



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:11 PM BST

PDB ID : 5A1W  
EMDB ID: : EMD-2987  
Title : The structure of the COPI coat linkage II  
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 : 18.00 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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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



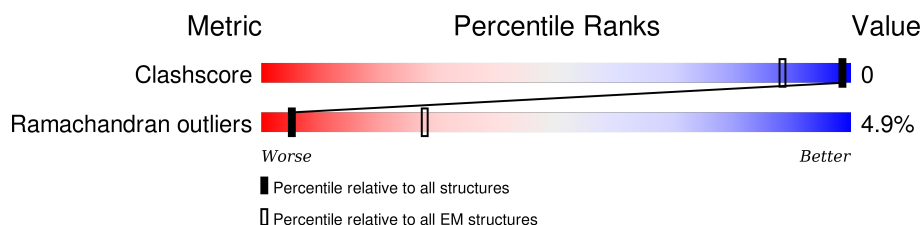
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 18.00 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  $\geq 3$ , 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	88% 12%
1	B	181	88% 12%
2	C	1262	59% 5% 36%
3	D	905	80% 9% 11%
4	E	874	58% 37%
5	F	177	75% 21%
6	G	968	73% 10% 16%
7	H	511	70% 26%



## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15258 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		

- Molecule 2 is a protein called COATOMER SUBUNIT ALPHA.

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

There are 38 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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- 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		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	550	Total	C	N	O	0	0
			2199	1100	550	549		

- 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		

- 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		

There are 15 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

- 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		















## 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
2	C	1.55	8/3250 (0.2%)	1.71	14/4061 (0.3%)
3	D	1.60	17/3210 (0.5%)	1.72	23/4011 (0.6%)
4	E	1.52	2/2198 (0.1%)	1.58	9/2746 (0.3%)
5	F	1.55	1/554 (0.2%)	1.74	3/691 (0.4%)
6	G	1.50	7/3248 (0.2%)	1.71	22/4057 (0.5%)
7	H	1.21	0/1518	1.34	8/1893 (0.4%)
All	All	1.45	35/15248 (0.2%)	1.60	79/19043 (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
3	D	0	2
4	E	0	4
5	F	0	1
6	G	0	14
All	All	0	25

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	621	VAL	C-N	6.92	1.45	1.33
3	D	330	MET	N-CA	-6.75	1.32	1.46
4	E	198	GLY	CA-C	-6.44	1.41	1.51
3	D	378	TYR	N-CA	-6.39	1.33	1.46
3	D	537	THR	N-CA	-6.33	1.33	1.46

The worst 5 of 79 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	496	GLU	N-CA-C	7.82	132.10	111.00
4	E	302	ALA	C-N-CA	7.06	139.35	121.70
2	C	54	VAL	N-CA-C	-6.92	92.31	111.00
6	G	486	ILE	O-C-N	-6.81	108.17	121.10
6	G	869	THR	N-CA-C	-6.73	92.83	111.00

There are no chirality outliers.

5 of 25 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
2	C	3251	0	869	0	0
3	D	3211	0	880	0	0
4	E	2199	0	570	1	0
5	F	555	0	148	0	0
6	G	3250	0	833	0	0
7	H	1520	0	406	4	0
All	All	15258	0	4068	5	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 0.

All (5) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:296:GLU:CA	7:H:368:THR:H	1.95	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:356:ASN:CA	7:H:362:LEU:H	2.10	0.65
7:H:356:ASN:C	7:H:362:LEU:H	2.20	0.45
4:E:249:SER:C	4:E:251:LEU:H	2.23	0.41
7:H:356:ASN:CA	7:H:362:LEU:N	2.83	0.41

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
2	C	811/1262 (64%)	671 (83%)	97 (12%)	43 (5%)	2	29
3	D	801/905 (88%)	700 (87%)	64 (8%)	37 (5%)	3	33
4	E	548/874 (63%)	492 (90%)	27 (5%)	29 (5%)	2	29
5	F	137/177 (77%)	128 (93%)	7 (5%)	2 (2%)	13	57
6	G	809/968 (84%)	658 (81%)	84 (10%)	67 (8%)	1	18
7	H	376/511 (74%)	336 (89%)	31 (8%)	9 (2%)	7	47
All	All	3796/5059 (75%)	3291 (87%)	318 (8%)	187 (5%)	5	31

5 of 187 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 [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 carbohydrates 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.