wwPDB EM Validation Summary Report (i)

May 4, 2024 – 06:07 pm BST

PDB ID	:	5NZS
EMDB ID	:	EMD-3721
Title	:	The structure of the COPI coat leaf in complex with the ArfGAP2 uncoating factor
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	:	10.10 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:

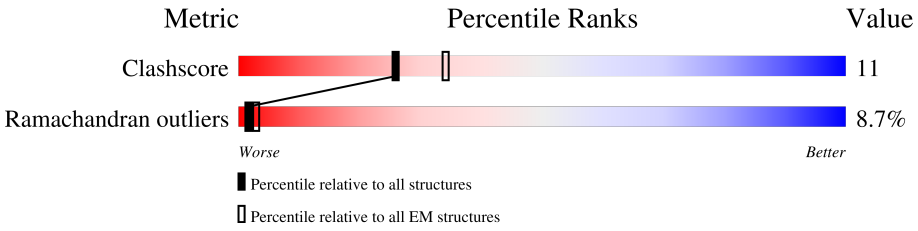
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 10.10 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.



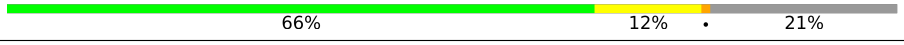
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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%

Mol	Chain	Length	Quality of chain
1	A	1262	49% 14% • 36%
2	B	968	66% 13% • 17%
3	C	905	77% 14% • 7%
4	D	511	29% 5% • 65%
5	F	181	77% 8% • 12%
5	M	181	65% 19% • 12%
5	R	181	54% 27% 7% 12%
6	G	874	75% 14% • 9%
6	K	874	52% 9% • 36%
7	L	177	66% 12% • 21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	Z	177	
8	P	520	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 19478 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	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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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	C	843	3371	1686	843	842	0	0

- Molecule 4 is a protein called Coatomer subunit delta.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	177	Total 706	C 354	N 177	O 175	0	0

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

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

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

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

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

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

- Molecule 8 is a protein called ADP-ribosylation factor GTPase-activating protein 2.

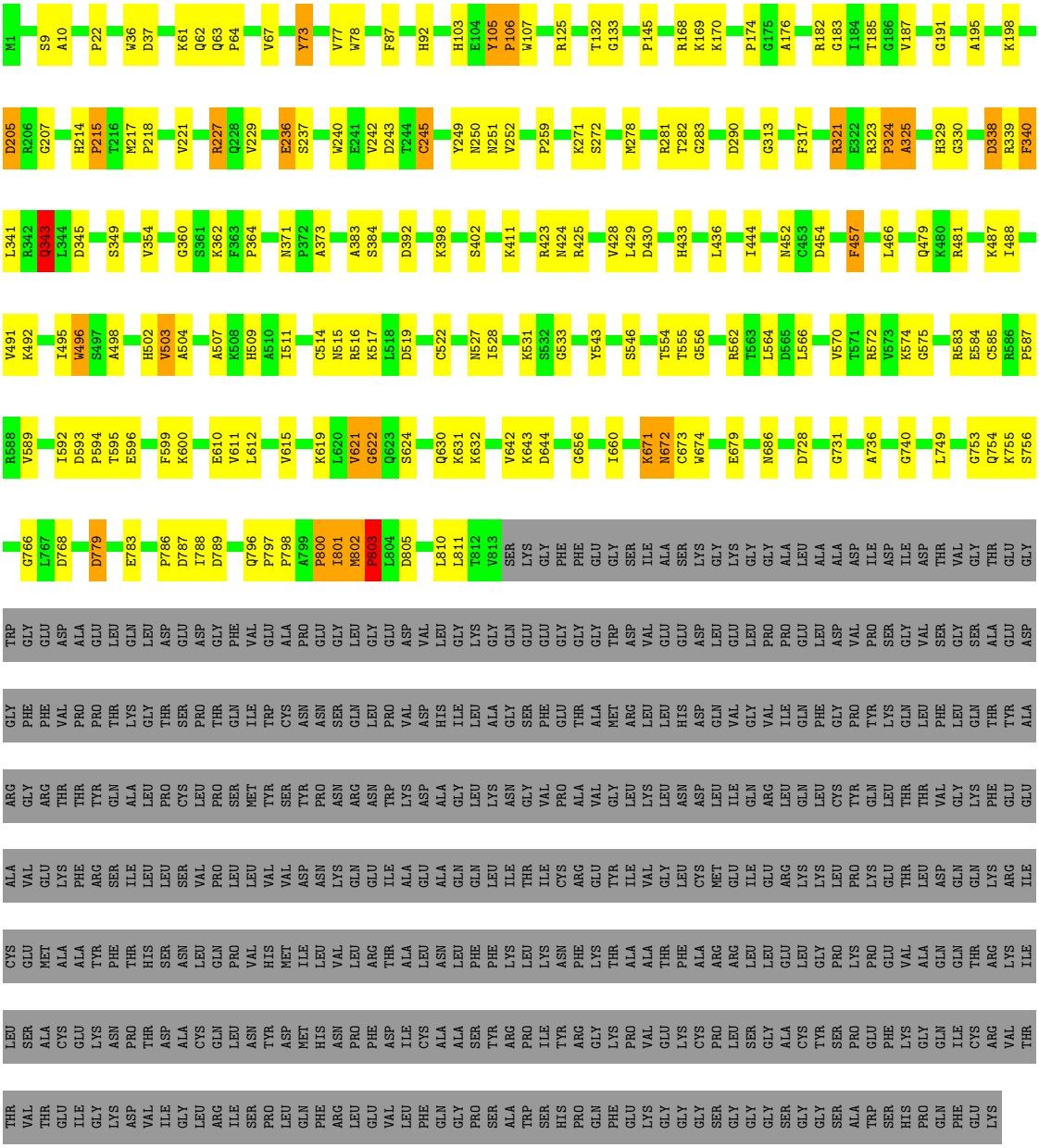
Mol	Chain	Residues	Atoms				AltConf	Trace
8	P	127	Total 508	C 254	N 127	O 127	0	0

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. 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. 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.

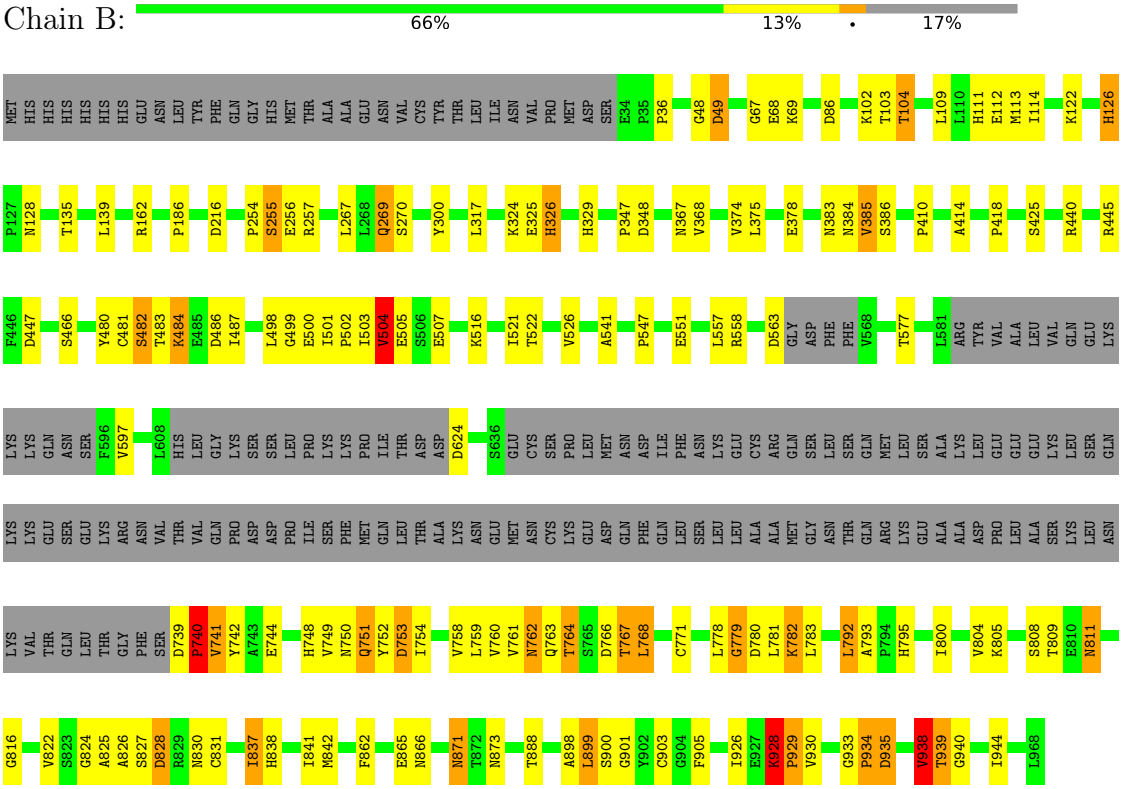
- Molecule 1: Coatomer subunit alpha

Chain A:



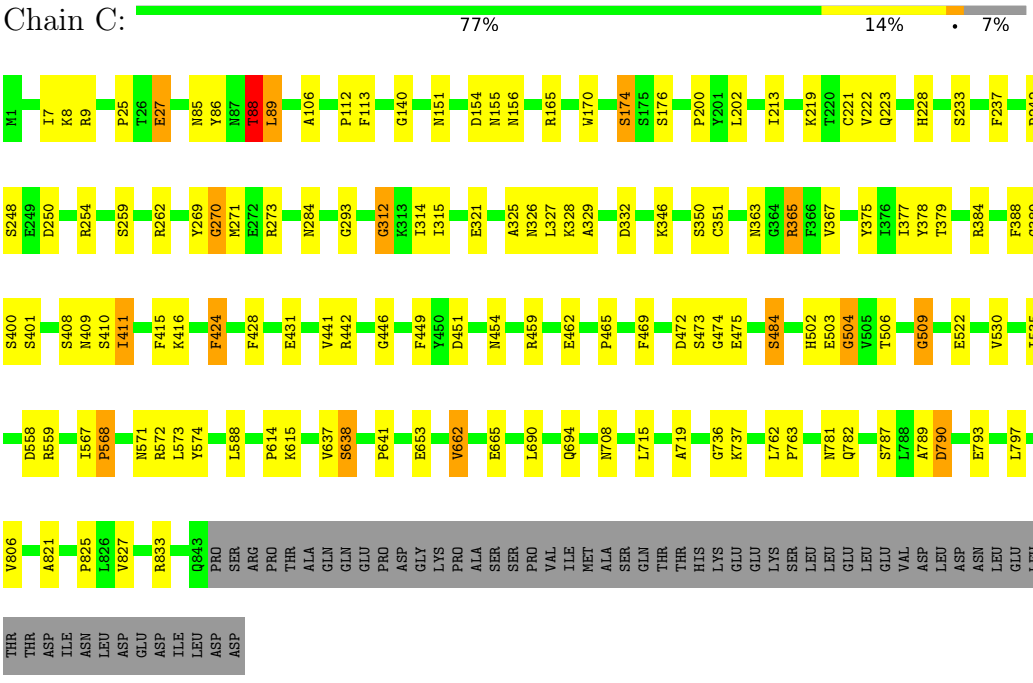
• Molecule 2: Coatomer subunit beta

Chain B:



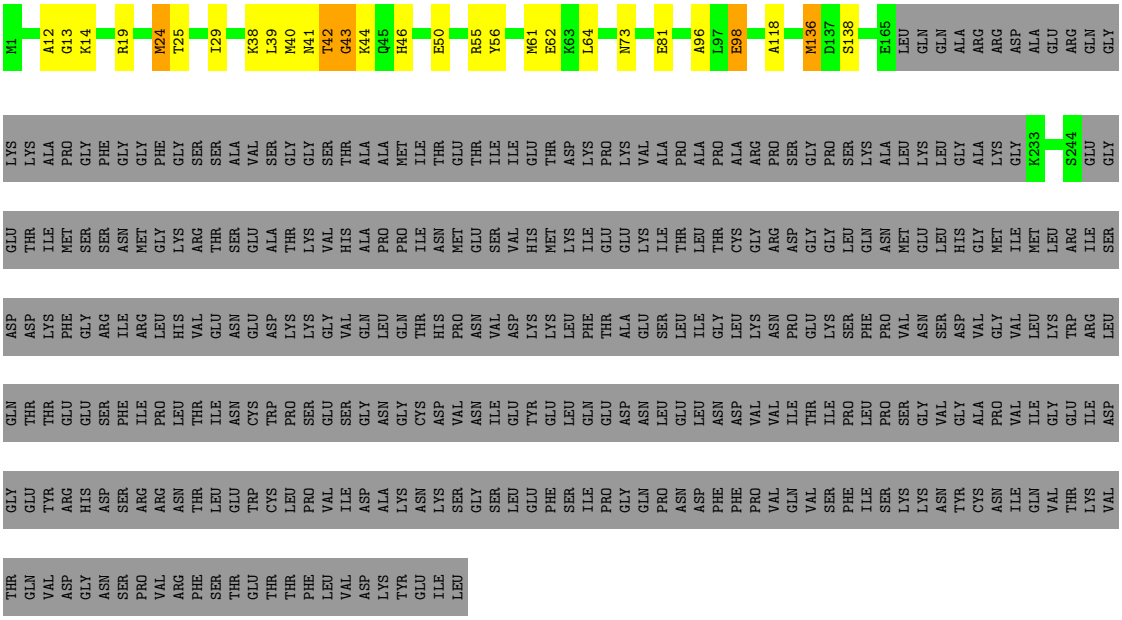
• Molecule 3: Coatomer subunit beta'

Chain C:



• Molecule 4: Coatomer subunit delta

Chain D:

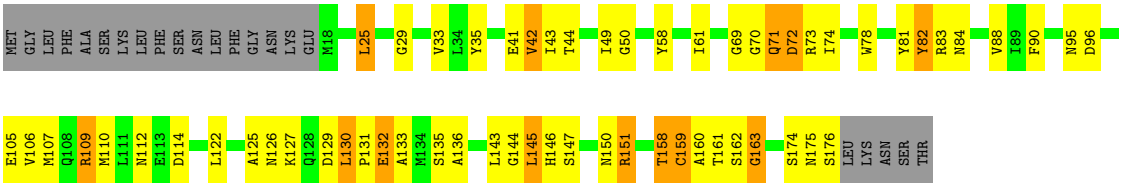


• Molecule 5: ADP-ribosylation factor 1

Chain F:

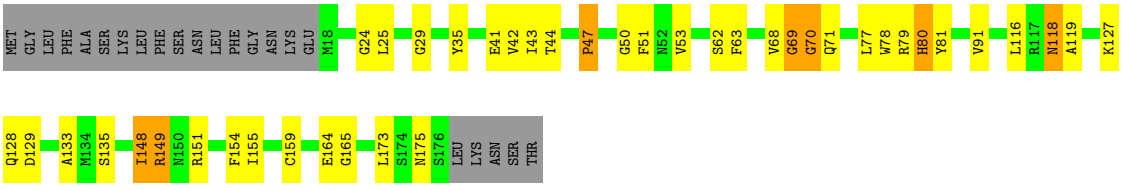
• Molecule 5: ADP-ribosylation factor 1

Chain R:



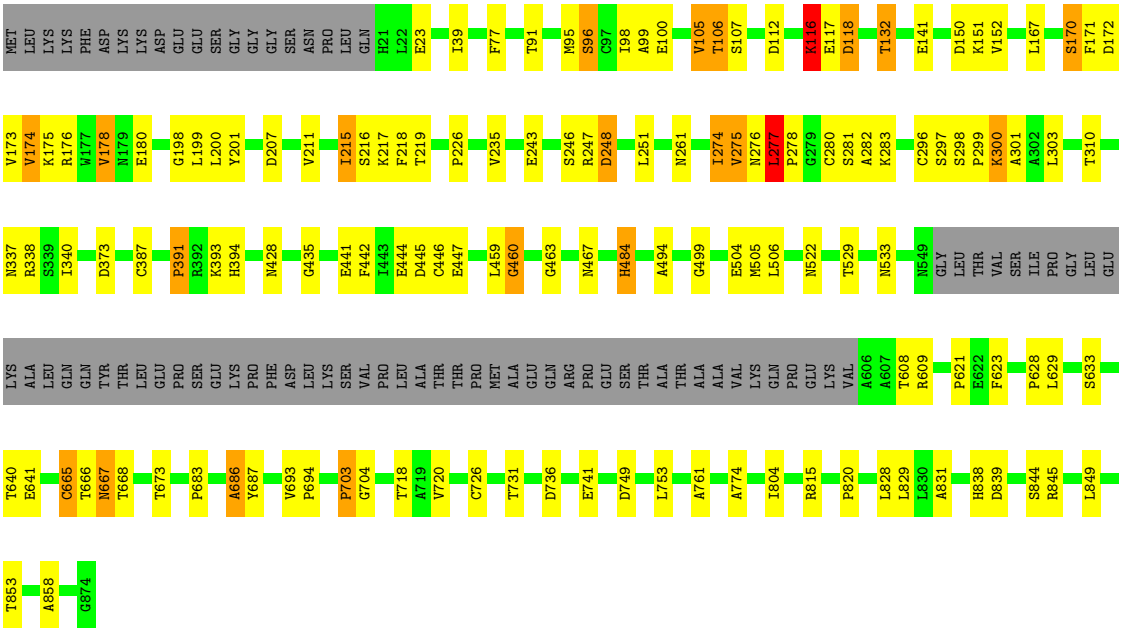
• Molecule 5: ADP-ribosylation factor 1

Chain M:



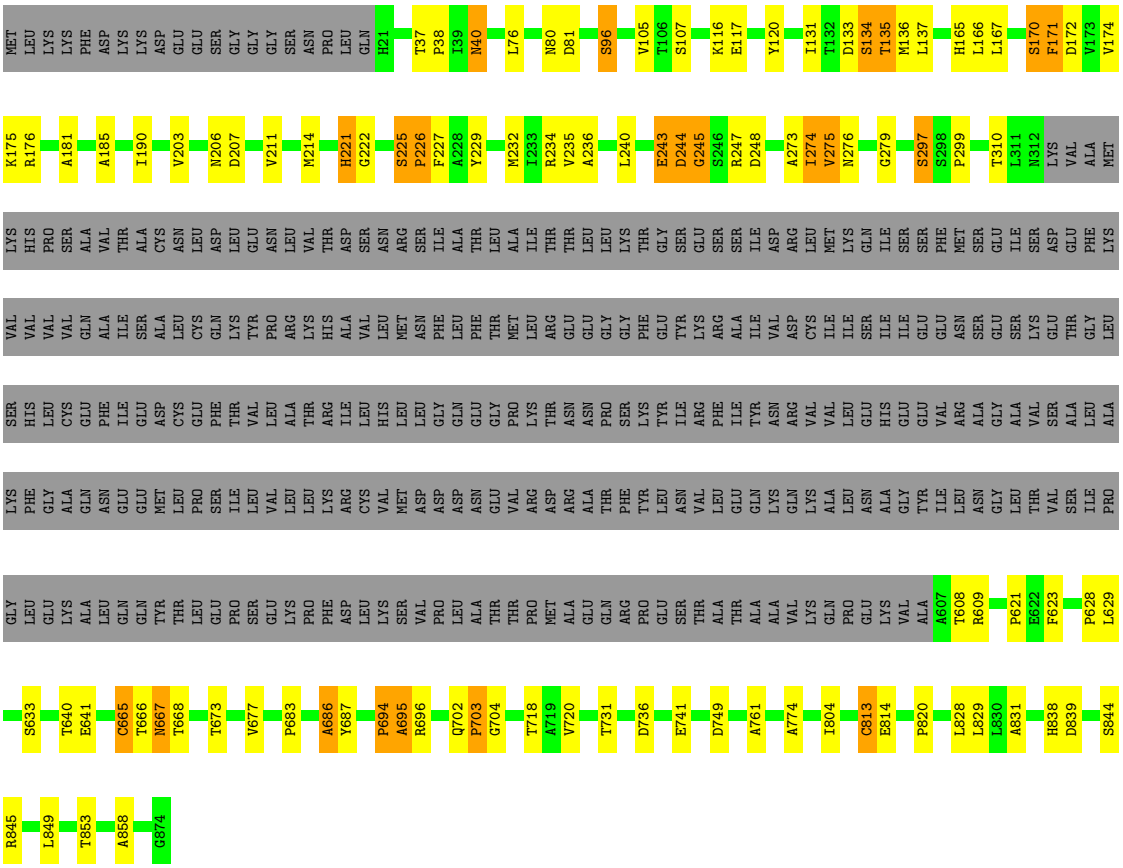
• Molecule 6: Coatomer subunit gamma-1

Chain G:



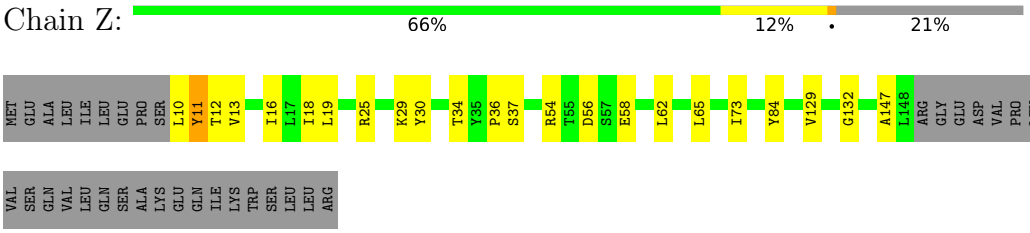
• Molecule 6: Coatomer subunit gamma-1

Chain K:



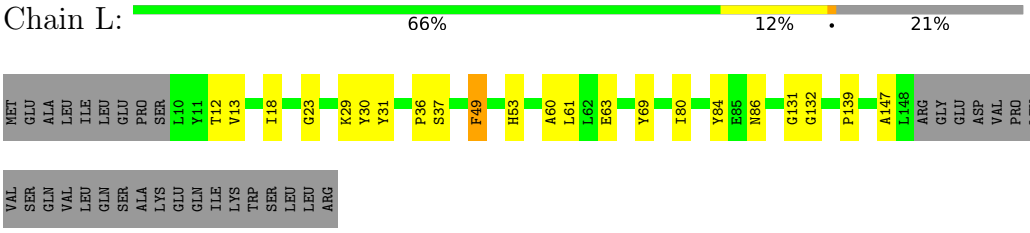
• Molecule 7: Coatomer subunit zeta-1

Chain Z:



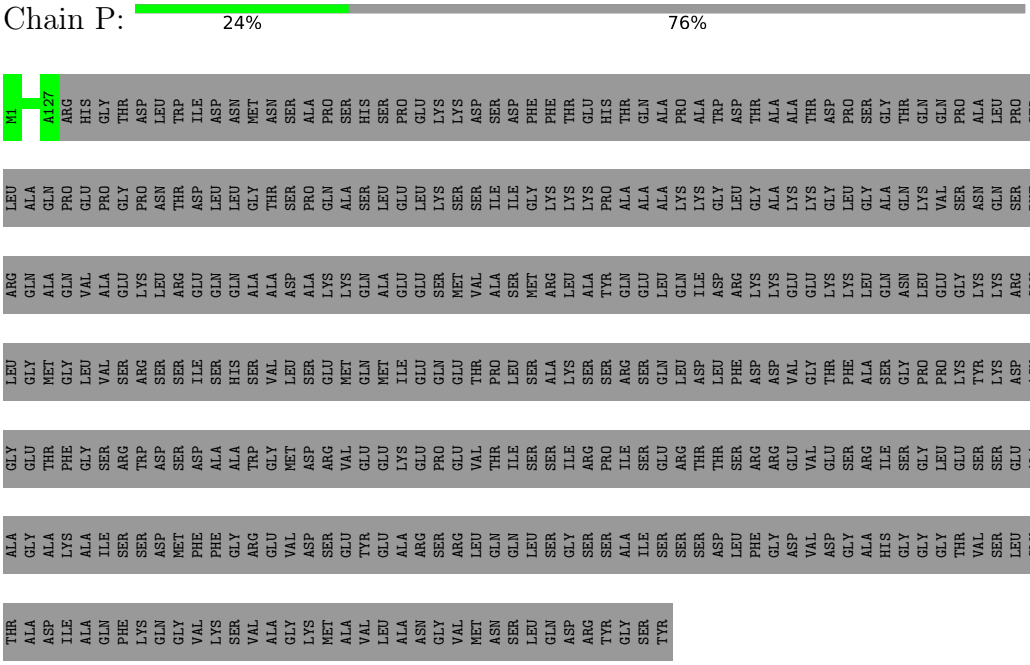
• Molecule 7: Coatomer subunit zeta-1

Chain L:



• Molecule 8: ADP-ribosylation factor GTPase-activating protein 2

Chain P:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	12372	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

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	1.56	15/3250 (0.5%)	1.81	74/4061 (1.8%)
2	B	1.71	19/3193 (0.6%)	1.55	45/3983 (1.1%)
3	C	1.76	23/3370 (0.7%)	1.70	60/4211 (1.4%)
4	D	1.67	3/704 (0.4%)	1.65	10/877 (1.1%)
5	F	1.56	1/634 (0.2%)	1.71	9/791 (1.1%)
5	M	1.60	4/634 (0.6%)	1.65	10/791 (1.3%)
5	R	1.88	10/634 (1.6%)	1.81	15/791 (1.9%)
6	G	1.62	11/3188 (0.3%)	1.59	45/3982 (1.1%)
6	K	1.72	9/2237 (0.4%)	1.69	44/2793 (1.6%)
7	L	2.05	3/554 (0.5%)	1.72	7/691 (1.0%)
7	Z	1.87	3/554 (0.5%)	1.69	10/691 (1.4%)
8	P	0.85	0/507	0.66	0/632
All	All	1.68	101/19459 (0.5%)	1.66	329/24294 (1.4%)

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	B	0	3

The worst 5 of 101 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	940	GLY	N-CA	-7.80	1.34	1.46
5	R	29	GLY	CA-C	-7.62	1.39	1.51
5	R	35	TYR	CA-C	-7.33	1.33	1.52
1	A	191	GLY	CA-C	-7.04	1.40	1.51
3	C	572	ARG	CA-C	-6.59	1.35	1.52

The worst 5 of 329 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	343	GLN	N-CA-C	-9.86	84.38	111.00
6	K	117	GLU	C-N-CA	9.76	146.10	121.70
2	B	326	HIS	N-CA-C	-9.59	85.12	111.00
6	G	96	SER	N-CA-C	9.10	135.56	111.00
2	B	940	GLY	N-CA-C	-9.03	90.52	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	898	ALA	Peptide
2	B	903	CYS	Peptide
2	B	938	VAL	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	3251	0	869	36	0
2	B	3198	0	810	58	0
3	C	3371	0	919	23	0
4	D	706	0	182	9	0
5	F	635	0	181	3	0
5	M	635	0	181	19	0
5	R	635	0	181	37	0
6	G	3190	0	822	57	0
6	K	2239	0	572	39	0
7	L	555	0	148	2	0
7	Z	555	0	147	15	0
8	P	508	0	144	0	0
All	All	19478	0	5156	279	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 279 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:K:107:SER:N	5:M:50:GLY:HA3	1.28	1.43
6:G:107:SER:N	5:R:50:GLY:HA3	1.16	1.43
6:G:107:SER:H	5:R:50:GLY:CA	1.31	1.41
6:K:167:LEU:CA	6:K:170:SER:O	1.73	1.35
1:A:145:PRO:CA	1:A:215:PRO:O	1.80	1.30

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	811/1262 (64%)	590 (73%)	112 (14%)	109 (13%)	0 5
2	B	790/968 (82%)	648 (82%)	68 (9%)	74 (9%)	0 10
3	C	841/905 (93%)	681 (81%)	91 (11%)	69 (8%)	1 12
4	D	173/511 (34%)	144 (83%)	16 (9%)	13 (8%)	1 13
5	F	157/181 (87%)	134 (85%)	14 (9%)	9 (6%)	1 18
5	M	157/181 (87%)	126 (80%)	13 (8%)	18 (12%)	0 6
5	R	157/181 (87%)	120 (76%)	17 (11%)	20 (13%)	0 5
6	G	794/874 (91%)	678 (85%)	61 (8%)	55 (7%)	1 15
6	K	556/874 (64%)	475 (85%)	42 (8%)	39 (7%)	1 14
7	L	137/177 (77%)	117 (85%)	11 (8%)	9 (7%)	1 16
7	Z	137/177 (77%)	119 (87%)	11 (8%)	7 (5%)	2 19
8	P	125/520 (24%)	124 (99%)	1 (1%)	0	100 100
All	All	4835/6811 (71%)	3956 (82%)	457 (10%)	422 (9%)	1 11

5 of 422 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	64	PRO
1	A	92	HIS
1	A	106	PRO
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

This section contains visualisations of the EMDB entry EMD-3721. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

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

9 Map-model fit

This section was not generated.