

wwPDB EM Validation Summary Report (i)

Sep 18, 2021 – 08:10 am BST

PDB ID	:	7PE7
EMDB ID	:	EMD-13347
Title	:	cryo-EM structure of DEPTOR bound to human mTOR complex 2, overall
		refinement
Authors	:	Waelchli, M.; Maier, T.
Deposited on	:	2021-08-09
Resolution	:	3.41 Å(reported)
Based on initial model	:	6ZWM

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 following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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 3.41 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.



Motria	Whole archive	EM structures		
	$(\# \mathbf{Entries})$	$(\# { m Entries})$		
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%

Mol	Chain	Length			Quality of	chain		
1	А	2571			77%		8%	15%
1	В	2571			77%		8%	15%
2	С	326			76%		21	% ••
2	D	326			76%		21	% ••
3	Е	1708		57%		8%	35%	
3	F	1708		57%		8%	35%	
4	G	522	17% •			81%		
4	Н	522	17% •			81%		
5	Ι	409	20%	6%		74%		

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Mol	Chain	Length	Quality of chain						
5	J	409	20%	6%	74%				



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 58582 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 Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues		At		AltConf	Trace		
1	В	2194	Total 16419	m C 10414	N 2922	O 2984	S 99	0	0
1	А	2194	Total 16419	C 10414	N 2922	O 2984	S 99	0	0

Chain	Residue	Modelled	Actual	Comment	Reference
В	246 M	GLY	-	insertion	UNP P42345
В	246N	SER	-	insertion	UNP P42345
В	2460	THR	-	insertion	UNP P42345
В	246P	SER	-	insertion	UNP P42345
В	246Q	GLY	-	insertion	UNP P42345
В	246R	SER	-	insertion	UNP P42345
В	246S	GLY	-	insertion	UNP P42345
В	246T	ASP	-	insertion	UNP P42345
В	246U	TYR	-	insertion	UNP P42345
В	246V	LYS	-	insertion	UNP P42345
В	246W	ASP	-	insertion	UNP P42345
В	246X	ASP	-	insertion	UNP P42345
В	246Y	ASP	-	insertion	UNP P42345
В	246Z	ASP	-	insertion	UNP P42345
В	247A	LYS	-	insertion	UNP P42345
В	247B	GLY	-	insertion	UNP P42345
В	247C	SER	-	insertion	UNP P42345
В	247D	THR	-	insertion	UNP P42345
В	247E	SER	-	insertion	UNP P42345
В	247F	GLY	-	insertion	UNP P42345
В	247G	SER	-	insertion	UNP P42345
В	247H	GLY	-	insertion	UNP P42345
A	246 M	GLY	-	insertion	UNP P42345
A	246N	SER	-	insertion	UNP P42345
A	2460	THR	-	insertion	UNP P42345
A	246P	SER	-	insertion	UNP P42345

There are 44 discrepancies between the modelled and reference sequences:

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Chain	Residue	Modelled	Actual	Comment	Reference
А	246Q	GLY	-	insertion	UNP P42345
A	246R	SER	-	insertion	UNP P42345
А	246S	GLY	-	insertion	UNP P42345
А	246T	ASP	-	insertion	UNP P42345
А	246U	TYR	-	insertion	UNP P42345
А	246V	LYS	-	insertion	UNP P42345
A	246W	ASP	-	insertion	UNP P42345
А	246X	ASP	-	insertion	UNP P42345
A	246Y	ASP	-	insertion	UNP P42345
А	246Z	ASP	-	insertion	UNP P42345
А	247A	LYS	-	insertion	UNP P42345
А	247B	GLY	-	insertion	UNP P42345
А	247C	SER	-	insertion	UNP P42345
A	247D	THR	-	insertion	UNP P42345
A	247E	SER	-	insertion	UNP P42345
A	247F	GLY	-	insertion	UNP P42345
А	247G	SER	-	insertion	UNP P42345
А	247H	GLY	-	insertion	UNP P42345

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• Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

Mol	Chain	Residues		At	oms		AltConf	Trace	
9	п	210	Total	С	Ν	Ο	\mathbf{S}	0	0
	519	2465	1533	437	477	18	0	0	
9	C	210	Total	С	Ν	Ο	S	0	0
		519	2465	1533	437	477	18		U

• Molecule 3 is a protein called Rapamycin-insensitive companion of mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	1115	Total	С	Ν	Ο	\mathbf{S}	0	0
1 6	T,	1115	8917	5680	1582	1608	47		
2	Б	1115	Total	С	Ν	Ο	S	0	0
D D		1110	8917	5680	1582	1608	47	0	0

• Molecule 4 is a protein called Target of rapamycin complex 2 subunit MAPKAP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	ц	98	Total	С	Ν	Ο	\mathbf{S}	0	0
	90	655	399	125	127	4	0	0	
4	C	0.8	Total	С	Ν	0	S	0	0
4 G	G	90	655	399	125	127	4	0	



• Molecule 5 is a protein called DEP domain-containing mTOR-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	т	I 106	Total	С	Ν	Ο	\mathbf{S}	0	0
0 1	L	100	795	504	138	146	7	0	
5	т	106	Total	С	Ν	Ο	S	0	0
Э	J	100	795	504	138	146	7		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ι	204	SER	ASN	variant	UNP Q8TB45
Ι	389	ASN	SER	variant	UNP Q8TB45
J	204	SER	ASN	variant	UNP Q8TB45
J	389	ASN	SER	variant	UNP Q8TB45

• Molecule 6 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms	AltConf
6	В	1	Total C O P	0
0	D	1	36 6 24 6	0
6	Λ	1	Total C O P	0
6	A		36 6 24 6	0

• Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).



Mol	Chain	Residues	Atoms	AltConf
7	F	1	Total Zn 1 1	0
7	Е	1	Total Zn 1 1	0

 $\bullet\,$ Molecule 8 is ACETYL GROUP (three-letter code: ACE) (formula: ${\rm C_2H_4O}).$



Mol	Chain	Residues	Atoms	AltConf
8	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 2 & 1 \end{array}$	0
8	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 2 & 1 \end{array}$	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: Serine/threonine-protein kinase mTOR





 \bullet Molecule 1: Serine/threen ine-protein kinase mTOR





D2244 V1963 D2241 11960 R2561 11970 R2339 R2036 R2342 R2036 R2343 R2036 R2344 R2036 R2343 R2036 R2344 R2042 R2343 R2042 R2344 R2042 R2343 R2043 R2344 R2043 R2345 R2046 R2346 R2046 R2341 R2049 R2343 R2049 R2344 R2044 R2344 R2045 R2345 R2046 R2346 R2046 R2347 R2046 R2348 R2046 R2349 R2046 R2346 R2046 R244</td

• Molecule 2: Target of rapamycin complex subunit LST8



• Molecule 2: Target of rapamycin complex subunit LST8



 \bullet Molecule 3: Rapamy cin-insensitive companion of mTOR







• Molecule 3: Rapamycin-insensitive companion of mTOR





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• Molecule 4: Target of rapamycin complex 2 subunit MAPKAP1



• Molecule 5: DEP domain-containing mTOR-interacting protein





• Molecule 5: DEP domain-containing mTOR-interacting protein





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	467078	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 K2 SUMMIT (4k x 4k)	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, IHP, ACE

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	Choin	Bond	lengths	Bond angles	
WIOI	Cham	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.23	0/16719	0.43	0/22710
1	В	0.23	0/16719	0.43	0/22710
2	С	0.24	0/2523	0.49	0/3438
2	D	0.24	0/2523	0.49	0/3438
3	Е	0.23	0/9078	0.44	0/12281
3	F	0.23	0/9078	0.44	0/12281
4	G	0.22	0/660	0.45	0/900
4	Н	0.22	0/660	0.45	0/900
5	Ι	0.24	0/811	0.49	0/1104
5	J	0.24	0/811	0.49	0/1104
All	All	0.23	0/59582	0.44	0/80866

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	А	16419	0	15461	119	0
1	В	16419	0	15461	121	0
2	C	2465	0	2351	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2465	0	2351	42	0
3	Е	8917	0	9064	80	0
3	F	8917	0	9064	79	0
4	G	655	0	519	7	0
4	Н	655	0	519	8	0
5	Ι	795	0	812	12	0
5	J	795	0	812	13	0
6	А	36	0	6	0	0
6	В	36	0	6	0	0
7	Е	1	0	0	0	0
7	F	1	0	0	0	0
8	G	3	0	3	0	0
8	Н	3	0	3	0	0
All	All	58582	0	56432	493	0

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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 4.

The worst 5 of 493 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:E:556:LYS:HB2	3:E:607:GLN:HE21	1.54	0.73
3:F:556:LYS:HB2	3:F:607:GLN:HE21	1.54	0.73
1:A:2192:LEU:HD22	1:A:2235:GLY:HA3	1.72	0.72
1:B:2192:LEU:HD22	1:B:2235:GLY:HA3	1.72	0.72
1:A:1722:GLN:O	1:A:1726:GLN:NE2	2.24	0.70

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	ntiles
1	А	2152/2571~(84%)	2101 (98%)	51 (2%)	0	100	100
1	В	2152/2571~(84%)	2100~(98%)	52 (2%)	0	100	100
2	С	317/326~(97%)	301~(95%)	16~(5%)	0	100	100
2	D	317/326~(97%)	301~(95%)	16 (5%)	0	100	100
3	Е	1101/1708~(64%)	1056~(96%)	44 (4%)	1 (0%)	51	83
3	F	1101/1708~(64%)	1056~(96%)	44 (4%)	1 (0%)	51	83
4	G	94/522~(18%)	91~(97%)	3(3%)	0	100	100
4	Н	94/522~(18%)	91 (97%)	3 (3%)	0	100	100
5	Ι	104/409~(25%)	92~(88%)	11 (11%)	1 (1%)	15	51
5	J	104/409~(25%)	92 (88%)	11 (11%)	1 (1%)	15	51
All	All	7536/11072~(68%)	7281 (97%)	251 (3%)	4 (0%)	54	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
3	F	642	PRO
3	Е	642	PRO
5	Ι	308	SER
5	J	308	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain 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	\mathbf{ntiles}
1	А	1571/2236~(70%)	1556~(99%)	15~(1%)	76	88
1	В	1571/2236~(70%)	1556~(99%)	15~(1%)	76	88
2	С	269/276~(98%)	266~(99%)	3~(1%)	73	87
2	D	269/276~(98%)	266~(99%)	3~(1%)	73	87
3	Ε	985/1539~(64%)	979~(99%)	6 (1%)	86	94
3	F	985/1539~(64%)	979~(99%)	6~(1%)	86	94
4	G	50/471~(11%)	50 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
4	Н	50/471~(11%)	50~(100%)	0	100	100
5	Ι	89/364~(24%)	87~(98%)	2(2%)	52	78
5	J	89/364~(24%)	87~(98%)	2(2%)	52	78
All	All	5928/9772~(61%)	5876 (99%)	52 (1%)	79	90

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5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	\mathbf{Type}
1	А	854	VAL
1	А	1665	ARG
5	Ι	319	LEU
1	А	863	THR
1	А	1203	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	В	1726	GLN
3	F	607	GLN
3	F	889	HIS
3	Е	607	GLN
3	Е	889	HIS

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)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Turne	Chain	Dec	Tink	Bo	ond leng	$_{\rm sths}$	Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	IHP	В	2601	-	36,36,36	0.77	1 (2%)	$54,\!60,\!60$	0.30	0
6	IHP	А	2601	-	36,36,36	0.77	1 (2%)	$54,\!60,\!60$	0.30	0
8	ACE	Н	601	4	1,2,2	0.74	0	$1,\!1,\!1$	0.24	0
8	ACE	G	601	4	1,2,2	0.74	0	$1,\!1,\!1$	0.24	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	IHP	В	2601	-	-	1/30/54/54	0/1/1/1
6	IHP	А	2601	-	-	1/30/54/54	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
6	В	2601	IHP	P3-O13	3.00	1.65	1.59
6	А	2601	IHP	P3-O13	2.99	1.65	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	В	2601	IHP	C2-O12-P2-O22
6	А	2601	IHP	C2-O12-P2-O22

There are no ring outliers.



No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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.

