



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 03:57 am BST

PDB ID : 6NO6  
Title : K46bE&K114bD mutant ATP-grasp fold of Blastocystis hominis succinyl-CoA synthetase  
Authors : Huang, J.; Fraser, M.E.  
Deposited on : 2019-01-15  
Resolution : 1.91 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

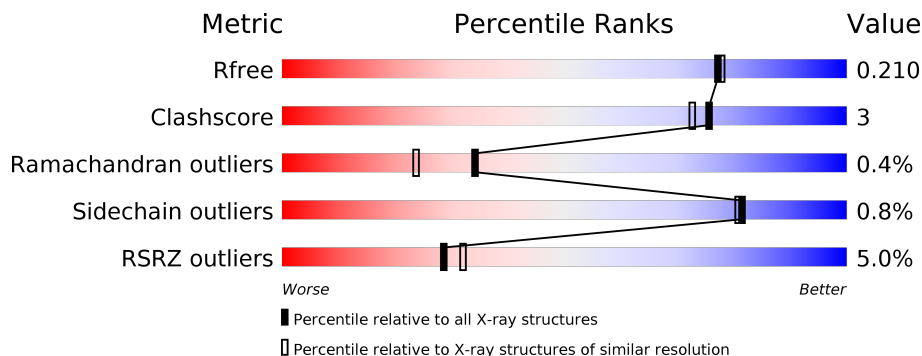
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


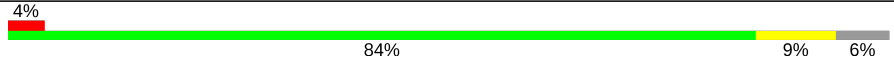
The reported resolution of this entry is 1.91 Å.

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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	
1	B	250	

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 7331 atoms, of which 3622 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Succinate–CoA ligase [ADP-forming] subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	229	3534	1111	1784	296	327	16	0	0	0
1	B	234	3641	1140	1838	308	337	18	0	3	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP B3FHP0
A	46	GLU	LYS	engineered mutation	UNP B3FHP0
A	114	ASP	LYS	engineered mutation	UNP B3FHP0
A	240	GLY	-	expression tag	UNP B3FHP0
A	241	LEU	-	expression tag	UNP B3FHP0
A	242	GLU	-	expression tag	UNP B3FHP0
A	243	HIS	-	expression tag	UNP B3FHP0
A	244	HIS	-	expression tag	UNP B3FHP0
A	245	HIS	-	expression tag	UNP B3FHP0
A	246	HIS	-	expression tag	UNP B3FHP0
A	247	HIS	-	expression tag	UNP B3FHP0
A	248	HIS	-	expression tag	UNP B3FHP0
A	249	HIS	-	expression tag	UNP B3FHP0
A	250	HIS	-	expression tag	UNP B3FHP0
B	1	MET	-	initiating methionine	UNP B3FHP0
B	46	GLU	LYS	engineered mutation	UNP B3FHP0
B	114	ASP	LYS	engineered mutation	UNP B3FHP0
B	240	GLY	-	expression tag	UNP B3FHP0
B	241	LEU	-	expression tag	UNP B3FHP0
B	242	GLU	-	expression tag	UNP B3FHP0
B	243	HIS	-	expression tag	UNP B3FHP0
B	244	HIS	-	expression tag	UNP B3FHP0
B	245	HIS	-	expression tag	UNP B3FHP0
B	246	HIS	-	expression tag	UNP B3FHP0
B	247	HIS	-	expression tag	UNP B3FHP0

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	248	HIS	-	expression tag	UNP B3FHP0
B	249	HIS	-	expression tag	UNP B3FHP0
B	250	HIS	-	expression tag	UNP B3FHP0

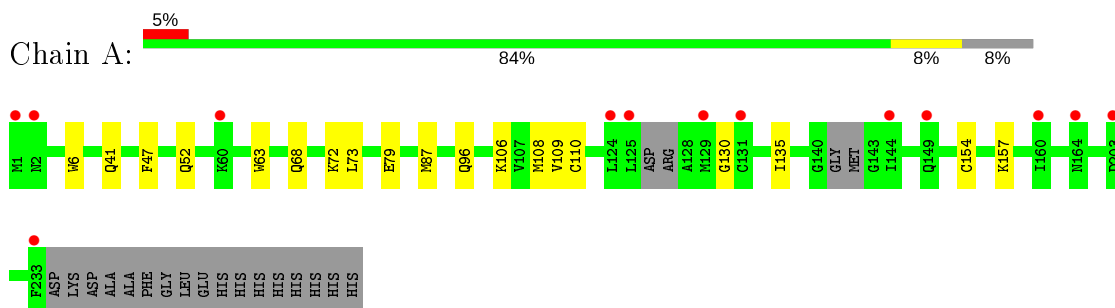
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	71	Total O 71 71	0	0
2	B	85	Total O 85 85	0	0

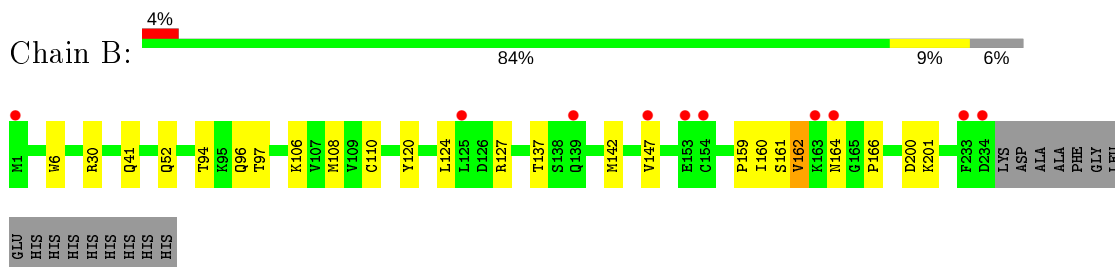
### 3 Residue-property plots [i](#)

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 and electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: Succinate–CoA ligase [ADP-forming] subunit beta



- Molecule 1: Succinate–CoA ligase [ADP-forming] subunit beta



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.99Å 97.54Å 67.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.31 – 1.91 52.31 – 1.91	Depositor EDS
% Data completeness (in resolution range)	99.9 (52.31-1.91) 99.9 (52.31-1.91)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 1.91Å)	Xtrriage
Refinement program	PHENIX dev_3318	Depositor
R, $R_{free}$	0.181 , 0.210 0.181 , 0.210	Depositor DCC
$R_{free}$ test set	2136 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtrriage
Anisotropy	0.398	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 49.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7331	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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	A	0.56	0/1777	0.69	0/2392
1	B	0.55	0/1839	0.68	0/2476
All	All	0.55	0/3616	0.68	0/4868

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	A	1750	1784	1784	9	1
1	B	1803	1838	1834	15	1
2	A	71	0	0	0	0
2	B	85	0	0	1	0
All	All	3709	3622	3618	22	1

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 3.

All (22) 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:B:120:TYR:HB3	1:B:137:THR:HG22	1.63	0.81

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ILE:HD12	1:B:166:PRO:HB3	1.66	0.77
1:A:135:ILE:HG22	1:A:157:LYS:HG2	1.80	0.63
1:B:94:THR:OG1	1:B:97:THR:HG23	2.02	0.60
1:B:96:GLN:OE1	1:B:96:GLN:N	2.37	0.58
1:A:110:CYS:HA	1:B:41:GLN:OE1	2.07	0.55
1:A:41:GLN:OE1	1:B:110[B]:CYS:HA	2.08	0.54
1:A:96:GLN:N	1:A:96:GLN:OE1	2.42	0.53
1:A:108:MET:HG2	1:A:109:VAL:N	2.25	0.51
1:B:124:LEU:HD23	1:B:124:LEU:N	2.26	0.51
1:B:162:VAL:HG13	1:B:162:VAL:O	2.11	0.51
1:A:52:GLN:HB2	1:A:106:LYS:HG3	1.92	0.51
1:B:159:PRO:O	1:B:160:ILE:HD13	2.14	0.47
1:A:47:PHE:O	1:A:73:LEU:HD12	2.16	0.46
1:B:108:MET:SD	1:B:110[A]:CYS:SG	3.14	0.45
1:A:63:TRP:CZ2	1:A:87:MET:HG2	2.52	0.44
1:B:142:MET:CE	1:B:147:VAL:HG22	2.47	0.44
1:A:68:GLN:O	1:A:72:LYS:HD3	2.18	0.44
1:B:52:GLN:HB2	1:B:106:LYS:HG3	2.00	0.44
1:B:200:ASP:OD2	1:B:201:LYS:NZ	2.49	0.42
1:B:161:SER:HB3	1:B:164:ASN:HB2	2.02	0.41
1:B:30:ARG:HG2	2:B:343:HOH:O	2.19	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLU:OE2	1:B:127[A]:ARG:HH22[4_454]	1.53	0.07

## 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 X-ray entries followed by that with respect to entries of similar resolution.

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	223/250 (89%)	218 (98%)	4 (2%)	1 (0%)	34	24
1	B	235/250 (94%)	229 (97%)	5 (2%)	1 (0%)	34	24
All	All	458/500 (92%)	447 (98%)	9 (2%)	2 (0%)	34	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	162	VAL
1	A	130	GLY

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	191/208 (92%)	189 (99%)	2 (1%)	76	75
1	B	197/208 (95%)	196 (100%)	1 (0%)	88	89
All	All	388/416 (93%)	385 (99%)	3 (1%)	81	81

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	TRP
1	A	154	CYS
1	B	6	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	229/250 (91%)	0.48	13 (5%) 23 26	32, 53, 93, 141	0
1	B	234/250 (93%)	0.47	10 (4%) 35 38	29, 53, 87, 148	0
All	All	463/500 (92%)	0.47	23 (4%) 28 32	29, 53, 90, 148	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	CYS	4.0
1	A	125	LEU	4.0
1	A	60	LYS	3.6
1	A	233	PHE	3.4
1	B	234	ASP	3.1
1	A	1	MET	3.1
1	B	154	CYS	3.1
1	B	1	MET	3.1
1	B	164	ASN	3.1
1	B	163	LYS	2.9
1	A	203	ASP	2.8
1	B	147	VAL	2.4
1	B	125	LEU	2.4
1	A	129	MET	2.4
1	B	153	GLU	2.3
1	A	160	ILE	2.3
1	A	164	ASN	2.3
1	B	233	PHE	2.2
1	B	139	GLN	2.2
1	A	124	LEU	2.1
1	A	2	ASN	2.1
1	A	149	GLN	2.1
1	A	144	ILE	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.