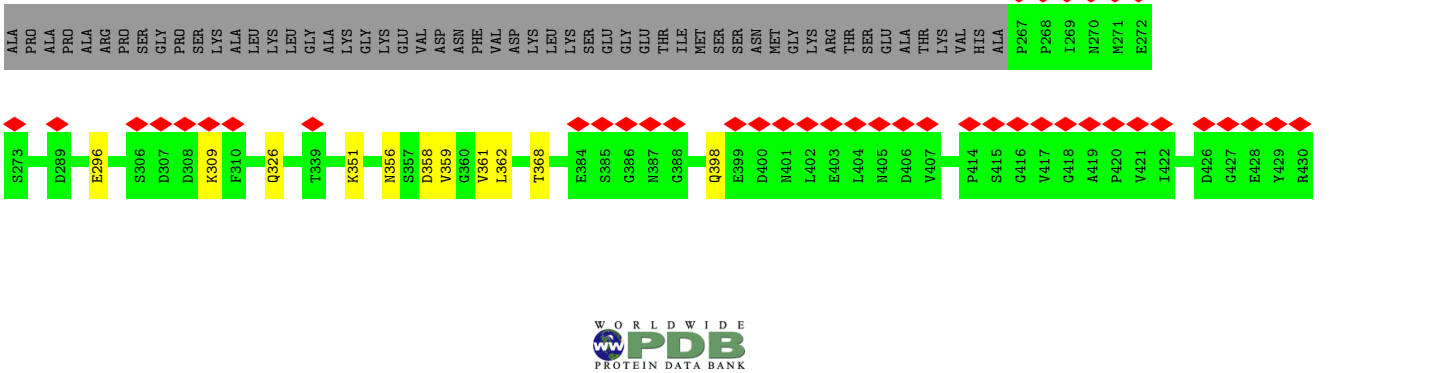
• Molecule 6: COATOMER SUBUNIT BETA

Chain O:



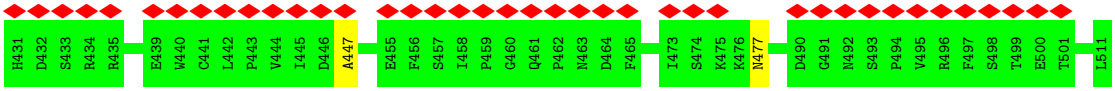




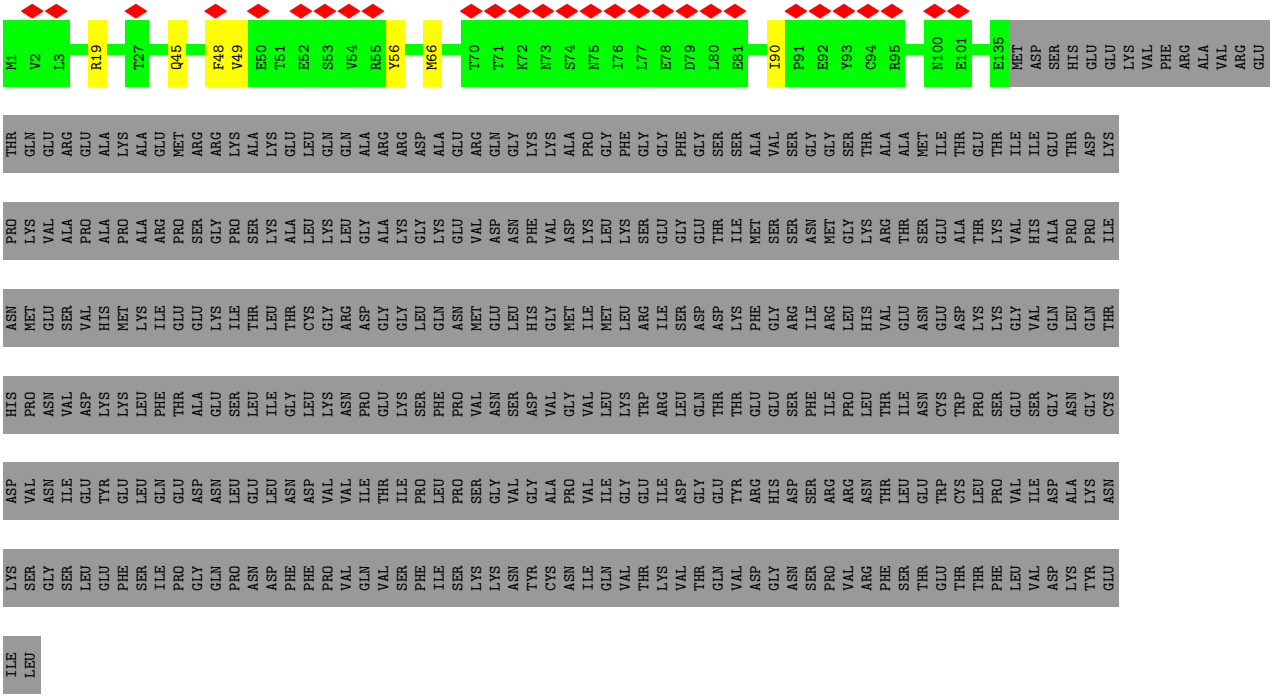


• Molecule 7: COATOMER SUBUNIT DELTA

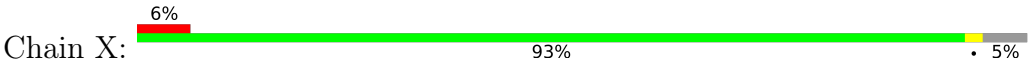
Chain H:

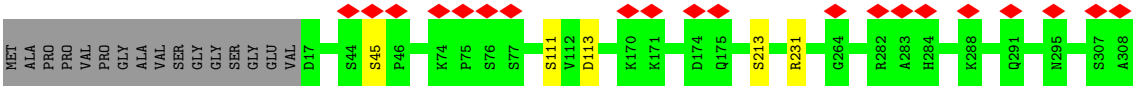


• Molecule 7: COATOMER SUBUNIT DELTA

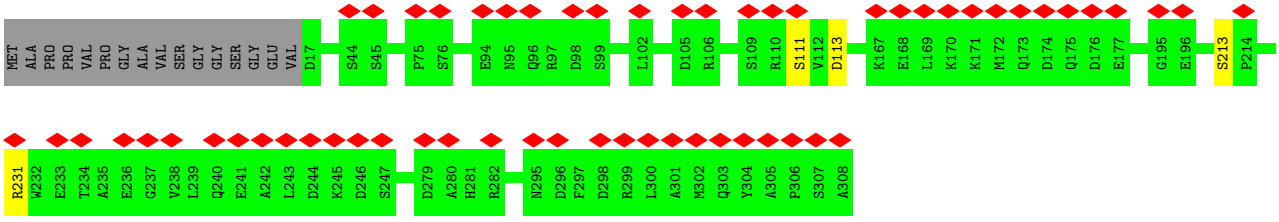


• Molecule 8: COATOMER SUBUNIT EPSILON





• Molecule 8: COATOMER SUBUNIT EPSILON



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of tilted images used	1205	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING OF INDIVIDUAL TILTS	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	42000	Depositor
Image detector	GATAN MULTISCAN	Depositor
Maximum voxel value	6.961	Depositor
Minimum voxel value	-5.585	Depositor
Average voxel value	0.033	Depositor
Voxel value standard deviation	0.924	Depositor
Recommended contour level	1.5	Depositor
Tomogram size (Å)	403.80002, 403.80002, 403.80002	wwPDB
Tomogram dimensions	200, 200, 200	wwPDB
Tomogram angles (°)	90.0, 90.0, 90.0	wwPDB
Grid spacing (Å)	2.019, 2.019, 2.019	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.43	0/635	0.69	0/792
1	B	0.43	0/635	0.69	0/792
1	I	0.43	0/635	0.69	0/792
1	J	0.43	0/635	0.69	0/792
1	R	0.43	0/635	0.69	0/792
2	C	1.40	8/4501 (0.2%)	1.50	13/5623 (0.2%)
2	K	1.40	8/4501 (0.2%)	1.50	14/5623 (0.2%)
3	D	1.60	16/3210 (0.5%)	1.72	24/4011 (0.6%)
3	L	1.60	16/3210 (0.5%)	1.72	23/4011 (0.6%)
4	E	1.52	4/3292 (0.1%)	1.63	19/4112 (0.5%)
4	M	1.52	2/2198 (0.1%)	1.58	9/2746 (0.3%)
4	V	1.52	4/3292 (0.1%)	1.63	19/4112 (0.5%)
5	F	1.55	1/554 (0.2%)	1.74	3/691 (0.4%)
5	N	1.55	1/554 (0.2%)	1.74	3/691 (0.4%)
5	W	1.55	1/554 (0.2%)	1.74	3/691 (0.4%)
6	G	1.50	7/3248 (0.2%)	1.71	23/4057 (0.6%)
6	O	1.50	7/3248 (0.2%)	1.71	23/4057 (0.6%)
7	H	1.21	0/1518	1.34	8/1893 (0.4%)
7	P	1.46	0/538	1.76	7/671 (1.0%)
8	X	0.91	0/1168	0.63	0/1457
8	Z	0.91	0/1168	0.63	0/1457
All	All	1.40	75/39929 (0.2%)	1.53	191/49863 (0.4%)

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	C	0	4
2	K	0	4
3	D	0	2
3	L	0	2

Continued on next page...

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	E	0	4
4	M	0	4
4	V	0	4
5	F	0	1
5	N	0	1
5	W	0	1
6	G	0	14
6	O	0	14
All	All	0	55

The worst 5 of 75 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	621	VAL	C-N	6.95	1.45	1.33
2	C	621	VAL	C-N	6.95	1.45	1.33
3	D	330	MET	N-CA	-6.82	1.32	1.46
3	L	330	MET	N-CA	-6.80	1.32	1.46
4	V	198	GLY	CA-C	-6.48	1.41	1.51

The worst 5 of 191 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	O	496	GLU	N-CA-C	7.83	132.14	111.00
6	G	496	GLU	N-CA-C	7.82	132.12	111.00
4	M	302	ALA	C-N-CA	7.05	139.32	121.70
4	V	302	ALA	C-N-CA	7.04	139.31	121.70
4	E	302	ALA	C-N-CA	7.04	139.29	121.70

There are no chirality outliers.

5 of 55 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	317	PHE	Mainchain
2	C	380	CYS	Mainchain
2	C	559	GLY	Mainchain
2	C	63	GLN	Peptide
3	D	44	HIS	Mainchain

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	636	0	181	0	0
1	B	636	0	181	0	0
1	I	636	0	181	0	0
1	J	636	0	181	2	0
1	R	636	0	181	0	0
2	C	4503	0	1194	3	0
2	K	4503	0	1194	0	0
3	D	3211	0	880	2	0
3	L	3211	0	880	17	0
4	E	3294	0	852	1	0
4	M	2199	0	570	1	0
4	V	3294	0	852	18	0
5	F	555	0	148	0	0
5	N	555	0	148	0	0
5	W	555	0	148	0	0
6	G	3250	0	833	0	0
6	O	3250	0	833	0	0
7	H	1520	0	406	3	0
7	P	539	0	142	0	0
8	X	1169	0	303	0	0
8	Z	1169	0	303	0	0
All	All	39957	0	10591	28	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 1.

The worst 5 of 28 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)
3:L:349:GLY:HA2	4:V:206:ASN:C	1.53	1.27
3:L:349:GLY:HA2	4:V:206:ASN:O	1.39	1.18
3:L:350:SER:H	4:V:207:ASP:N	1.42	1.16
3:L:350:SER:H	4:V:207:ASP:CA	1.58	1.14
3:L:351:CYS:N	4:V:210:ALA:CA	2.24	1.01

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	157/181 (87%)	153 (98%)	4 (2%)	0	100	100
1	B	157/181 (87%)	153 (98%)	4 (2%)	0	100	100
1	I	157/181 (87%)	153 (98%)	4 (2%)	0	100	100
1	J	157/181 (87%)	153 (98%)	4 (2%)	0	100	100
1	R	157/181 (87%)	153 (98%)	4 (2%)	0	100	100
2	C	1122/1262 (89%)	972 (87%)	104 (9%)	46 (4%)	3	23
2	K	1122/1262 (89%)	972 (87%)	104 (9%)	46 (4%)	3	23
3	D	801/905 (88%)	700 (87%)	64 (8%)	37 (5%)	2	21
3	L	801/905 (88%)	701 (88%)	63 (8%)	37 (5%)	2	21
4	E	820/874 (94%)	749 (91%)	40 (5%)	31 (4%)	3	24
4	M	548/874 (63%)	492 (90%)	27 (5%)	29 (5%)	2	19
4	V	820/874 (94%)	749 (91%)	40 (5%)	31 (4%)	3	24
5	F	137/177 (77%)	128 (93%)	7 (5%)	2 (2%)	10	46
5	N	137/177 (77%)	128 (93%)	7 (5%)	2 (2%)	10	46
5	W	137/177 (77%)	128 (93%)	7 (5%)	2 (2%)	10	46
6	G	809/968 (84%)	658 (81%)	84 (10%)	67 (8%)	1	12
6	O	809/968 (84%)	658 (81%)	84 (10%)	67 (8%)	1	12
7	H	376/511 (74%)	336 (89%)	31 (8%)	9 (2%)	6	33
7	P	133/511 (26%)	116 (87%)	16 (12%)	1 (1%)	19	60
8	X	290/308 (94%)	276 (95%)	9 (3%)	5 (2%)	9	42
8	Z	290/308 (94%)	276 (95%)	10 (3%)	4 (1%)	11	46
All	All	9937/11966 (83%)	8804 (89%)	717 (7%)	416 (4%)	5	22

5 of 416 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	11	ARG
2	C	227	ARG
2	C	526	GLU
2	C	572	ARG
2	C	686	ASN

5.3.2 Protein sidechains

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

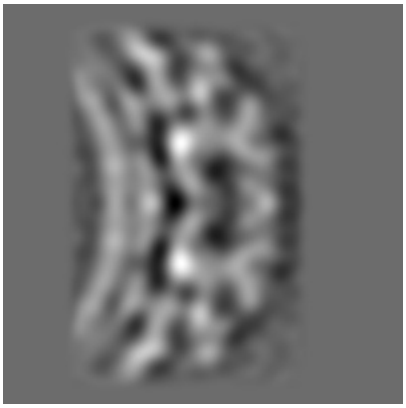
There are no chain breaks in this entry.

6 Tomogram visualisation

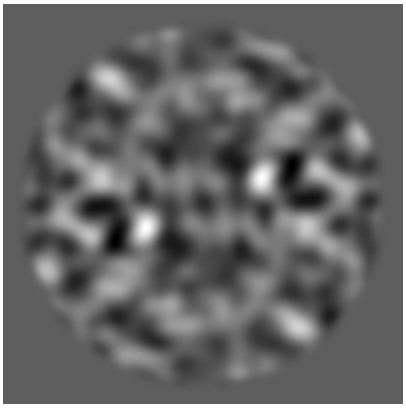
This section contains visualisations of the EMDB entry EMD-2989. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections

X



Y



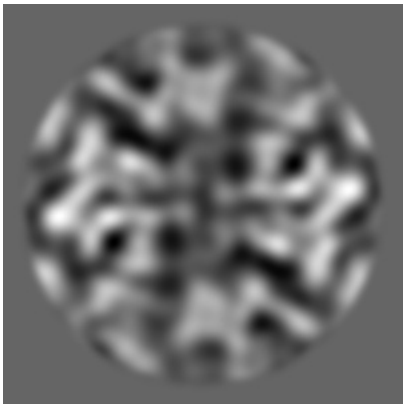
Z

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

6.2 Central slices

X Index: 100

Y Index: 100



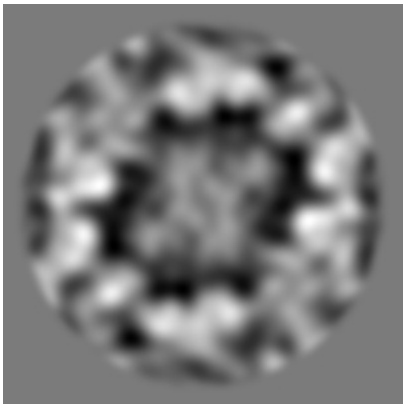
Z Index: 100

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

6.3 Largest variance slices (i)

X Index: 70

Y Index: 108



Z Index: 78

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

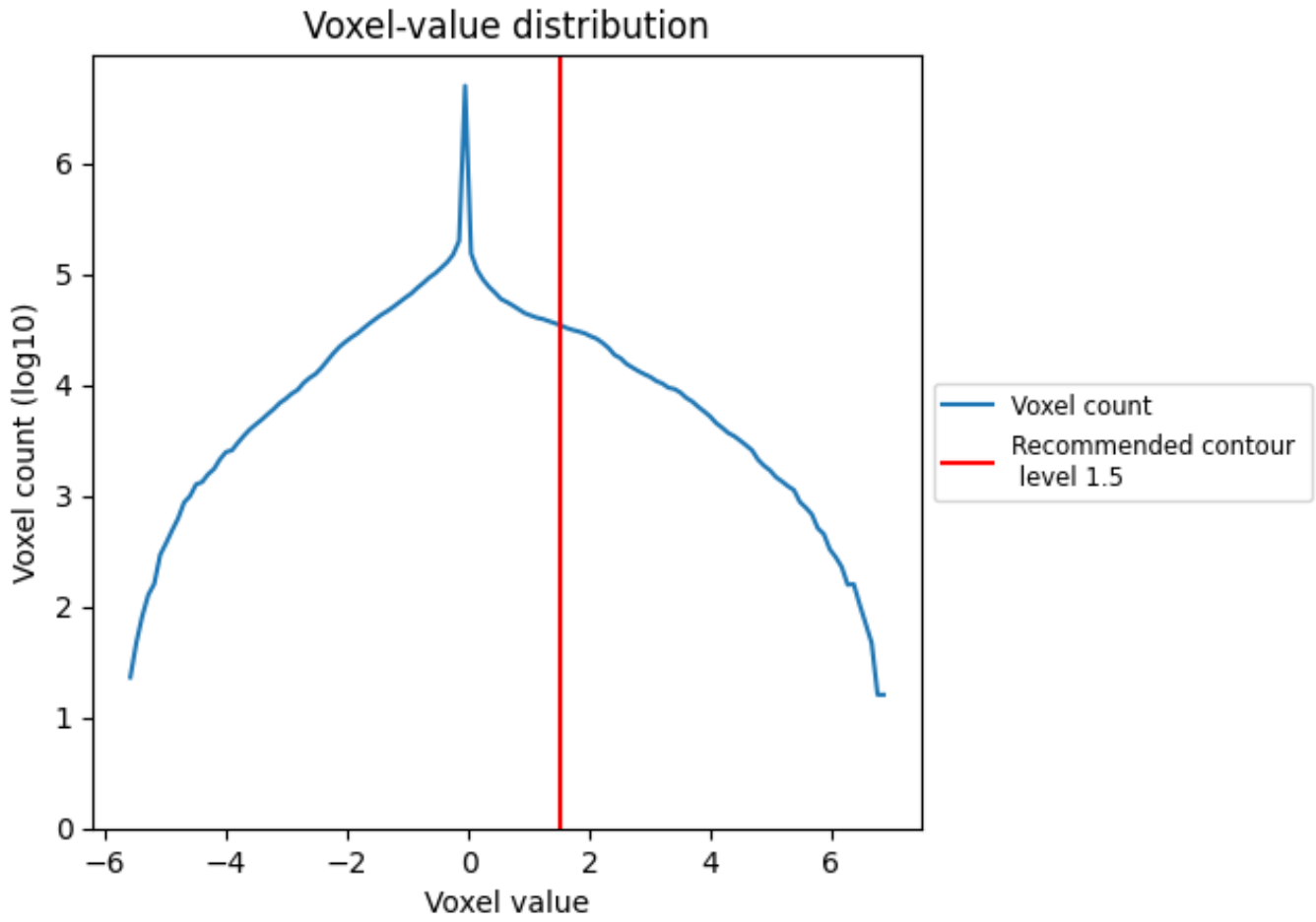
6.4 Mask visualisation (i)

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

7 Tomogram analysis (i)

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

7.1 Voxel-value distribution (i)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

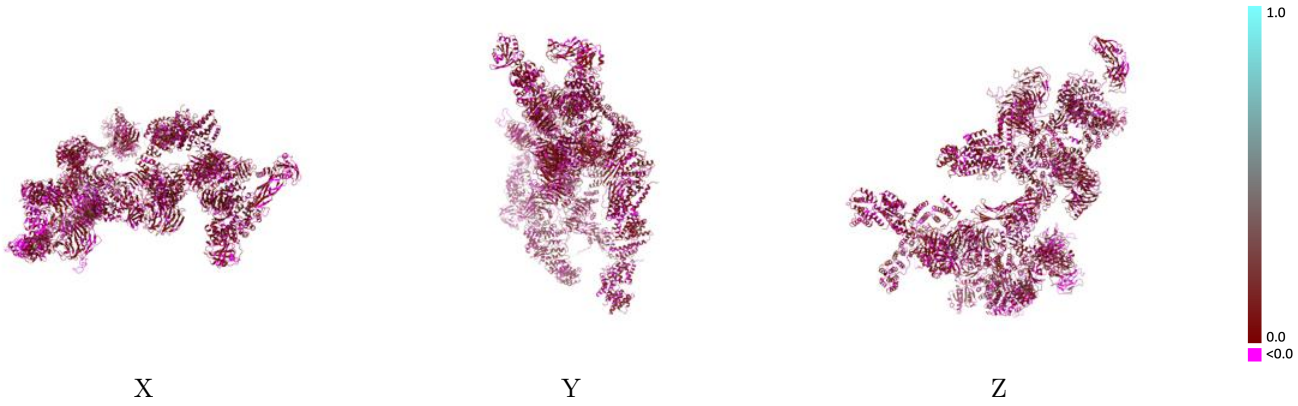
8 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2989 and PDB model 5A1Y. Per-residue inclusion information can be found in section 3 on page 9.

8.1 Map-model overlay

This section was not generated.

8.2 Q-score mapped to coordinate model

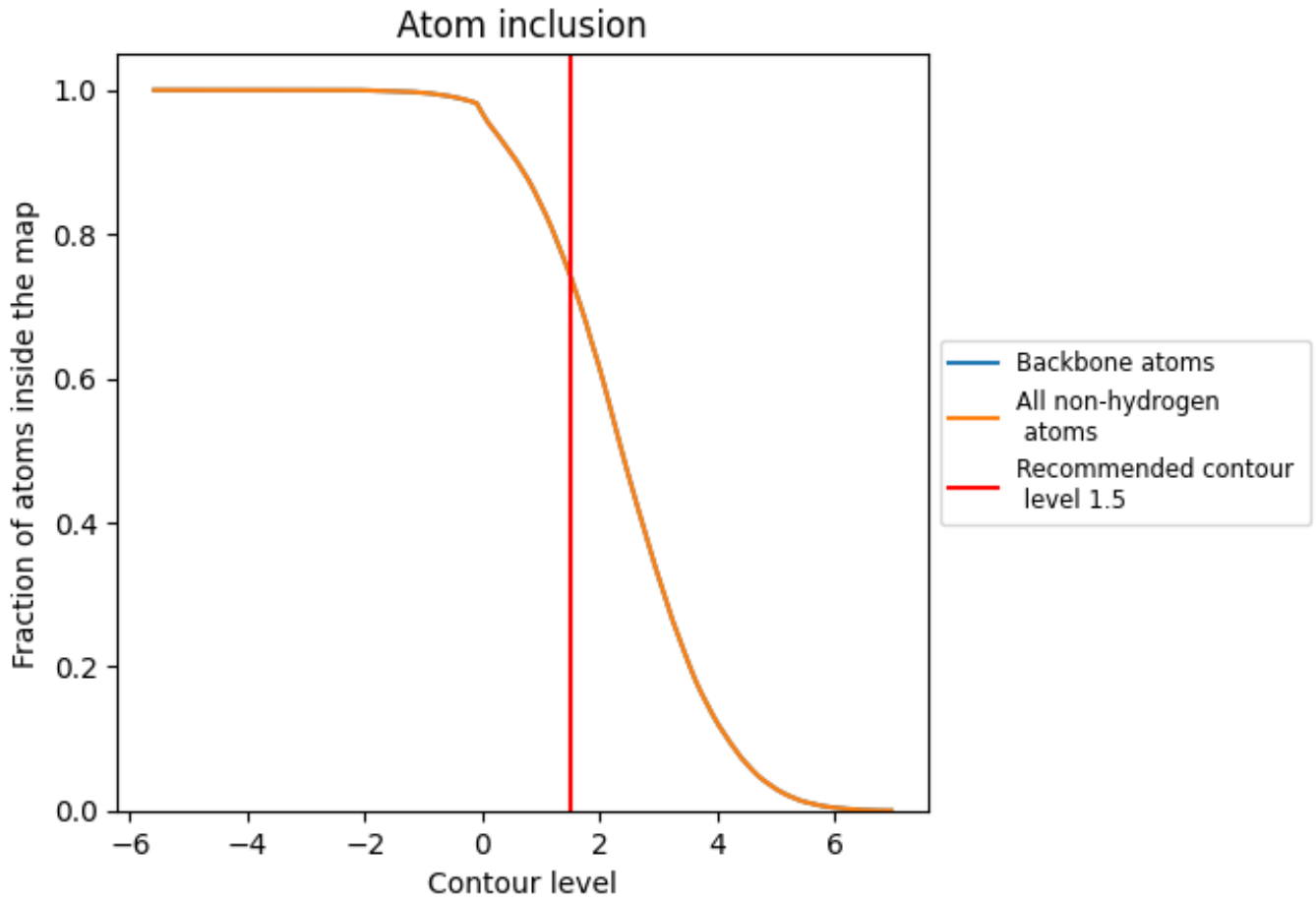


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

8.3 Atom inclusion mapped to coordinate model

This section was not generated.

8.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7414	0.0600
A	0.6965	0.0490
B	0.8899	0.0590
C	0.8899	0.0680
D	0.8708	0.0730
E	0.7790	0.0660
F	0.7856	0.0710
G	0.8631	0.0710
H	0.7164	0.0640
I	0.2280	0.0330
J	0.4827	0.0500
K	0.6960	0.0530
L	0.8184	0.0690
M	0.3997	0.0220
N	0.5279	0.0670
O	0.5502	0.0470
P	0.7737	0.0440
R	0.6887	0.0540
V	0.7413	0.0680
W	0.8306	0.0590
X	0.9153	0.0690
Z	0.7819	0.0490