



wwPDB EM Map/Model Validation Report ⓘ

Apr 26, 2016 – 06:29 PM BST

PDB ID : 5FVM
EMDB ID: : EMD-3329
Title : Cryo electron microscopy of a complex of Tor and Lst8
Authors : Baretic, D.; Berndt, A.; Ohashi, Y.; Johnson, C.M.; Williams, R.L.
Deposited on : 2016-02-09
Resolution : 6.70 Å(reported)
Based on PDB ID : 4JSV

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) : trunk27461

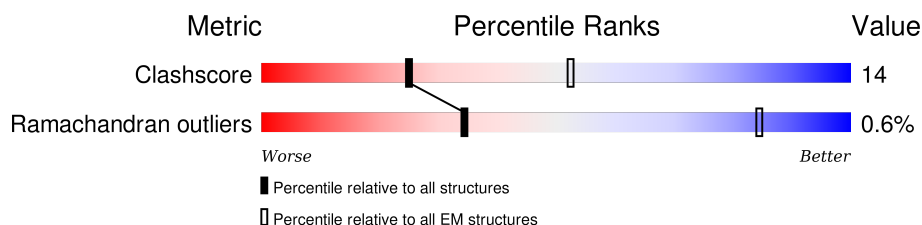
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.70 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	2471	72% 13% 14%
1	B	2471	72% 14% 14%
2	C	303	72% 27% .
2	D	303	71% 28% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23974 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 TOR2.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	2117	Total 10508	C 6274	N 2117	O 2117	0	0
1	B	2117	Total 10508	C 6274	N 2117	O 2117	0	0

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	GLU	-	EXPRESSION TAG	UNP A0A090BKR
A	-19	LEU	-	EXPRESSION TAG	UNP A0A090BKR
A	-18	LEU	-	EXPRESSION TAG	UNP A0A090BKR
A	-17	GLU	-	EXPRESSION TAG	UNP A0A090BKR
A	-16	GLY	-	EXPRESSION TAG	UNP A0A090BKR
A	-15	GLU	-	EXPRESSION TAG	UNP A0A090BKR
A	-14	LEU	-	EXPRESSION TAG	UNP A0A090BKR
A	-13	LYS	-	EXPRESSION TAG	UNP A0A090BKR
A	-12	THR	-	EXPRESSION TAG	UNP A0A090BKR
A	-11	ALA	-	EXPRESSION TAG	UNP A0A090BKR
A	-10	ALA	-	EXPRESSION TAG	UNP A0A090BKR
A	-9	LEU	-	EXPRESSION TAG	UNP A0A090BKR
A	-8	ALA	-	EXPRESSION TAG	UNP A0A090BKR
A	-7	GLN	-	EXPRESSION TAG	UNP A0A090BKR
A	-6	HIS	-	EXPRESSION TAG	UNP A0A090BKR
A	-5	ASP	-	EXPRESSION TAG	UNP A0A090BKR
A	-4	GLU	-	EXPRESSION TAG	UNP A0A090BKR
A	-3	ALA	-	EXPRESSION TAG	UNP A0A090BKR
A	-2	MET	-	EXPRESSION TAG	UNP A0A090BKR
A	-1	GLY	-	EXPRESSION TAG	UNP A0A090BKR
A	0	GLY	-	EXPRESSION TAG	UNP A0A090BKR
A	1	SER	-	EXPRESSION TAG	UNP A0A090BKR
A	34	ALA	THR	CONFLICT	UNP A0A090BKR
A	44	ALA	PRO	CONFLICT	UNP A0A090BKR
A	48	MET	ILE	CONFLICT	UNP A0A090BKR
A	125	ASP	GLU	CONFLICT	UNP A0A090BKR

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Chain	Residue	Modelled	Actual	Comment	Reference
A	557	ARG	THR	CONFLICT	UNP A0A090BKR
A	998	LEU	VAL	CONFLICT	UNP A0A090BKR
A	1063	VAL	ALA	CONFLICT	UNP A0A090BKR
B	-20	GLU	-	EXPRESSION TAG	UNP A0A090BKR
B	-19	LEU	-	EXPRESSION TAG	UNP A0A090BKR
B	-18	LEU	-	EXPRESSION TAG	UNP A0A090BKR
B	-17	GLU	-	EXPRESSION TAG	UNP A0A090BKR
B	-16	GLY	-	EXPRESSION TAG	UNP A0A090BKR
B	-15	GLU	-	EXPRESSION TAG	UNP A0A090BKR
B	-14	LEU	-	EXPRESSION TAG	UNP A0A090BKR
B	-13	LYS	-	EXPRESSION TAG	UNP A0A090BKR
B	-12	THR	-	EXPRESSION TAG	UNP A0A090BKR
B	-11	ALA	-	EXPRESSION TAG	UNP A0A090BKR
B	-10	ALA	-	EXPRESSION TAG	UNP A0A090BKR
B	-9	LEU	-	EXPRESSION TAG	UNP A0A090BKR
B	-8	ALA	-	EXPRESSION TAG	UNP A0A090BKR
B	-7	GLN	-	EXPRESSION TAG	UNP A0A090BKR
B	-6	HIS	-	EXPRESSION TAG	UNP A0A090BKR
B	-5	ASP	-	EXPRESSION TAG	UNP A0A090BKR
B	-4	GLU	-	EXPRESSION TAG	UNP A0A090BKR
B	-3	ALA	-	EXPRESSION TAG	UNP A0A090BKR
B	-2	MET	-	EXPRESSION TAG	UNP A0A090BKR
B	-1	GLY	-	EXPRESSION TAG	UNP A0A090BKR
B	0	GLY	-	EXPRESSION TAG	UNP A0A090BKR
B	1	SER	-	EXPRESSION TAG	UNP A0A090BKR
B	34	ALA	THR	CONFLICT	UNP A0A090BKR
B	44	ALA	PRO	CONFLICT	UNP A0A090BKR
B	48	MET	ILE	CONFLICT	UNP A0A090BKR
B	125	ASP	GLU	CONFLICT	UNP A0A090BKR
B	557	ARG	THR	CONFLICT	UNP A0A090BKR
B	998	LEU	VAL	CONFLICT	UNP A0A090BKR
B	1063	VAL	ALA	CONFLICT	UNP A0A090BKR

- Molecule 2 is a protein called TARGET OF RAPAMYCIN COMPLEX SUBUNIT LST8.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	299	Total	C	N	O	0	0
			1479	881	299	299		
2	D	299	Total	C	N	O	0	0
			1479	881	299	299		

There are 2 discrepancies between the modelled and reference sequences:

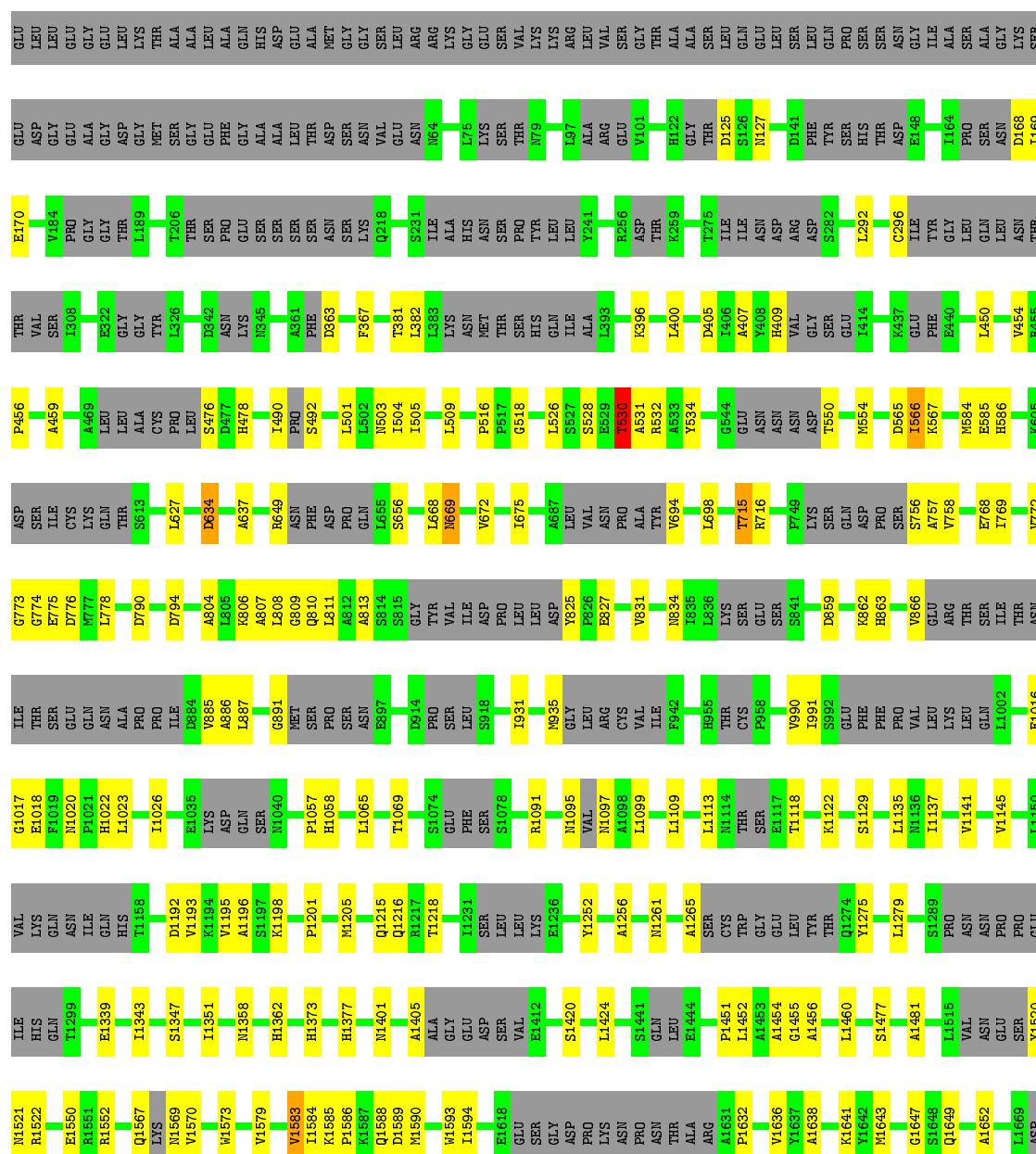
Chain	Residue	Modelled	Actual	Comment	Reference
C	221	ASN	HIS	CONFLICT	UNP A0A090BJK
D	221	ASN	HIS	CONFLICT	UNP A0A090BJK

3 Residue-property plots

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: SERINE/THREONINE-PROTEIN KINASE TOR2

Chain A: 



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE (GCTF), Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	47000	Depositor
Image detector	FEI FALCON II (4K X 4K)	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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.40	0/10457	0.62	4/14512 (0.0%)
1	B	0.40	0/10457	0.62	4/14512 (0.0%)
2	C	0.29	0/1478	0.60	1/2058 (0.0%)
2	D	0.29	0/1478	0.60	1/2058 (0.0%)
All	All	0.39	0/23870	0.61	10/33140 (0.0%)

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
1	A	0	19
1	B	0	19
2	C	0	3
2	D	0	3
All	All	0	44

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	106	SER	C-N-CA	8.81	158.99	122.00
2	C	106	SER	C-N-CA	8.80	158.97	122.00
1	B	2341	ASP	C-N-CA	7.80	154.77	122.00
1	A	2341	ASP	C-N-CA	7.79	154.74	122.00
1	A	530	THR	C-N-CA	5.91	136.47	121.70

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	509	LEU	Peptide
1	A	530	THR	Peptide
1	A	566	ILE	Peptide
1	A	567	LYS	Peptide
1	A	627	LEU	Peptide

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	10508	0	4629	184	0
1	B	10508	0	4629	187	0
2	C	1479	0	673	52	0
2	D	1479	0	673	53	0
All	All	23974	0	10604	476	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 14.

The worst 5 of 476 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)
2:D:264:TYR:HA	2:D:278:ASP:HA	1.57	0.87
2:C:264:TYR:HA	2:C:278:ASP:HA	1.57	0.84
1:B:2407:ASP:O	1:B:2412:ASN:N	2.11	0.82
1:A:2407:ASP:O	1:A:2412:ASN:N	2.10	0.82
1:A:1955:PHE:HA	1:A:1961:THR:H	1.45	0.82

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	2017/2471 (82%)	1594 (79%)	411 (20%)	12 (1%)	30	74
1	B	2017/2471 (82%)	1594 (79%)	411 (20%)	12 (1%)	30	74
2	C	297/303 (98%)	253 (85%)	41 (14%)	3 (1%)	19	65
2	D	297/303 (98%)	253 (85%)	41 (14%)	3 (1%)	19	65
All	All	4628/5548 (83%)	3694 (80%)	904 (20%)	30 (1%)	34	74

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	ILE
1	A	454	VAL
1	A	490	ILE
1	A	1855	VAL
1	A	1890	VAL

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.