

wwPDB EM Validation Summary Report (i)

Nov 22, 2022 – 04:13 AM JST

PDB ID	:	7E8T
EMDB ID	:	EMD-31022
Title	:	Monomer of Ypt32-TRAPPII
Authors	:	Mi, C.C.; Sui, S.F.
Deposited on	:	2021-03-02
Resolution	:	3.80 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 (1)) were used in the production of this report:

:	0.0.1. dev 43
:	4.02b-467
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	1.9.9
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	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 3.80 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	L	222	10% 58%	25%	• 13%						
2	Ι	1102	65%	6% •	28%						
3	J	1289	56%	11% •	32%						
4	K	560	7% 39% 5% •	55%							
5	В	268	• 58%	14% •	26%						
6	G	283	• 63%	8%	29%						
7	Е	219	 58%	15%	26%						
8	Н	175	• 68%	16%	16%						



Contr	nued from	n previous	page	
Mol	Chain	Length	Quality of chain	
			20%	
9	А	152	74%	20% • 5%
	-		<u>.</u>	
10	D	159	67%	28% • •
	a	100	📥	
11	C	193	81%	13% • •
		100	i	
11	F,	193	79%	14% • 5%



2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 24894 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 GTP-binding protein YPT32/YPT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	194	Total 1484	C 930	N 254	O 296	$\begin{array}{c} \mathrm{S} \\ \mathrm{4} \end{array}$	0	0

• Molecule 2 is a protein called Trafficking protein particle complex II-specific subunit 130.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ι	788	Total 4199	C 2553	N 811	O 833	${ m S} { m 2}$	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ι	464	LYS	TRP	conflict	UNP Q03660

• Molecule 3 is a protein called Trafficking protein particle complex II-specific subunit 120.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	882	Total 6452	C 4114	N 1113	O 1206	S 19	0	0

• Molecule 4 is a protein called Trafficking protein particle complex II-specific subunit 65.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	251	Total 1649	C 1041	N 291	0 315	${S \over 2}$	0	0

• Molecule 5 is a protein called Trafficking protein particle complex subunit 33.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	В	197	Total 1590	C 1027	N 268	0 287	S 8	0	0

• Molecule 6 is a protein called Trafficking protein particle complex subunit 31.



Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	202	Total 1624	C 1035	N 280	O 300	S 9	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled Actual		Comment	Reference	
G	108	SER	VAL	conflict	UNP Q03337	

• Molecule 7 is a protein called Trafficking protein particle complex subunit 23.

Mol	Chain	Residues	Atoms				AltConf	Trace	
7	Е	163	Total 1317	C 851	N 210	0 246	S 10	0	0

• Molecule 8 is a protein called Trafficking protein particle complex subunit 20.

Mol	Chain	Residues	Atoms				AltConf	Trace	
8	Н	147	Total 1180	C 763	N 195	0 217	${f S}{5}$	0	0

• Molecule 9 is a protein called TRAPP-associated protein TCA17.

Mol	Chain	Residues	Atoms				AltConf	Trace	
9	А	144	Total 1160	C 753	N 182	0 221	$\frac{S}{4}$	0	0

• Molecule 10 is a protein called Trafficking protein particle complex subunit BET5.

Mol	Chain	Residues	Atoms				AltConf	Trace	
10	D	156	Total 1273	C 813	N 216	0 238	S 6	0	0

• Molecule 11 is a protein called Trafficking protein particle complex subunit BET3.

Mol	Chain	Residues	Atoms				AltConf	Trace	
11	Б	192	Total	С	Ν	0	\mathbf{S}	0	0
	105	1478	945	243	279	11	0	0	
11	C	195	Total	С	Ν	0	S	0	0
	100	1488	950	242	285	11		U	



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: GTP-binding protein YPT32/YPT11

















• Molecule 10: Trafficking protein particle complex subunit BET5



• Molecule 11: Trafficking protein particle complex subunit BET3





• Molecule 11: Trafficking protein particle complex subunit BET3





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81870	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 $(6k \ge 4k)$	Depositor
Maximum map value	0.048	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	521.82, 521.82, 521.82	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8697, 0.8697, 0.8697	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).

Mal	Chain	Bo	nd lengths	B	ond angles
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	L	0.56	0/1507	0.78	3/2038~(0.1%)
2	Ι	0.32	0/4219	0.65	14/5852~(0.2%)
3	J	0.45	2/6562~(0.0%)	0.86	28/8927~(0.3%)
4	Κ	0.34	0/1663	0.83	11/2268~(0.5%)
5	В	0.43	0/1617	0.91	7/2174~(0.3%)
6	G	0.45	0/1658	0.82	3/2236~(0.1%)
7	Е	0.49	0/1341	0.79	1/1807~(0.1%)
8	Н	0.48	0/1211	0.95	5/1643~(0.3%)
9	А	0.39	0/1180	0.87	4/1592~(0.3%)
10	D	0.50	0/1302	0.76	2/1758~(0.1%)
11	С	0.47	0/1515	0.81	1/2049~(0.0%)
11	F	0.45	0/1505	0.80	4/2035~(0.2%)
All	All	0.44	$2/2\overline{5280}\ (0.0\%)$	0.81	$83/\overline{34379}~(0.2\%)$

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
11	С	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
3	J	1100	PRO	N-CD	-10.29	1.33	1.47
3	J	738	PRO	N-CD	-7.32	1.37	1.47

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
8	Н	46	ASP	CB-CG-OD1	10.25	127.53	118.30
11	С	186	ASP	CB-CG-OD1	9.62	126.95	118.30



	J	1	I J				
Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	J	783	LEU	CA-CB-CG	8.98	135.96	115.30
3	J	815	ILE	CG1-CB-CG2	-8.86	91.90	111.40
10	D	119	LEU	CA-CB-CG	7.96	133.62	115.30

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There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	С	43	GLN	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	L	1484	0	1410	44	0
2	Ι	4199	0	2172	26	0
3	J	6452	0	5798	224	0
4	K	1649	0	1338	21	0
5	В	1590	0	1612	27	0
6	G	1624	0	1601	16	0
7	Е	1317	0	1323	24	0
8	Н	1180	0	1132	15	0
9	А	1160	0	1184	20	0
10	D	1273	0	1245	23	0
11	С	1488	0	1487	24	0
11	F	1478	0	1487	20	0
All	All	24894	0	21789	436	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 9.

The worst 5 of 436 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:J:903:PRO:HB3	3:J:1098:ILE:CG1	1.13	1.58



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:903:PRO:CA	3:J:1098:ILE:HG21	1.37	1.50
3:J:915:TYR:H	3:J:1102:ARG:NH2	1.09	1.45
3:J:903:PRO:CB	3:J:1098:ILE:HG12	1.44	1.44
3:J:915:TYR:N	3:J:1102:ARG:HH22	1.07	1.39

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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	Perce	entiles
1	L	192/222~(86%)	170 (88%)	17 (9%)	5(3%)	5	36
2	Ι	782/1102 (71%)	649 (83%)	120 (15%)	13 (2%)	9	43
3	J	868/1289~(67%)	730 (84%)	129 (15%)	9 (1%)	15	52
4	Κ	243/560~(43%)	205 (84%)	33 (14%)	5 (2%)	7	40
5	В	191/268~(71%)	172 (90%)	19 (10%)	0	100	100
6	G	198/283~(70%)	181 (91%)	17 (9%)	0	100	100
7	Е	155/219~(71%)	140 (90%)	13 (8%)	2(1%)	12	48
8	Н	143/175~(82%)	134 (94%)	9~(6%)	0	100	100
9	А	142/152~(93%)	131 (92%)	11 (8%)	0	100	100
10	D	154/159~(97%)	139 (90%)	14 (9%)	1 (1%)	25	62
11	С	183/193~(95%)	165 (90%)	17 (9%)	1 (0%)	29	66
11	F	181/193 (94%)	162 (90%)	19 (10%)	0	100	100
All	All	3432/4815 (71%)	2978 (87%)	418 (12%)	36 (1%)	20	52

 $5~{\rm of}~36$ Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	42	SER
	<i>a</i>	-	



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	5	1	1 5
Mol	Chain	Res	Type
1	L	199	PRO
2	Ι	346	PRO
2	Ι	483	PRO
2	Ι	976	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	L	152/189~(80%)	125~(82%)	27 (18%)	2	12
2	Ι	78/1023~(8%)	77~(99%)	1 (1%)	69	82
3	J	594/1213~(49%)	573~(96%)	21 (4%)	36	64
4	Κ	121/518~(23%)	121 (100%)	0	100	100
5	В	176/248~(71%)	175~(99%)	1 (1%)	86	92
6	G	179/249~(72%)	179 (100%)	0	100	100
7	Ε	149/199~(75%)	140 (94%)	9~(6%)	19	50
8	Н	127/152~(84%)	125~(98%)	2(2%)	62	79
9	А	134/142~(94%)	131 (98%)	3(2%)	52	72
10	D	142/145~(98%)	124 (87%)	18 (13%)	4	23
11	С	170/178~(96%)	168 (99%)	2(1%)	71	84
11	F	169/178~(95%)	165~(98%)	4 (2%)	49	71
All	All	2191/4434 (49%)	2103 (96%)	88 (4%)	35	59

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
7	Ε	56	GLN
10	D	35	LYS
8	Н	12	ASP
10	D	22	THR
10	D	39	GLU



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
7	Ε	65	ASN
7	Ε	113	ASN
10	D	37	ASN
3	J	1092	ASN
3	J	736	GLN

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-31022. 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.

Orthogonal projections (i) 6.1

6.1.1Primary map



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

6.2Central slices (i)

6.2.1**Primary** map



X Index: 300

Y Index: 300



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: 203

Y Index: 378

Z Index: 327

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



The images above show the 3D surface view of the map at the recommended contour level 0.009. 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 220 $\rm nm^3;$ this corresponds to an approximate mass of 198 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 0.263 \AA^{-1}



8 Fourier-Shell correlation (i)

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



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-31022 and PDB model 7E8T. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.009 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)



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.

9.3 Atom inclusion mapped to coordinate model (i)



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 (0.009).



9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 77% 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 (0.009) and Q-score for the entire model and for each chain.

	Q-score	Atom inclusion	Chain
	0.3940	0.7731	All
1.0	0.3760	0.6207	А
	0.3940	0.7399	В
	0.4330	0.7866	С
	0.4220	0.8119	D
	0.4520	0.8114	Е
	0.4340	0.7993	F
	0.4390	0.8049	G
	0.4210	0.8034	Н
0.0	0.3710	0.8459	I
<0.0	0.3700	0.7532	J
	0.3390	0.7052	K
	0.4070	0.7167	L

