



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 14, 2021 – 08:04 PM EDT

PDB ID : 6WQI
Title : Xanthomonas citri Methionyl-tRNA synthetase (apo)
Authors : Mercaldi, G.F.; Benedetti, C.E.
Deposited on : 2020-04-28
Resolution : 2.00 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 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	:	2.18
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)	:	2.18

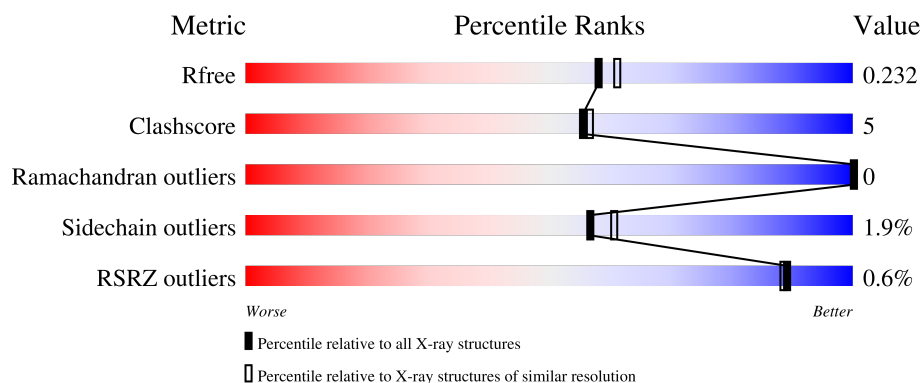
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	711	 68% 8% 23%
1	B	711	 65% 11% 23%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8988 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 Methionine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	0	0
			4244	2713	730	782	19			
1	B	547	Total	C	N	O	S	0	0	0
			4244	2713	730	782	19			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP Q8PMP0
A	-15	GLY	-	expression tag	UNP Q8PMP0
A	-14	HIS	-	expression tag	UNP Q8PMP0
A	-13	HIS	-	expression tag	UNP Q8PMP0
A	-12	HIS	-	expression tag	UNP Q8PMP0
A	-11	HIS	-	expression tag	UNP Q8PMP0
A	-10	HIS	-	expression tag	UNP Q8PMP0
A	-9	HIS	-	expression tag	UNP Q8PMP0
A	-8	GLY	-	expression tag	UNP Q8PMP0
A	-7	GLU	-	expression tag	UNP Q8PMP0
A	-6	ASN	-	expression tag	UNP Q8PMP0
A	-5	LEU	-	expression tag	UNP Q8PMP0
A	-4	TYR	-	expression tag	UNP Q8PMP0
A	-3	PHE	-	expression tag	UNP Q8PMP0
A	-2	GLN	-	expression tag	UNP Q8PMP0
A	-1	GLY	-	expression tag	UNP Q8PMP0
A	0	SER	-	expression tag	UNP Q8PMP0
B	-16	MET	-	initiating methionine	UNP Q8PMP0
B	-15	GLY	-	expression tag	UNP Q8PMP0
B	-14	HIS	-	expression tag	UNP Q8PMP0
B	-13	HIS	-	expression tag	UNP Q8PMP0
B	-12	HIS	-	expression tag	UNP Q8PMP0
B	-11	HIS	-	expression tag	UNP Q8PMP0
B	-10	HIS	-	expression tag	UNP Q8PMP0
B	-9	HIS	-	expression tag	UNP Q8PMP0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	expression tag	UNP Q8PMP0
B	-7	GLU	-	expression tag	UNP Q8PMP0
B	-6	ASN	-	expression tag	UNP Q8PMP0
B	-5	LEU	-	expression tag	UNP Q8PMP0
B	-4	TYR	-	expression tag	UNP Q8PMP0
B	-3	PHE	-	expression tag	UNP Q8PMP0
B	-2	GLN	-	expression tag	UNP Q8PMP0
B	-1	GLY	-	expression tag	UNP Q8PMP0
B	0	SER	-	expression tag	UNP Q8PMP0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	276	Total	O	0	0
			276	276		
3	B	222	Total	O	0	0
			222	222		

ALA
GLY
PHE
ASP
GLY
GLY
ALA
LEU
ALA
LEU
LEU
ASP
ALA
ASP
SER
GLY
ALA
GLN
PRO
GLY
MET
PRO
VAL
ARG

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.02Å 95.25Å 84.08Å 90.00° 90.52° 90.00°	Depositor
Resolution (Å)	47.83 – 2.00 47.83 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.3 (47.83-2.00) 94.3 (47.83-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.185 , 0.230 0.192 , 0.232	Depositor DCC
R_{free} test set	3766 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.885	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.340 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8988	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.75	0/4356	0.89	3/5921 (0.1%)
1	B	0.76	0/4356	0.90	0/5921
All	All	0.76	0/8712	0.90	3/11842 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	ARG	NE-CZ-NH2	6.27	123.44	120.30
1	A	496	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	A	317	ARG	NE-CZ-NH1	-6.04	117.28	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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	4244	0	4130	39	0
1	B	4244	0	4130	46	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	276	0	0	5	0
3	B	222	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8988	0	8260	85	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 5.

All (85) 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:19:HIS:H	1:A:22:HIS:HD2	1.38	0.70
1:B:19:HIS:H	1:B:22:HIS:HD2	1.42	0.65
1:B:377:ILE:HD11	1:B:539:ILE:HG13	1.81	0.63
1:A:19:HIS:H	1:A:22:HIS:CD2	2.22	0.57
1:A:13:TYR:CZ	1:A:56:ILE:HD12	2.39	0.57
1:B:203:LEU:HD12	1:B:220:LEU:HD11	1.87	0.55
1:B:291:ILE:O	1:B:320:VAL:HA	2.06	0.55
1:B:389:VAL:HG13	1:B:527:TYR:OH	2.08	0.54
1:A:426:PRO:HB2	1:A:442:GLN:HE22	1.71	0.54
1:B:389:VAL:CG1	1:B:527:TYR:OH	2.56	0.54
1:A:369:LEU:HD23	1:A:369:LEU:C	2.28	0.54
1:B:428:ARG:HD3	1:B:512:TRP:CD1	2.43	0.53
1:B:19:HIS:HA	1:B:340:MET:HA	1.91	0.53
1:A:369:LEU:HD23	1:A:370:ASP:N	2.24	0.53
1:A:28:GLN:HE22	1:A:321:ASN:HB3	1.74	0.53
1:B:440:ILE:HD11	1:B:493:ILE:HD13	1.91	0.52
1:A:192:VAL:HG12	1:A:226:LEU:HD13	1.93	0.51
1:B:381:ASN:O	1:B:385:VAL:HB	2.10	0.51
1:A:155:ASN:ND2	3:A:808:HOH:O	2.40	0.51
1:A:384:LEU:HD21	1:A:494:LEU:HD11	1.91	0.51
1:B:220:LEU:HD23	1:B:226:LEU:HD11	1.92	0.51
1:A:390:ASN:HA	3:A:902:HOH:O	2.11	0.50
1:A:420:PHE:CE2	1:A:446:LEU:HB3	2.47	0.49
1:A:426:PRO:HB2	1:A:442:GLN:NE2	2.28	0.49
1:B:68:GLU:HA	1:B:71:ILE:HG12	1.94	0.49
1:A:330:LYS:HE3	3:A:1032:HOH:O	2.13	0.48
1:B:189:PHE:HB3	1:B:228:ALA:HB1	1.95	0.48
1:B:142:ILE:HB	1:B:169:LYS:HB2	1.94	0.48
1:A:54:THR:N	1:A:55:PRO:CD	2.77	0.48
1:B:122:VAL:CG2	1:B:187:HIS:CD2	2.96	0.47
1:A:506:SER:O	1:A:522:HIS:CE1	2.67	0.47
1:B:127:ASP:HB2	1:B:134:LEU:HD21	1.96	0.47
1:A:506:SER:O	1:A:522:HIS:HE1	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ALA:HB2	1:B:290:PHE:CG	2.50	0.47
1:A:467:GLY:HA2	3:A:921:HOH:O	2.14	0.46
1:A:253:TRP:O	1:A:298:PHE:HZ	1.98	0.46
1:B:385:VAL:HG11	1:B:533:ARG:HG3	1.97	0.46
1:A:130:LYS:HD3	1:A:175:ILE:HG21	1.97	0.46
1:A:313:ARG:HD3	1:A:314:ALA:O	2.15	0.46
1:A:130:LYS:HD3	1:A:175:ILE:CG2	2.46	0.46
1:B:28:GLN:NE2	3:B:812:HOH:O	2.49	0.46
1:B:117:ILE:HA	1:B:189:PHE:O	2.16	0.46
1:B:313:ARG:HD3	1:B:314:ALA:O	2.17	0.45
1:B:18:LEU:HD12	1:B:81:ASP:HB2	1.99	0.45
1:B:512:TRP:O	1:B:515:VAL:HG22	2.16	0.45
1:A:137:ARG:HD2	1:A:138:TYR:CE2	2.52	0.45
1:B:28:GLN:HE22	1:B:321:ASN:HB3	1.82	0.45
1:A:125:PHE:HD2	1:A:139:ILE:HD13	1.81	0.44
1:B:295:ILE:HD12	1:B:299:HIS:CE1	2.52	0.44
1:B:459:PRO:HA	1:B:462:ILE:HD12	1.99	0.44
1:A:223:GLU:O	1:A:223:GLU:HG3	2.16	0.44
1:A:24:VAL:O	1:A:28:GLN:HG3	2.19	0.43
1:B:453:TYR:CZ	1:B:478:GLN:HG2	2.54	0.43
1:B:276:GLU:CD	1:B:276:GLU:H	2.19	0.43
1:B:54:THR:N	1:B:55:PRO:CD	2.82	0.43
1:A:459:PRO:HA	1:A:462:ILE:HD12	2.01	0.43
1:B:271:MET:HE3	1:B:273:GLU:HB2	2.01	0.43
1:B:494:LEU:HB3	1:B:497:THR:HB	2.01	0.43
1:B:356:TYR:CE1	1:B:384:LEU:HD21	2.54	0.42
1:A:440:ILE:HD11	1:A:493:ILE:HD13	2.01	0.42
1:B:215:LYS:HE3	1:B:218:GLU:OE1	2.19	0.42
1:A:268:CYS:HA	1:A:271:MET:HE2	2.01	0.42
1:B:356:TYR:CD1	1:B:384:LEU:HD21	2.54	0.42
1:A:398:PHE:O	1:A:402:ARG:HB2	2.19	0.42
1:A:399:ILE:HG22	1:A:405:GLY:HA2	2.01	0.42
1:A:384:LEU:HD23	1:A:384:LEU:HA	1.82	0.42
1:A:491:LYS:HE2	1:A:502:GLU:OE2	2.20	0.42
1:B:171:PRO:O	1:B:172:LYS:HD3	2.19	0.41
1:A:86:GLY:HA3	3:A:950:HOH:O	2.20	0.41
1:B:140:LYS:HA	1:B:151:GLN:O	2.20	0.41
1:B:250:PHE:CD1	1:B:254:LEU:HD23	2.55	0.41
1:B:252:VAL:HG13	1:B:256:ALA:HB2	2.02	0.41
1:B:425:ALA:HB3	1:B:426:PRO:CD	2.50	0.41
1:B:331:MET:HB3	1:B:338:PHE:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ARG:HD3	1:B:233:ARG:HA	1.90	0.41
1:B:334:SER:O	1:B:547:LYS:HD2	2.20	0.41
1:A:38:LEU:HD21	1:A:491:LYS:HD3	2.03	0.41
1:B:403:PHE:CZ	1:B:473:GLN:HB2	2.55	0.41
1:A:68:GLU:HA	1:A:71:ILE:HG12	2.02	0.41
1:A:125:PHE:HD1	1:A:125:PHE:HA	1.72	0.41
1:B:350:GLU:HA	1:B:351:PRO:HD2	1.99	0.41
1:A:512:TRP:O	1:A:515:VAL:HG22	2.21	0.40
1:B:426:PRO:HB2	1:B:442:GLN:HE22	1.85	0.40
1:A:507:ALA:N	1:A:508:PRO:HD3	2.36	0.40
1:B:420:PHE:HB3	1:B:485:ILE:HG21	2.03	0.40

There are no symmetry-related clashes.

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	545/711 (77%)	533 (98%)	12 (2%)	0	100	100
1	B	545/711 (77%)	532 (98%)	13 (2%)	0	100	100
All	All	1090/1422 (77%)	1065 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	432/553 (78%)	422 (98%)	10 (2%)	50	53
1	B	432/553 (78%)	426 (99%)	6 (1%)	67	72
All	All	864/1106 (78%)	848 (98%)	16 (2%)	57	61

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASP
1	A	54	THR
1	A	125	PHE
1	A	169	LYS
1	A	252	VAL
1	A	262	CYS
1	A	313	ARG
1	A	330	LYS
1	A	334	SER
1	A	531	PHE
1	B	125	PHE
1	B	201	GLU
1	B	276	GLU
1	B	313	ARG
1	B	369	LEU
1	B	379	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	28	GLN
1	A	96	ASN
1	A	442	GLN
1	A	471	GLN
1	A	525	GLN
1	B	22	HIS
1	B	28	GLN
1	B	390	ASN
1	B	442	GLN

5.3.3 RNA ⓘ

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

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	547/711 (76%)	-0.07	2 (0%) 92 92	23, 33, 48, 68	0
1	B	547/711 (76%)	-0.02	5 (0%) 84 83	25, 34, 52, 70	0
All	All	1094/1422 (76%)	-0.05	7 (0%) 89 88	23, 33, 50, 70	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	336	GLY	3.4
1	A	463	ALA	3.1
1	B	465	GLN	2.5
1	B	462	ILE	2.2
1	B	338	PHE	2.1
1	A	219	TRP	2.1
1	B	198	PHE	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	B	701	1/1	0.99	0.05	34,34,34,34	0
2	ZN	A	701	1/1	1.00	0.05	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.