wwPDB EM Validation Summary Report

May 14, 2024 – 02:45 pm BST

PDB ID	:	9F48
EMDB ID	:	EMD-50185
Title	:	KS + AT di-domain of polyketide synthase 13 in Mycobacterium tuberculosis
Authors	:	Johnston, H.E.; Futterer, K.
Deposited on	:	2024-04-26
Resolution	:	3.40 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 (i)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

PERCENTILES INFOmissingINFO

1 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 13803 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 Polyketide synthase Pks13.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	922	Total	C	N	O	S	0	0
			6900	4350	1215	1315	20		
1	B	923	Total	C	N	O	S	0	0
			6903	4351	1216	1316	20		

SEQUENCE-PLOTS INFOmissingINFO

2 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	168566	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	16.5	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

3 Model quality

3.1 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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.26	0/7048	0.50	0/9593
1	B	0.27	0/7051	0.50	0/9597
All	All	0.27	0/14099	0.50	0/19190

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	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	328	GLU	Peptide
1	A	449	ASP	Peptide
1	B	201	ILE	Peptide

3.2 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	6900	0	6750	113	0
1	B	6903	0	6745	107	0
All	All	13803	0	13495	215	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 8.

The worst 5 of 215 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)
1:A:892:ALA:HB1	1:A:897:LYS:HB2	1.66	0.77
1:B:127:ARG:HG2	1:B:180:LEU:HD21	1.67	0.77
1:B:202:ASP:HB3	1:B:203:PRO:HA	1.69	0.73
1:B:336:ASP:N	1:B:336:ASP:OD1	2.24	0.71
1:B:317:LEU:HG	1:B:353:GLU:HB3	1.72	0.70

There are no symmetry-related clashes.

3.3 Torsion angles (i)

3.3.1 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	918/1733 (53%)	837 (91%)	80 (9%)	1 (0%)	51 82
1	B	919/1733 (53%)	852 (93%)	64 (7%)	3 (0%)	41 72
All	All	1837/3466 (53%)	1689 (92%)	144 (8%)	4 (0%)	50 78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	159	GLU
1	B	286	ALA
1	B	202	ASP

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Mol	Chain	Res	Type
1	A	329	ILE

3.3.2 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	Percentiles
1	A	698/1358 (51%)	670 (96%)	28 (4%)	31 60
1	B	697/1358 (51%)	681 (98%)	16 (2%)	50 74
All	All	1395/2716 (51%)	1351 (97%)	44 (3%)	42 67

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	207	MET
1	B	497	TYR
1	B	241	ASP
1	B	340	LYS
1	B	648	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	971	HIS
1	B	277	HIS

3.3.3 RNA (i)

There are no RNA molecules in this entry.

3.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

3.5 Carbohydrates (i)

There are no monosaccharides in this entry.

3.6 Ligand geometry (i)

There are no ligands in this entry.

3.7 Other polymers (i)

There are no such residues in this entry.

3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

4 Map visualisation

This section contains visualisations of the EMDB entry EMD-50185. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

4.1 Orthogonal projections

This section was not generated.

4.2 Central slices

This section was not generated.

4.3 Largest variance slices

This section was not generated.

4.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

4.5 Orthogonal surface views

This section was not generated.

4.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

5 Map analysis

This section contains the results of statistical analysis of the map.

5.1 Map-value distribution

This section was not generated.

5.2 Volume estimate versus contour level

This section was not generated.

5.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

6 Fourier-Shell correlation (i)

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

7 Map-model fit

This section was not generated.