



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:16 PM BST

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 Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

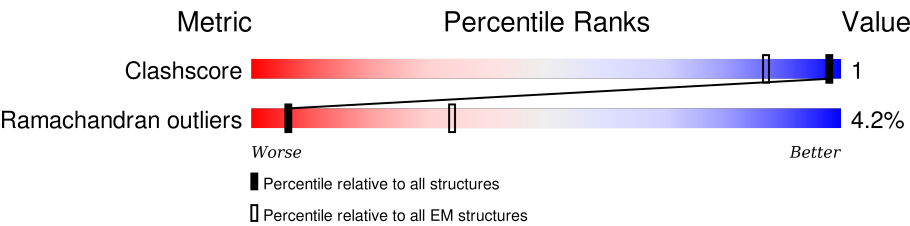
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

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	114402	924
Ramachandran outliers	111179	726

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	181	<div><div>88%12%</div></div>
1	B	181	<div><div>88%12%</div></div>
1	I	181	<div><div>88%12%</div></div>
1	J	181	<div><div>87%12%</div></div>
1	R	181	<div><div>88%12%</div></div>
2	C	1262	<div><div>84%5%11%</div></div>
2	K	1262	<div><div>84%5%11%</div></div>
3	D	905	<div><div>80%9%11%</div></div>
3	L	905	<div><div>80%9%11%</div></div>
4	E	874	<div><div>88%5%6%</div></div>
4	M	874	<div><div>58%37%</div></div>

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Mol	Chain	Length	Quality of chain
4	V	874	 88% 6% • 6%
5	F	177	 75% • 21%
5	N	177	 75% • 21%
5	W	177	 75% • 21%
6	G	968	 73% 10% • 16%
6	O	968	 73% 10% • 16%
7	H	511	 70% • 26%
7	P	511	 25% • 74%
8	X	308	 93% • 5%
8	Z	308	 94% • 5%

2 Entry composition

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	C	N	O	0	0
			636	318	159	159		
1	B	159	Total	C	N	O	0	0
			636	318	159	159		
1	I	159	Total	C	N	O	0	0
			636	318	159	159		
1	J	159	Total	C	N	O	0	0
			636	318	159	159		
1	R	159	Total	C	N	O	0	0
			636	318	159	159		

- Molecule 2 is a protein called COATOMER SUBUNIT ALPHA.

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

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	C	N	O	0	0
			555	278	139	138		
5	N	139	Total	C	N	O	0	0
			555	278	139	138		
5	W	139	Total	C	N	O	0	0
			555	278	139	138		

- Molecule 6 is a protein called COATOMER SUBUNIT BETA.

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

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.

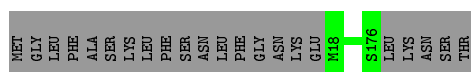
Mol	Chain	Residues	Atoms				AltConf	Trace
8	X	292	Total	C	N	O	0	0
			1169	584	292	293		
8	Z	292	Total	C	N	O	0	0
			1169	584	292	293		

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

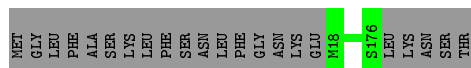
- Molecule 1: ADP-RIBOSYLATION FACTOR 1

Chain A: 




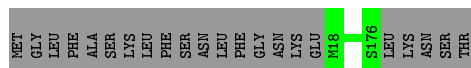
- Molecule 1: ADP-RIBOSYLATION FACTOR 1

Chain B: 




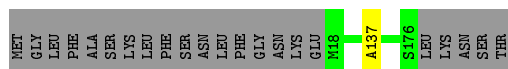
- Molecule 1: ADP-RIBOSYLATION FACTOR 1

Chain I: 




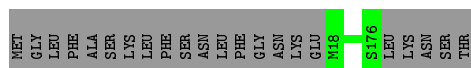
- Molecule 1: ADP-RIBOSYLATION FACTOR 1

Chain J: 




- Molecule 1: ADP-RIBOSYLATION FACTOR 1

Chain R: 

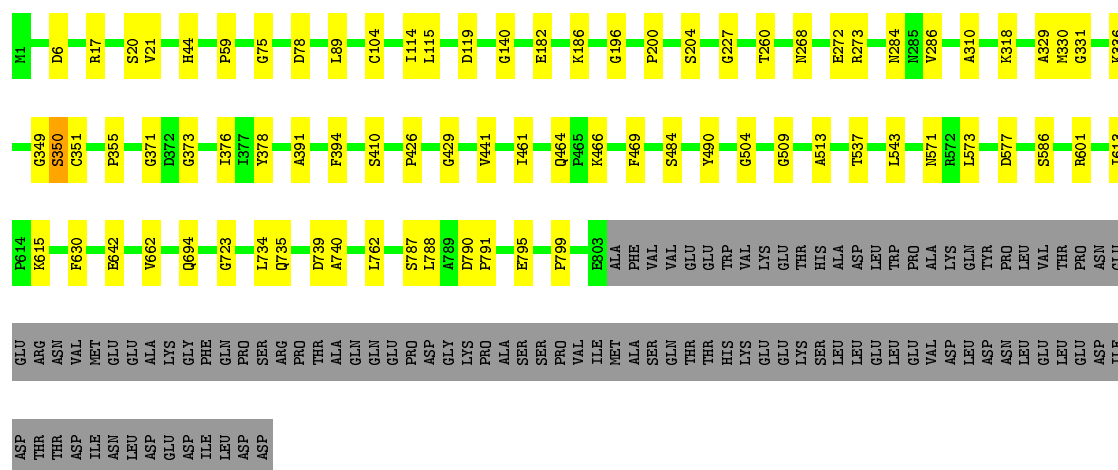


- Molecule 2: COATOMER SUBUNIT ALPHA

Chain C: 

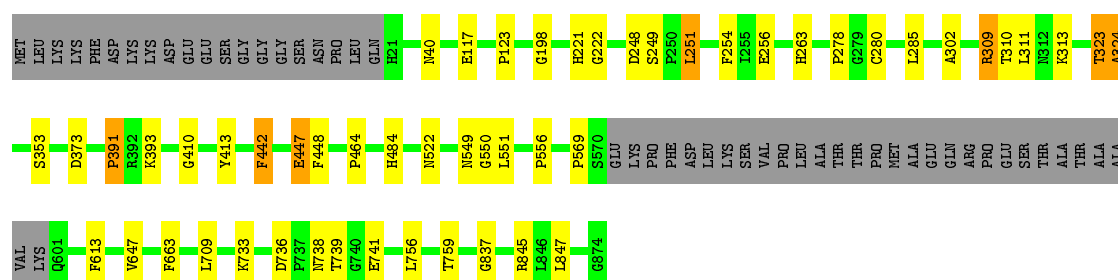


Chain L:



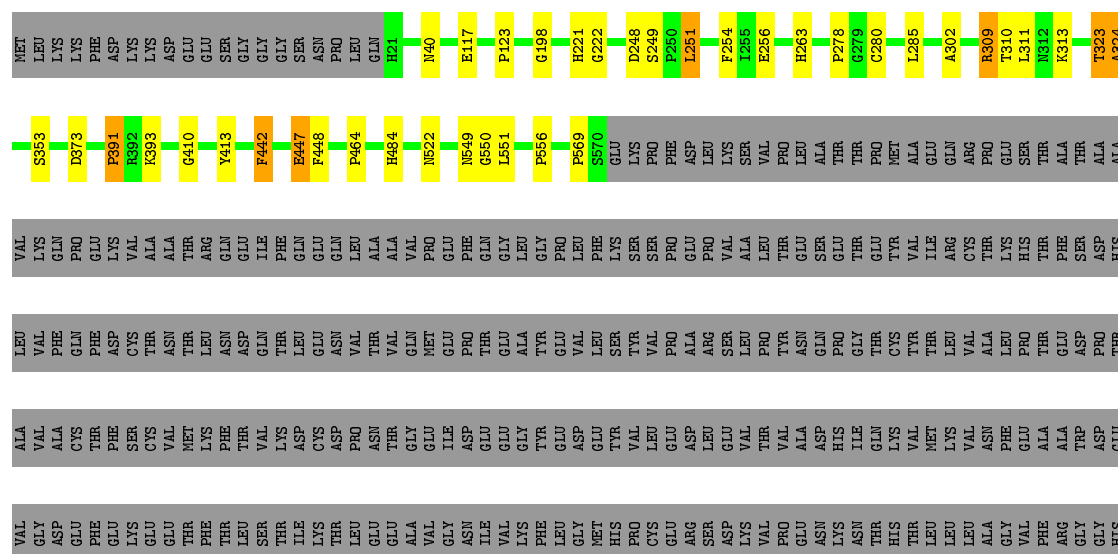
- Molecule 4: COATOMER SUBUNIT GAMMA-1

Chain E:




- Molecule 4: COATOMER SUBUNIT GAMMA-1

Chain M:



ASP
ILE
LEU
VAL
ARG
SER
ARG
LEU
LEU
LEU
LEU
ASP
THR
VAL
THR
MET
SER
GLN
VAL
THR
ALA
ARG
SER
SER
GLU
GLU
LEU
PRO
VAL
VAL
ILE
ILE
LEU
ALA
SER
VAL
GLY

• Molecule 4: COATOMER SUBUNIT GAMMA-1

Chain V:  88% 6% • 6%

MET
LEU
LYS
PHE
ASP
LYS
ASP
GLU
GLU
SER
GLY
GLY
GLY
SER
ASN
PRO
LEU
GLN
H21
N40
E117
P123
G198
N206
D207
A210
H221
G222
G245
D248
S249
P250
L251
F254
I255
E256
H263
P278
G279
C280
L285
A302
R309

T310
L311
N312
K313
T323
A324
S353
D373
P391
K392
K393
G410
Y413
F442
E447
F448
P464
H484
N522
N549
G550
L551
P556
P569
S570
LYS
PRO
PHE
ASP
LEU
LYS
SER
GLN
VAL
PRO
LEU
ALA
THR
THR
PRO
MET
ALA
GLU
GLN
ARG
PRO

GLU
SER
THR
THR
ALA
ALA
VAL
LYS
Q601
F613
V647
F663
L709
K733
D736
F737
N738
T739
G740
E741
L756
T759
G837
R845
L846
L847
G874

• Molecule 5: COATOMER SUBUNIT ZETA-1

Chain F:  75% • 21%


MET
GLU
ALA
ILE
LEU
GLU
PRO
SER
L140
P36
T55
I59
Y69
I80
E110
G132
L143
ARG
GLY
GLU
ASP
VAL
PRO
LEU
THR
GLU
GLN
THR
VAL
SER
GLN
VAL
LEU
LEU
GLN
SER
SER
ALA
LYS
GLU
GLN
ILE
LYS
TRP
SER
LEU
LEU
ARG

• Molecule 5: COATOMER SUBUNIT ZETA-1

Chain N:  75% • 21%

MET
GLU
ALA
ILE
LEU
GLU
PRO
SER
L140
P36
T55
I59
Y69
I80
E110
G132
L143
ARG
GLY
GLU
ASP
VAL
PRO
LEU
THR
GLU
GLN
THR
VAL
SER
GLN
VAL
LEU
LEU
GLN
SER
SER
ALA
LYS
GLU
GLN
ILE
LYS
TRP
SER
LEU
LEU
ARG

• Molecule 5: COATOMER SUBUNIT ZETA-1

Chain W:  75% • 21%

MET
GLU
ALA
ILE
LEU
GLU
PRO
SER
L140
P36
T55
I59
Y69
I80
E110
G132
L143
ARG
GLY
GLU
ASP
VAL
PRO
LEU
THR
GLU
GLN
THR
VAL
SER
GLN
VAL
LEU
LEU
GLN
SER
SER
ALA
LYS
GLU
GLN
ILE
LYS
TRP
SER
LEU
LEU
ARG

• Molecule 6: COATOMER SUBUNIT BETA

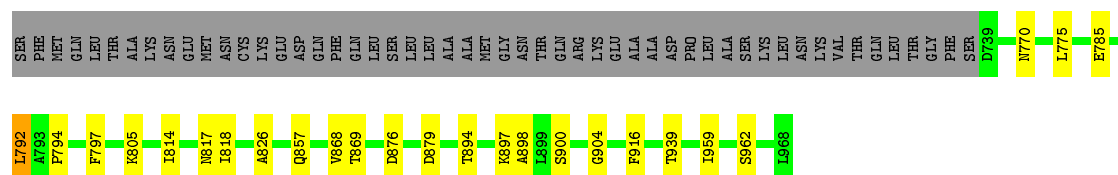
Chain G:  73% 10% • 16%

MET
HIS
HIS
HIS
HIS
HIS
HIS
ASN
LEU
TYR
PHE
GLN
GLY
HIS
MET
THR
ALA
ALA
GLU
ASN
VAL
CYS
TYR
THR
LEU
ILE
ASN
VAL
PRO
M16
D17
S13
P21
S22
K32
L42
L55
P56
G57
R64
F65
L69
E83
I84
V85
P90
D91
I99
C102

D103
G118
Y160
M165
L169
I170
A173
P174
L181
F194
M195
M196
L197
Y216
E229
L230
C235
E236
A237
N238
L253
Q254
S257
P258
A259
Y262
A274
P275
E307
L308
K309
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E311
V317
L318
L329
S330
T331
P332
V348
E372

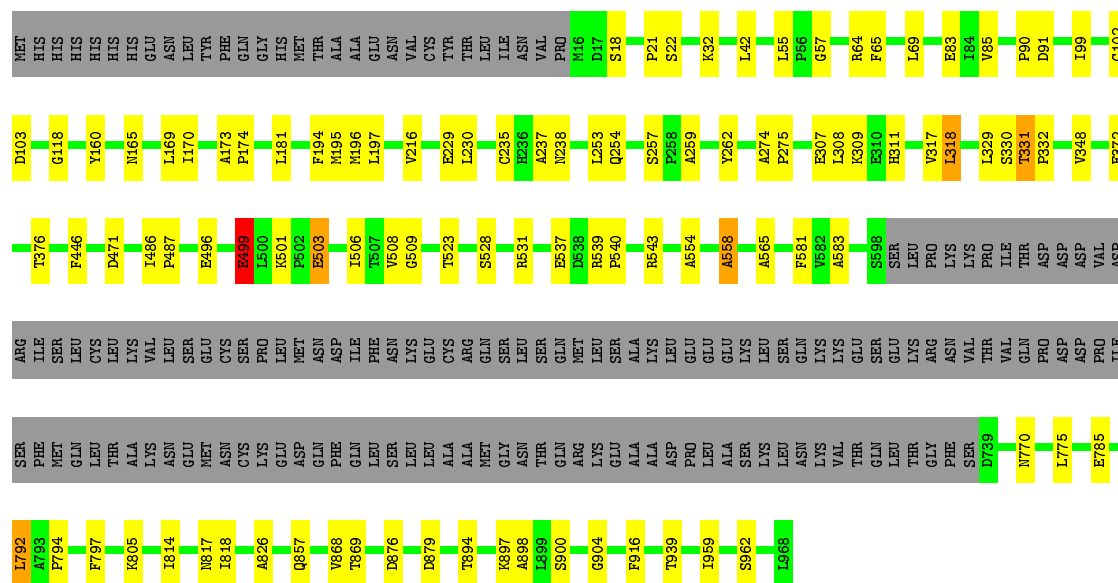
T376
F446
D471
I486
P487
E496
E499
L500
K501
P502
E503
I506
T507
V508
G509
T523
S528
R531
A537
E537
P538
R539
P540
R543
A554
A558
A565
F581
Y582
A583
S598
SER
LEU
PRO
LYS
LYS
VAL
THR
VAL
ILE
THR
GLN
PRO
ASP
ASP
ASP
VAL
ASP
ILE

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



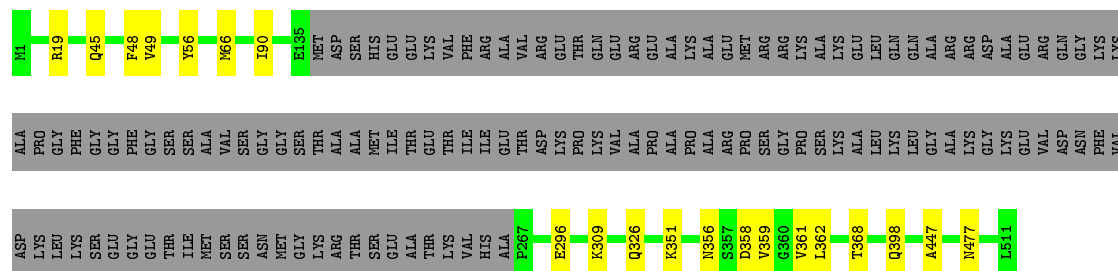
• Molecule 6: COATOMER SUBUNIT BETA

Chain O: 73% 10% 16%



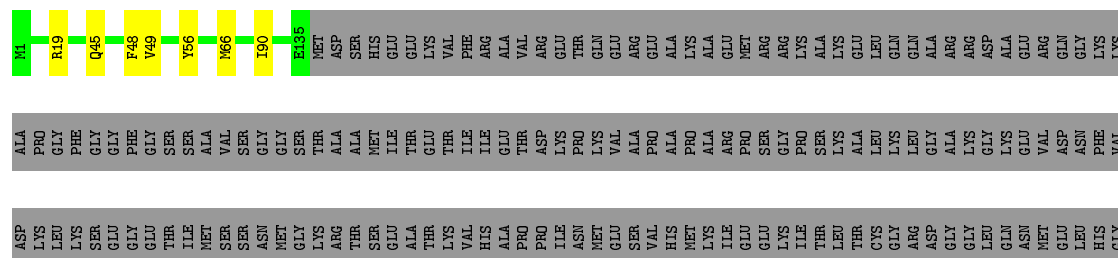
• Molecule 7: COATOMER SUBUNIT DELTA

Chain H: 70% 26%



• Molecule 7: COATOMER SUBUNIT DELTA

Chain P: 25% 74%



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

● Molecule 8: COATOMER SUBUNIT EPSILON

Chain X:

93%

• 5%

MET	ALA	PRO	PRO	VAL	PRO	GLY	ALA	VAL	SER	GLY	SER	GLY	GLU	VAL	D17	S45	S111	V112	D113	D113	S213	R231	A308
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● Molecule 8: COATOMER SUBUNIT EPSILON

Chain Z:

94%

• 5%

MET	ALA	PRO	PRO	VAL	PRO	GLY	ALA	VAL	SER	GLY	SER	GLY	GLU	VAL	D17	S111	V112	D113	S213	R231	A308
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4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PHASE FLIPPING OF INDIVIDUAL TILTS	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	42000	Depositor
Image detector	GATAN MULTISCAN	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 > 2$	RMSZ	# $ Z > 2$
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

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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(°)	Ideal(°)
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 ⓘ

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	35
2	K	1122/1262 (89%)	972 (87%)	104 (9%)	46 (4%)	3	35
3	D	801/905 (88%)	700 (87%)	64 (8%)	37 (5%)	3	33
3	L	801/905 (88%)	701 (88%)	63 (8%)	37 (5%)	3	33
4	E	820/874 (94%)	749 (91%)	40 (5%)	31 (4%)	4	37
4	M	548/874 (63%)	492 (90%)	27 (5%)	29 (5%)	2	29
4	V	820/874 (94%)	749 (91%)	40 (5%)	31 (4%)	4	37
5	F	137/177 (77%)	128 (93%)	7 (5%)	2 (2%)	13	57
5	N	137/177 (77%)	128 (93%)	7 (5%)	2 (2%)	13	57
5	W	137/177 (77%)	128 (93%)	7 (5%)	2 (2%)	13	57
6	G	809/968 (84%)	658 (81%)	84 (10%)	67 (8%)	1	18
6	O	809/968 (84%)	658 (81%)	84 (10%)	67 (8%)	1	18
7	H	376/511 (74%)	336 (89%)	31 (8%)	9 (2%)	7	47
7	P	133/511 (26%)	116 (87%)	16 (12%)	1 (1%)	24	69
8	X	290/308 (94%)	276 (95%)	9 (3%)	5 (2%)	11	55
8	Z	290/308 (94%)	276 (95%)	10 (3%)	4 (1%)	14	58
All	All	9937/11966 (83%)	8804 (89%)	717 (7%)	416 (4%)	6	34

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 carbohydrates 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.