



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2022 – 08:49 PM JST

PDB ID : 7WRS
Title : Crystal structure of the chicken isoleucyl-tRNA synthetase 1 (IARS1) UNE-I complexed with glutamyl-tRNA synthetase 1 (EARS1)
Authors : Chung, S.; Cho, Y.
Deposited on : 2022-01-27
Resolution : 2.40 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
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)	:	2.31.2

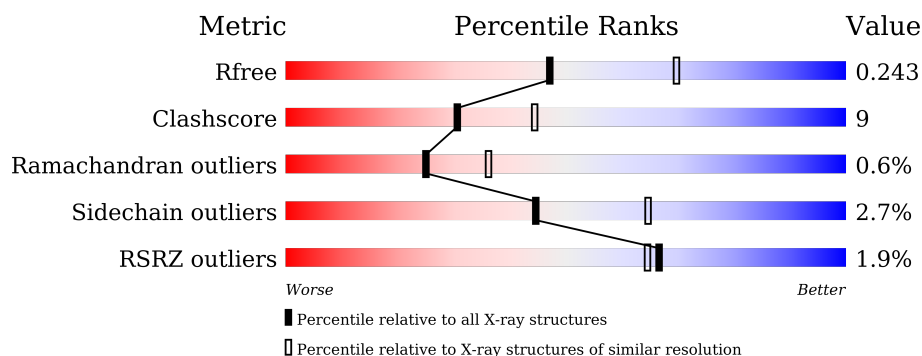
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	531	
2	B	301	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6384 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 Glutamyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	0	0	0
			4194	2668	720	780	26			

- Molecule 2 is a protein called Isoleucyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	280	Total	C	N	O	S	0	0	0
			2164	1368	369	417	10			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	26	Total	O	0	0
			26	26		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	143.02Å 155.55Å 44.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.51 – 2.40 77.78 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (71.51-2.40) 93.1 (77.78-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.14-3260_1069, PHENIX 1.14-3260_1069	Depositor
R, R_{free}	0.191 , 0.244 0.193 , 0.243	Depositor DCC
R_{free} test set	1988 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6384	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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	0.45	0/4293	0.59	0/5811
2	B	0.40	0/2191	0.63	1/2965 (0.0%)
All	All	0.43	0/6484	0.61	1/8776 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1224	ARG	NE-CZ-NH1	5.89	123.24	120.30

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	4194	0	4171	54	0
2	B	2164	0	2240	64	1
3	A	26	0	0	2	0
All	All	6384	0	6411	117	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 9.

All (117) 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:B:1142:ILE:HG22	2:B:1145:THR:HG23	1.47	0.97
1:A:196:GLY:O	1:A:197:LYS:HE2	1.71	0.91
2:B:1031:THR:HG23	2:B:1042:LEU:HD12	1.64	0.77
1:A:549:LYS:HG3	1:A:612:GLU:HB3	1.69	0.75
1:A:210:LEU:HD22	1:A:255:ASP:HB2	1.68	0.74
1:A:231:LYS:HG3	1:A:264:ASP:HB2	1.68	0.73
1:A:239:THR:HG22	1:A:269:THR:HG21	1.72	0.72
2:B:1233:ASP:OD1	2:B:1236:GLU:N	2.24	0.70
1:A:493:TRP:CE2	1:A:703:PRO:HG2	2.28	0.69
2:B:998:LEU:HB3	2:B:1055:ILE:HD12	1.74	0.69
1:A:196:GLY:C	1:A:197:LYS:HE2	2.13	0.68
2:B:1179:LEU:HD11	2:B:1197:LEU:HG	1.75	0.66
2:B:1012:VAL:HG22	2:B:1070:LEU:HD22	1.77	0.65
2:B:1002:ARG:HD3	2:B:1055:ILE:HG23	1.80	0.64
2:B:1041:ALA:HB3	2:B:1075:LEU:HD21	1.77	0.64
2:B:1089:LYS:HE3	2:B:1098:ASP:OD1	1.97	0.64
2:B:1018:PRO:HG2	2:B:1064:SER:HA	1.80	0.64
1:A:205:GLU:O	1:A:205:GLU:HG2	1.97	0.63
1:A:245:LYS:HG3	1:A:247:ASP:HB3	1.79	0.63
2:B:998:LEU:HB3	2:B:1055:ILE:CD1	2.28	0.63
1:A:242:GLU:HG3	1:A:362:GLN:HE21	1.64	0.62
2:B:994:ARG:NH1	2:B:1061:LEU:HG	2.14	0.62
1:A:211:HIS:HA	1:A:457:THR:HA	1.82	0.61
1:A:216:LYS:HG3	1:A:475:ILE:HD12	1.82	0.60
2:B:998:LEU:HD22	2:B:1055:ILE:HD12	1.84	0.59
2:B:996:GLN:O	2:B:1000:LYS:HG2	2.03	0.57
1:A:298:GLN:O	1:A:302:GLU:HG3	2.03	0.57
2:B:1019:GLU:O	2:B:1021:ASP:N	2.38	0.56
2:B:1013:TYR:HE2	2:B:1071:VAL:HG21	1.71	0.55
1:A:549:LYS:NZ	1:A:612:GLU:OE1	2.31	0.55
2:B:1022:TYR:O	2:B:1026:VAL:HG23	2.05	0.55
1:A:242:GLU:HG3	1:A:362:GLN:NE2	2.21	0.55
1:A:536:ASN:OD1	1:A:538:ASP:HB2	2.07	0.55
1:A:683:PRO:O	2:B:1224:ARG:NH2	2.40	0.55
1:A:205:GLU:OE2	1:A:207:SER:HB3	2.08	0.54
1:A:580:ASN:HB2	1:A:589:SER:HB3	1.89	0.53
1:A:685:GLU:HB2	1:A:695:ALA:HB3	1.91	0.52
1:A:535:LYS:O	1:A:535:LYS:HG2	2.10	0.52
2:B:1085:TYR:O	2:B:1086:VAL:HG23	2.10	0.52
2:B:1183:ASN:HB2	2:B:1258:VAL:H	1.75	0.51
2:B:980:GLN:O	2:B:980:GLN:HG2	2.10	0.51
2:B:1024:ASP:O	2:B:1028:LYS:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:HD22	1:A:255:ASP:CB	2.40	0.50
2:B:1088:LEU:HD11	2:B:1101:LEU:HB2	1.94	0.50
2:B:1013:TYR:HA	2:B:1043:LYS:O	2.11	0.50
2:B:1114:LEU:O	2:B:1118:VAL:HG23	2.12	0.50
2:B:1075:LEU:HD22	2:B:1075:LEU:N	2.26	0.50
1:A:678:PHE:HB3	1:A:699:LEU:HB3	1.94	0.49
2:B:1055:ILE:HD11	2:B:1070:LEU:HD12	1.94	0.49
1:A:324:GLU:O	1:A:328:LYS:HG3	2.12	0.49
2:B:1248:ASN:O	2:B:1252:LYS:NZ	2.42	0.49
1:A:674:ARG:NH1	3:A:802:HOH:O	2.46	0.49
2:B:1128:LYS:HG3	2:B:1130:SER:HB2	1.94	0.49
2:B:994:ARG:NH2	2:B:1061:LEU:HD21	2.27	0.49
2:B:1002:ARG:HD3	2:B:1054:LEU:O	2.12	0.49
2:B:1128:LYS:O	2:B:1130:SER:N	2.45	0.49
1:A:312:ARG:HD2	1:A:353:ASP:OD2	2.13	0.48
2:B:1089:LYS:CE	2:B:1098:ASP:OD1	2.60	0.48
1:A:447:VAL:HG22	1:A:452:ASP:CB	2.43	0.48
1:A:522:GLU:OE2	1:A:593:LYS:HG2	2.12	0.48
2:B:1079:VAL:HG13	2:B:1178:ASN:HD22	1.77	0.48
1:A:210:LEU:HD11	1:A:252:ILE:HG23	1.96	0.48
2:B:1066:LEU:HD11	2:B:1068:ILE:HD11	1.96	0.47
1:A:532:LYS:HE3	1:A:541:LEU:O	2.14	0.47
1:A:447:VAL:HG22	1:A:452:ASP:CG	2.34	0.47
1:A:212:ILE:HD11	1:A:471:LEU:HD11	1.97	0.47
1:A:396:THR:HG23	1:A:398:GLU:HG2	1.97	0.47
1:A:619:ILE:O	1:A:621:THR:HG23	2.15	0.47
2:B:1136:ASN:OD1	2:B:1153:LYS:HE2	2.14	0.47
2:B:1034:ILE:HG23	2:B:1038:ILE:HD12	1.96	0.46
2:B:1002:ARG:HE	2:B:1002:ARG:HB3	1.49	0.46
2:B:1169:PRO:HG3	2:B:1173:LEU:HD21	1.96	0.46
1:A:518:VAL:HG22	1:A:590:ILE:HB	1.97	0.46
2:B:992:ILE:HA	2:B:1038:ILE:HD11	1.97	0.46
2:B:1061:LEU:HD23	2:B:1061:LEU:HA	1.82	0.45
1:A:372:LYS:HB2	1:A:372:LYS:HE2	1.83	0.45
1:A:522:GLU:HB2	1:A:594:LEU:HD12	1.98	0.45
1:A:208:GLY:HA2	1:A:248:PHE:CD2	2.52	0.45
1:A:265:GLN:HG2	1:A:267:THR:HG23	1.99	0.44
2:B:1109:ASP:OD2	2:B:1191:LYS:HB3	2.17	0.44
1:A:248:PHE:O	1:A:252:ILE:HG13	2.18	0.44
1:A:235:ARG:HA	1:A:267:THR:O	2.17	0.44
1:A:684:TYR:OH	1:A:694:GLU:OE2	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1022:TYR:O	2:B:1025:THR:OG1	2.24	0.44
2:B:1142:ILE:C	2:B:1144:LYS:H	2.20	0.44
1:A:560:LEU:HD22	1:A:566:VAL:HG21	1.99	0.43
1:A:416:ARG:O	1:A:418:PRO:HD3	2.19	0.43
1:A:199:ILE:HG22	1:A:390:VAL:HA	2.01	0.43
1:A:357:TYR:CE1	1:A:373:VAL:HG13	2.54	0.43
2:B:1142:ILE:HA	2:B:1142:ILE:HD12	1.59	0.43
2:B:1011:THR:HG21	2:B:1075:LEU:HD11	2.01	0.42
2:B:1079:VAL:HG13	2:B:1178:ASN:ND2	2.35	0.42
1:A:191:PRO:HG2	1:A:419:TYR:CE1	2.55	0.42
2:B:1017:HIS:O	2:B:1019:GLU:N	2.52	0.42
1:A:637:LYS:HD2	1:A:638:ASP:H	1.85	0.42
2:B:1081:PRO:HG3	2:B:1172:LEU:CD1	2.49	0.42
1:A:386:SER:O	1:A:416:ARG:NH1	2.49	0.42
2:B:1141:LEU:HD22	2:B:1145:THR:HG21	2.01	0.42
1:A:398:GLU:OE1	1:A:425:ARG:NE	2.45	0.42
2:B:1019:GLU:C	2:B:1021:ASP:H	2.22	0.42
2:B:1041:ALA:CB	2:B:1075:LEU:HD21	2.46	0.42
2:B:1035:PHE:CD1	2:B:1041:ALA:HA	2.54	0.42
1:A:618:LEU:HD13	3:A:804:HOH:O	2.20	0.41
2:B:1084:SER:HB3	2:B:1151:SER:HB2	2.02	0.41
2:B:1187:GLN:HB2	2:B:1222:GLY:O	2.20	0.41
1:A:554:GLY:O	1:A:558:GLU:HG3	2.20	0.41
1:A:190:LEU:HD22	1:A:392:HIS:CD2	2.55	0.41
1:A:362:GLN:OE1	1:A:363:PRO:HD2	2.20	0.41
2:B:1002:ARG:CD	2:B:1055:ILE:HG23	2.48	0.41
2:B:1142:ILE:HG23	2:B:1144:LYS:H	1.86	0.41
2:B:995:ILE:HD13	2:B:1012:VAL:HG11	2.01	0.41
2:B:1021:ASP:CG	2:B:1022:TYR:H	2.21	0.41
2:B:1146:ASP:O	2:B:1149:SER:OG	2.39	0.41
2:B:1156:HIS:CG	2:B:1163:PRO:HG3	2.56	0.40
2:B:1021:ASP:OD2	2:B:1022:TYR:N	2.41	0.40
2:B:1142:ILE:C	2:B:1144:LYS:N	2.75	0.40
2:B:1233:ASP:HB3	2:B:1238:GLN:OE1	2.22	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)
2:B:1093:ASN:O	2:B:1191:LYS:NZ[1_554]	2.18	0.02

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	516/531 (97%)	497 (96%)	18 (4%)	1 (0%)	47	62
2	B	272/301 (90%)	246 (90%)	22 (8%)	4 (2%)	10	14
All	All	788/832 (95%)	743 (94%)	40 (5%)	5 (1%)	25	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	PRO
2	B	1020	GLY
2	B	1189	CYS
2	B	1143	ASN
2	B	1137	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	462/472 (98%)	456 (99%)	6 (1%)	69	84
2	B	248/267 (93%)	235 (95%)	13 (5%)	23	38
All	All	710/739 (96%)	691 (97%)	19 (3%)	44	65

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	ARG

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Mol	Chain	Res	Type
1	A	229	LYS
1	A	357	TYR
1	A	455	PHE
1	A	593	LYS
1	A	615	ARG
2	B	994	ARG
2	B	1002	ARG
2	B	1072	ARG
2	B	1089	LYS
2	B	1107	LYS
2	B	1128	LYS
2	B	1130	SER
2	B	1131	LYS
2	B	1161	SER
2	B	1168	SER
2	B	1242	LYS
2	B	1243	ASP
2	B	1247	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	980	GLN
2	B	996	GLN
2	B	1238	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	518/531 (97%)	-0.11	7 (1%) 75 73	29, 50, 76, 98	0
2	B	280/301 (93%)	0.21	8 (2%) 51 50	38, 70, 96, 107	0
All	All	798/832 (95%)	-0.00	15 (1%) 66 64	29, 55, 89, 107	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	243	LYS	4.3
1	A	244	GLU	4.2
2	B	1038	ILE	3.7
2	B	1017	HIS	3.1
1	A	246	GLU	3.0
2	B	1093	ASN	2.8
1	A	484	VAL	2.7
2	B	1003	ASN	2.6
1	A	482	ARG	2.5
1	A	480	SER	2.3
2	B	1095	THR	2.2
2	B	1006	PRO	2.2
2	B	1077	GLU	2.1
2	B	1170	ASP	2.1
1	A	398	GLU	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 monosaccharides 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.