



Full wwPDB EM Model Validation Report ⓘ

May 26, 2020 – 04:40 PM EDT

PDB ID : 6WC7
EMDB ID : EMD-21602
Title : Acyl carrier protein (ACP) domain bound to dehydratase (DH) domain in fungal fatty acid synthase (FAS)
Authors : Lou, J.W.; Mazhab-Jafari, M.T.
Deposited on : 2020-03-29
Resolution : 5.80 Å(reported)
Based on initial model : 2UV8

This is a Full wwPDB EM Model Validation Report for a publicly released PDB/EMDB 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.10.1

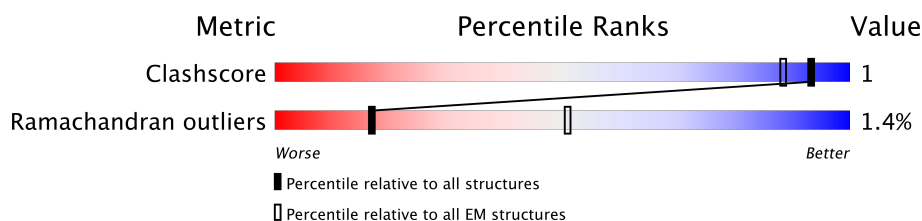
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.80 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	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663

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 on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	G	2057	 20% 79%
2	A	1887	 8% 91%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2879 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 Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	G	422	Total	C	N	O	0	0
			2078	1234	422	422		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	2052	HIS	-	expression tag	UNP P07149
G	2053	HIS	-	expression tag	UNP P07149
G	2054	HIS	-	expression tag	UNP P07149
G	2055	HIS	-	expression tag	UNP P07149
G	2056	HIS	-	expression tag	UNP P07149
G	2057	HIS	-	expression tag	UNP P07149

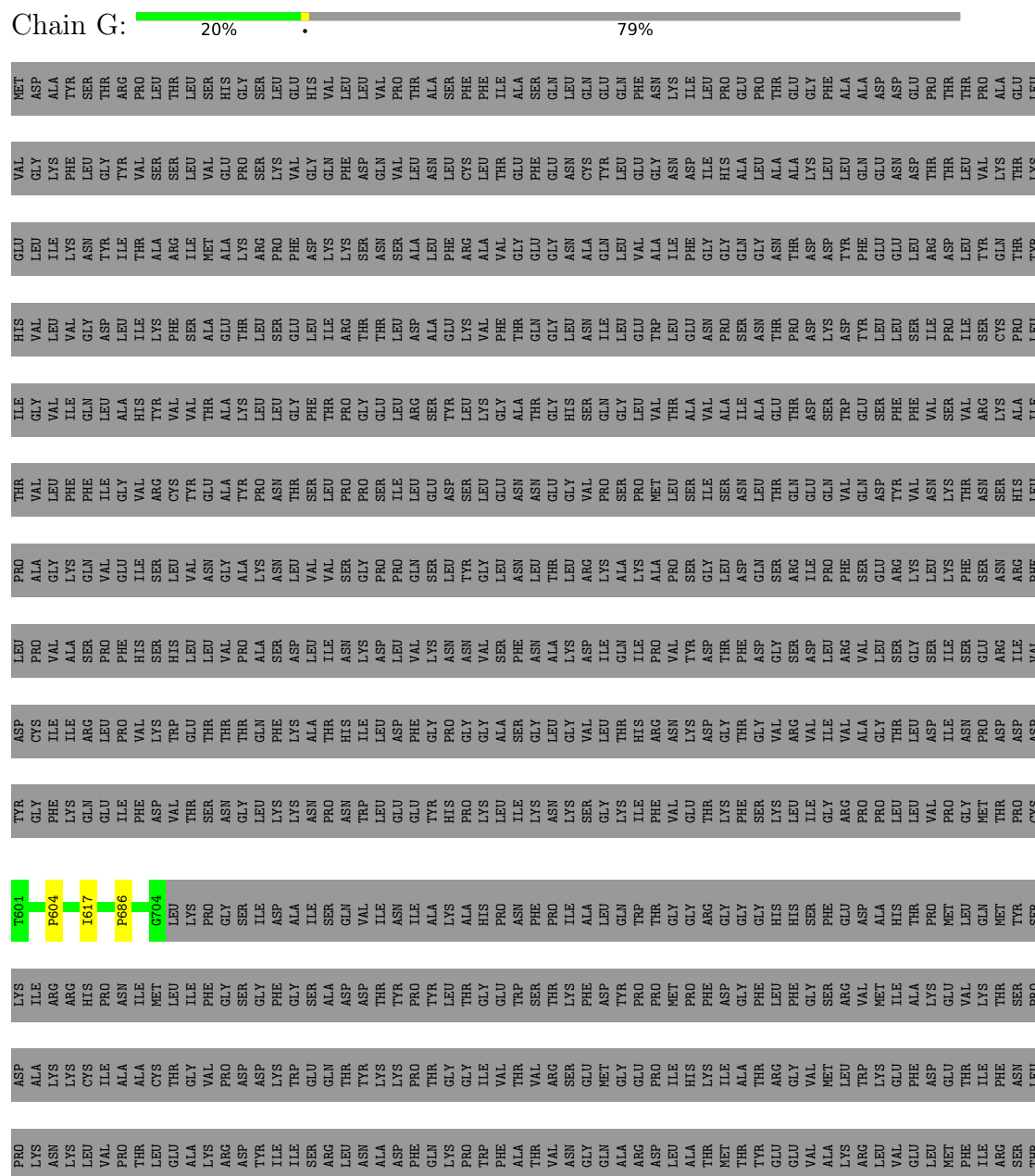
- Molecule 2 is a protein called Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	A	163	Total	C	N	O	0	0
			801	475	163	163		

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 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: Fatty acid synthase subunit beta





[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	15767	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	36	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (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 > 5$	RMSZ	# $ Z > 5$
1	G	0.24	0/2075	0.44	0/2881
2	A	0.23	0/800	0.39	0/1110
All	All	0.24	0/2875	0.42	0/3991

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	G	2078	0	936	4	0
2	A	801	0	373	2	0
All	All	2879	0	1309	6	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 1.

All (6) 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:A:171:THR:HA	2:A:205:PRO:HA	1.91	0.53
1:G:1395:THR:HA	1:G:1405:GLU:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1357:TYR:HA	1:G:1406:VAL:HA	1.95	0.48
1:G:1356:GLY:HA2	1:G:1609:THR:HA	1.97	0.47
1:G:1605:VAL:HA	1:G:1657:ILE:HA	2.00	0.43
2:A:148:SER:HA	2:A:210:ALA:HB1	2.01	0.42

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	G	416/2057 (20%)	351 (84%)	58 (14%)	7 (2%)	10	49
2	A	161/1887 (8%)	149 (92%)	11 (7%)	1 (1%)	27	70
All	All	577/3944 (15%)	500 (87%)	69 (12%)	8 (1%)	17	52

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	604	PRO
2	A	257	PRO
1	G	1250	PRO
1	G	617	ILE
1	G	1369	GLY
1	G	686	PRO
1	G	1377	VAL
1	G	1541	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.