wwPDB X-ray Structure Validation Summary Report (i)

Jun 13, 2024 – 10:14 AM EDT

PDB ID	:	1QE0
Title	:	CRYSTAL STRUCTURE OF APO S. AUREUS HISTIDYL-TRNA SYNTHETASE
Authors	:	Qiu, X.; Janson, C.A.; Blackburn, M.N.; Chohan, I.K.; Hibbs, M.; Abdel-Meguid, S.S.
Deposited on	:	1999-07-12
Resolution	:	2.70 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp
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:

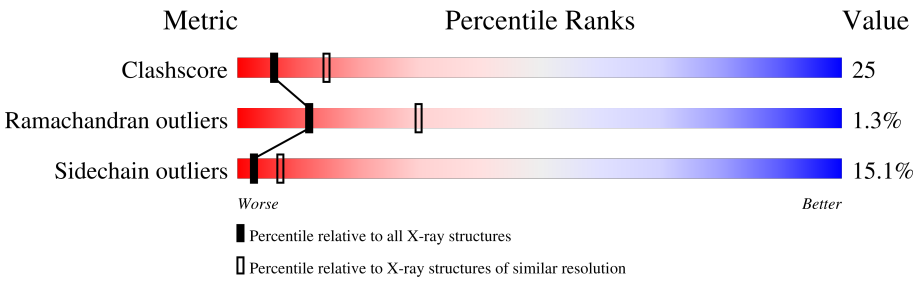
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	420	49% 36% 7% 7%
1	B	420	43% 31% 7% 19%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5996 atoms, of which 0 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 Histidine–tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	390	3150	2001	528	604	17	0	0	0
1	B	342	2746	1747	455	530	14	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	ASP	ASN	conflict	UNP P60911
A	250	THR	ILE	conflict	UNP P60911
B	201	ASP	ASN	conflict	UNP P60911
B	250	THR	ILE	conflict	UNP P60911

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	50	50	50	0	0
2	B	50	Total	O	0	0
			50	50		

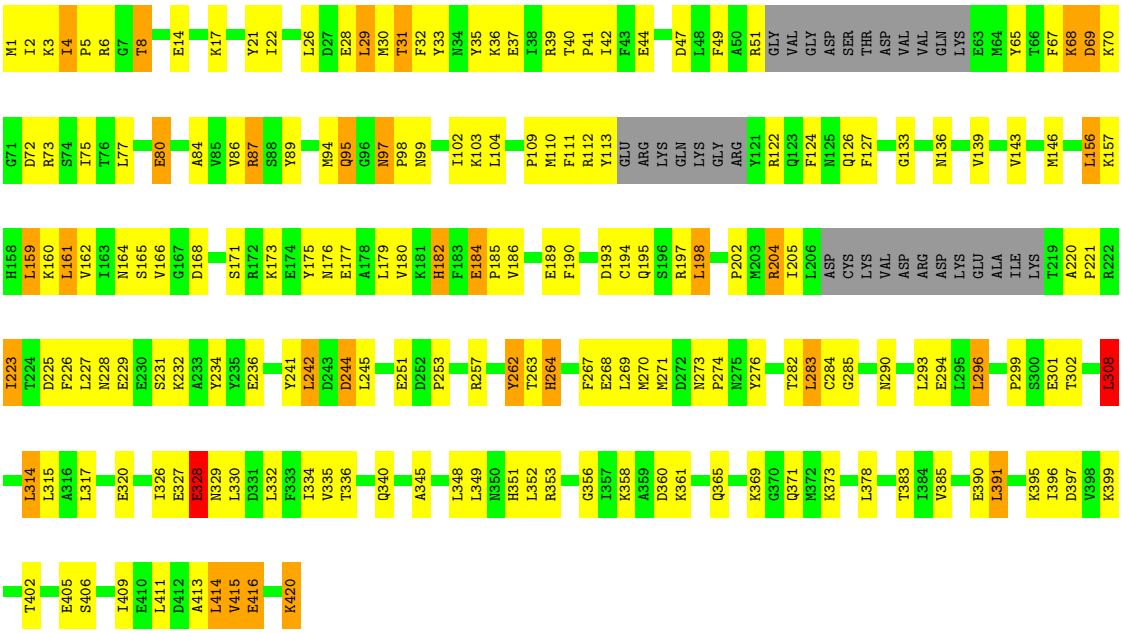
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

Note EDS was not executed.

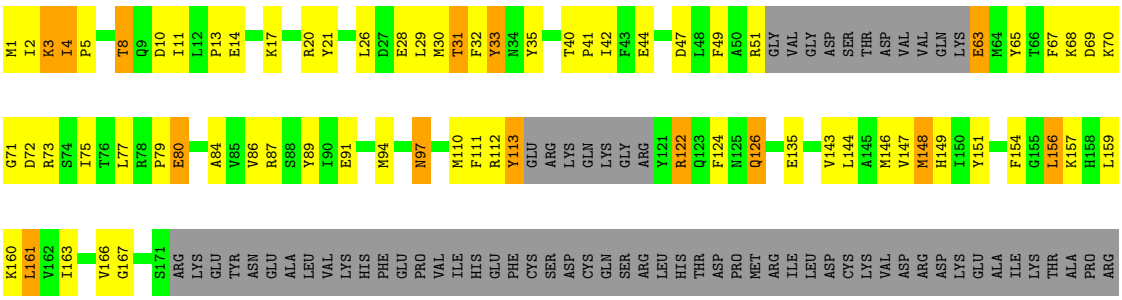
• Molecule 1: Histidine–tRNA ligase

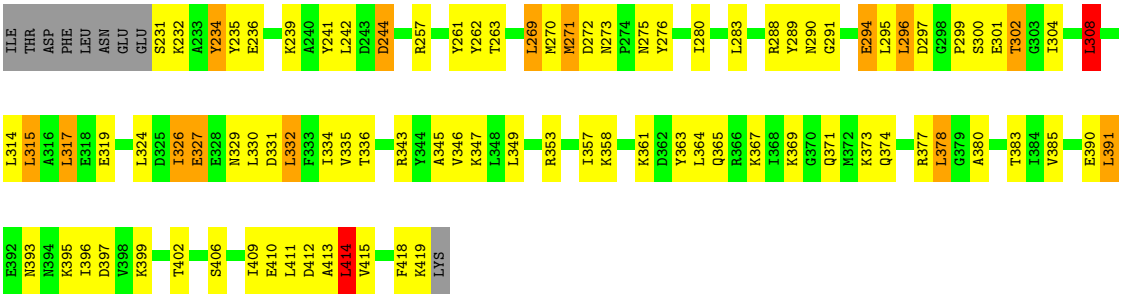
Chain A: 49% 36% 7% 7%



• Molecule 1: Histidine–tRNA ligase

Chain B: 43% 31% 7% 19%




ILE
THR
ASP
PHE
LEU
ASN
GLU
GLU
S231
K232
A233
Y234
Y235
E236
K239
A240
Y241
L242
D243
D244
R257
Y261
Y262
T263
L269
M270
M271
D272
N273
P274
N275
Y276
I280
L283
R288
Y289
N290
G291
E294
L295
L296
D297
G298
P299
S300
E301
T302
G303
I304
L308
L314
L315
A316
L317
E318
E319
L324
D325
I326
E327
E328
N329
L330
D331
L332
F333
I334
V335
T336
R343
Y344
A345
V346
K347
L348
L349
R353
I357
K358
K361
D362
Y363
L364
Q365
R366
K367
I368
K369
G370
Q371
M372
K373
Q374
R377
L378
G379
A380
T383
I384
V385
E390
L391
E392
N393
N394
K395
I396
D397
V398
K399
T402
S406
I409
E410
L411
D412
A413
L414
V415
F418
K419
LYS

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	125.65Å 125.65Å 115.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 2.70	Depositor
% Data completeness (in resolution range)	70.0 (7.00-2.70)	Depositor
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.197 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5996	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

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	0.66	0/3210	0.85	2/4327 (0.0%)
1	B	0.65	0/2796	0.85	3/3770 (0.1%)
All	All	0.65	0/6006	0.85	5/8097 (0.1%)

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	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	308	LEU	CA-CB-CG	8.05	133.81	115.30
1	B	308	LEU	CA-CB-CG	6.84	131.02	115.30
1	B	161	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	161	LEU	CA-CB-CG	5.02	126.85	115.30
1	B	363	TYR	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	33	TYR	Sidechain

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	3150	0	3097	167	0
1	B	2746	0	2698	163	0
2	A	50	0	0	0	0
2	B	50	0	0	4	0
All	All	5996	0	5795	288	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 25.

The worst 5 of 288 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:232:LYS:O	1:A:236:GLU:HG2	1.64	0.97
1:B:4:ILE:HG23	1:B:8:THR:HG22	1.47	0.97
1:B:44:GLU:HB2	1:B:49:PHE:HE2	1.42	0.83
1:B:257:ARG:HD3	1:B:262:TYR:CE2	2.13	0.82
1:B:40:THR:HG21	1:B:84:ALA:HB1	1.64	0.79

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 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	382/420 (91%)	339 (89%)	38 (10%)	5 (1%)	12 30
1	B	334/420 (80%)	300 (90%)	30 (9%)	4 (1%)	13 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	716/840 (85%)	639 (89%)	68 (10%)	9 (1%)	12 30

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	GLU
1	A	193	ASP
1	A	365	GLN
1	B	365	GLN
1	B	326	ILE

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	340/368 (92%)	286 (84%)	54 (16%)	2 6
1	B	294/368 (80%)	252 (86%)	42 (14%)	3 8
All	All	634/736 (86%)	538 (85%)	96 (15%)	3 7

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	29	LEU
1	B	159	LEU
1	B	47	ASP
1	B	122	ARG
1	B	269	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	329	ASN
1	B	365	GLN
1	B	354	HIS

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Mol	Chain	Res	Type
1	B	9	GLN
1	B	275	ASN

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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.