



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:59 PM EDT

PDB ID : 6NO6 / pdb_00006no6
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

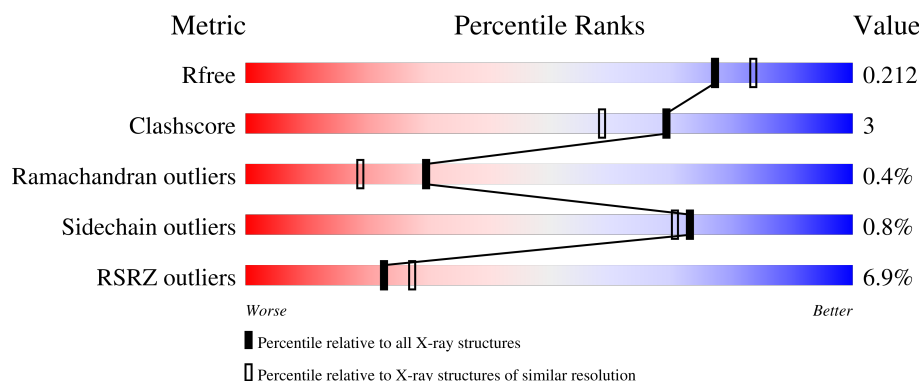
1 Overall quality at a glance

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}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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 of the lower 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 $\leq 5\%$. 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	9% 84% 7% 8%
1	B	250	4% 84% 9% 6%

2 Entry composition

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
1	A	229	Total	C	H	N	O	S	0	0	0
			3534	1111	1784	296	327	16			
1	B	234	Total	C	H	N	O	S	0	3	0
			3641	1140	1838	308	337	18			

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

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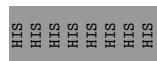
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Chain	Residue	Modelled	Actual	Comment	Reference
B	248	HIS	-	expression tag	UNP B3FHP0
B	249	HIS	-	expression tag	UNP B3FHP0
B	250	HIS	-	expression tag	UNP B3FHP0

- Molecule 2 is water.

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

- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 1.91Å)	Xtriage
Refinement program	PHENIX dev_3318	Depositor
R, R_{free}	0.181 , 0.210 0.184 , 0.212	Depositor DCC
R_{free} test set	2140 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7331	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.50	0/1777	0.65	0/2392
1	B	0.50	0/1839	0.65	0/2476
All	All	0.50	0/3616	0.65	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	18	1
2	A	71	0	0	0	0
2	B	85	0	0	1	0
All	All	3709	3622	3618	25	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 (25) 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

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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:N	1:B:96:GLN:OE1	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:B:6:TRP:CB	1:B:108:MET:HE2	2.38	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:O	1:B:162:VAL:HG13	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:6:TRP:HB2	1:B:108:MET:HE2	2.01	0.42
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
1:B:5:GLU:HG2	1:B:108:MET:HE1	2.03	0.40

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 ⓘ

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 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%)	30	19
1	B	235/250 (94%)	229 (97%)	5 (2%)	1 (0%)	30	19
All	All	458/500 (92%)	447 (98%)	9 (2%)	2 (0%)	30	19

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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%)	68	64
1	B	197/208 (95%)	196 (100%)	1 (0%)	81	80
All	All	388/416 (93%)	385 (99%)	3 (1%)	73	71

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

Mol	Chain	Res	Type
1	A	6	TRP
1	A	108	MET
1	B	6	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	4	HIS
1	B	85	ASN
1	B	168	ASN
1	B	197	GLN

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 oligosaccharides 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, 95th 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 ²)	Q<0.9
1	A	229/250 (91%)	0.52	22 (9%) 13 17	34, 58, 110, 165	0
1	B	234/250 (93%)	0.24	10 (4%) 40 44	18, 58, 98, 163	2 (0%)
All	All	463/500 (92%)	0.38	32 (6%) 23 27	18, 58, 105, 165	2 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	128	ALA	5.8
1	A	147	VAL	4.5
1	A	131	CYS	3.8
1	A	162	VAL	3.8
1	A	149	GLN	3.6
1	A	233	PHE	3.5
1	A	140	GLY	3.5
1	B	165	GLY	3.5
1	B	164	ASN	3.1
1	A	125	LEU	3.1
1	A	119	PHE	2.9
1	A	60	LYS	2.9
1	B	151	CYS	2.9
1	A	93	ILE	2.8
1	A	144	ILE	2.6
1	A	129	MET	2.6
1	B	163	LYS	2.6
1	B	144	ILE	2.5
1	A	6	TRP	2.4
1	A	148	ALA	2.3
1	B	1	MET	2.3
1	A	15	TYR	2.2
1	A	161	SER	2.2
1	B	148	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	142	MET	2.2
1	A	95	LYS	2.2
1	A	59	GLY	2.2
1	A	143	GLY	2.2
1	B	234	ASP	2.1
1	B	95	LYS	2.1
1	A	1	MET	2.1
1	A	130	GLY	2.0

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 oligosaccharides 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.