



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 15, 2023 – 10:30 AM JST

PDB ID : 6IY6
Title : Crystal structure of human cytosolic aspartyl-tRNA synthetase (DRS) in complex with glutathion-S transferase (GST) domains from Aminoacyl tRNA synthetase complex-interacting multifunctional protein 2 (AIMP2) and glutamyl-prolyl-tRNA synthetase (EPRS)
Authors : Park, S.H.; Hahn, H.; Han, B.W.
Deposited on : 2018-12-13
Resolution : 3.60 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 ⓘ 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

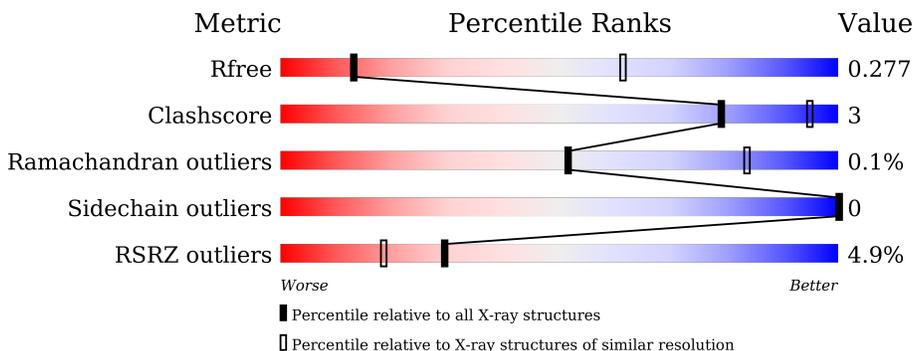
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	502	 3% 77% 7% 16%
1	B	502	 5% 76% 8% 17%
1	G	502	 6% 77% 6% 17%
1	H	502	 3% 77% 6% 17%
2	C	215	 3% 87% 11%

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Mol	Chain	Length	Quality of chain
2	D	215	
2	I	215	
2	J	215	
3	E	165	
3	F	165	
3	K	165	
3	L	165	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	A	605	-	-	-	X
5	PO4	A	607	-	-	-	X
5	PO4	B	602	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 24539 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 Aspartate-tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	421	3407	2165	600	622	20	0	0	0
1	B	419	3390	2156	595	619	20	0	0	0
1	G	417	3371	2145	589	617	20	0	0	0
1	H	417	3371	2145	589	617	20	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P14868
A	1	GLY	-	expression tag	UNP P14868
A	2	SER	-	expression tag	UNP P14868
A	3	SER	-	expression tag	UNP P14868
A	4	HIS	-	expression tag	UNP P14868
A	5	HIS	-	expression tag	UNP P14868
A	6	HIS	-	expression tag	UNP P14868
A	7	HIS	-	expression tag	UNP P14868
A	8	HIS	-	expression tag	UNP P14868
A	9	HIS	-	expression tag	UNP P14868
A	10	SER	-	expression tag	UNP P14868
A	11	SER	-	expression tag	UNP P14868
A	12	GLY	-	expression tag	UNP P14868
A	13	LEU	-	expression tag	UNP P14868
A	14	VAL	-	expression tag	UNP P14868
A	15	PRO	-	expression tag	UNP P14868
A	16	ARG	-	expression tag	UNP P14868
A	17	GLY	-	expression tag	UNP P14868
A	18	SER	-	expression tag	UNP P14868
A	19	HIS	-	expression tag	UNP P14868
A	20	MET	-	expression tag	UNP P14868

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P14868
B	1	GLY	-	expression tag	UNP P14868
B	2	SER	-	expression tag	UNP P14868
B	3	SER	-	expression tag	UNP P14868
B	4	HIS	-	expression tag	UNP P14868
B	5	HIS	-	expression tag	UNP P14868
B	6	HIS	-	expression tag	UNP P14868
B	7	HIS	-	expression tag	UNP P14868
B	8	HIS	-	expression tag	UNP P14868
B	9	HIS	-	expression tag	UNP P14868
B	10	SER	-	expression tag	UNP P14868
B	11	SER	-	expression tag	UNP P14868
B	12	GLY	-	expression tag	UNP P14868
B	13	LEU	-	expression tag	UNP P14868
B	14	VAL	-	expression tag	UNP P14868
B	15	PRO	-	expression tag	UNP P14868
B	16	ARG	-	expression tag	UNP P14868
B	17	GLY	-	expression tag	UNP P14868
B	18	SER	-	expression tag	UNP P14868
B	19	HIS	-	expression tag	UNP P14868
B	20	MET	-	expression tag	UNP P14868
G	0	MET	-	initiating methionine	UNP P14868
G	1	GLY	-	expression tag	UNP P14868
G	2	SER	-	expression tag	UNP P14868
G	3	SER	-	expression tag	UNP P14868
G	4	HIS	-	expression tag	UNP P14868
G	5	HIS	-	expression tag	UNP P14868
G	6	HIS	-	expression tag	UNP P14868
G	7	HIS	-	expression tag	UNP P14868
G	8	HIS	-	expression tag	UNP P14868
G	9	HIS	-	expression tag	UNP P14868
G	10	SER	-	expression tag	UNP P14868
G	11	SER	-	expression tag	UNP P14868
G	12	GLY	-	expression tag	UNP P14868
G	13	LEU	-	expression tag	UNP P14868
G	14	VAL	-	expression tag	UNP P14868
G	15	PRO	-	expression tag	UNP P14868
G	16	ARG	-	expression tag	UNP P14868
G	17	GLY	-	expression tag	UNP P14868
G	18	SER	-	expression tag	UNP P14868
G	19	HIS	-	expression tag	UNP P14868
G	20	MET	-	expression tag	UNP P14868

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Chain	Residue	Modelled	Actual	Comment	Reference
H	0	MET	-	initiating methionine	UNP P14868
H	1	GLY	-	expression tag	UNP P14868
H	2	SER	-	expression tag	UNP P14868
H	3	SER	-	expression tag	UNP P14868
H	4	HIS	-	expression tag	UNP P14868
H	5	HIS	-	expression tag	UNP P14868
H	6	HIS	-	expression tag	UNP P14868
H	7	HIS	-	expression tag	UNP P14868
H	8	HIS	-	expression tag	UNP P14868
H	9	HIS	-	expression tag	UNP P14868
H	10	SER	-	expression tag	UNP P14868
H	11	SER	-	expression tag	UNP P14868
H	12	GLY	-	expression tag	UNP P14868
H	13	LEU	-	expression tag	UNP P14868
H	14	VAL	-	expression tag	UNP P14868
H	15	PRO	-	expression tag	UNP P14868
H	16	ARG	-	expression tag	UNP P14868
H	17	GLY	-	expression tag	UNP P14868
H	18	SER	-	expression tag	UNP P14868
H	19	HIS	-	expression tag	UNP P14868
H	20	MET	-	expression tag	UNP P14868

- Molecule 2 is a protein called Aminoacyl tRNA synthase complex-interacting multifunctional protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	192	Total	C	N	O	S	0	0	0
			1499	968	258	265	8			
2	D	192	Total	C	N	O	S	0	0	0
			1499	968	258	265	8			
2	I	192	Total	C	N	O	S	0	0	0
			1499	968	258	265	8			
2	J	193	Total	C	N	O	S	0	0	0
			1508	973	259	268	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	114	MET	-	initiating methionine	UNP Q13155
C	321	LEU	-	expression tag	UNP Q13155
C	322	GLU	-	expression tag	UNP Q13155
C	323	HIS	-	expression tag	UNP Q13155

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Chain	Residue	Modelled	Actual	Comment	Reference
C	324	HIS	-	expression tag	UNP Q13155
C	325	HIS	-	expression tag	UNP Q13155
C	326	HIS	-	expression tag	UNP Q13155
C	327	HIS	-	expression tag	UNP Q13155
C	328	HIS	-	expression tag	UNP Q13155
D	114	MET	-	initiating methionine	UNP Q13155
D	321	LEU	-	expression tag	UNP Q13155
D	322	GLU	-	expression tag	UNP Q13155
D	323	HIS	-	expression tag	UNP Q13155
D	324	HIS	-	expression tag	UNP Q13155
D	325	HIS	-	expression tag	UNP Q13155
D	326	HIS	-	expression tag	UNP Q13155
D	327	HIS	-	expression tag	UNP Q13155
D	328	HIS	-	expression tag	UNP Q13155
I	114	MET	-	initiating methionine	UNP Q13155
I	321	LEU	-	expression tag	UNP Q13155
I	322	GLU	-	expression tag	UNP Q13155
I	323	HIS	-	expression tag	UNP Q13155
I	324	HIS	-	expression tag	UNP Q13155
I	325	HIS	-	expression tag	UNP Q13155
I	326	HIS	-	expression tag	UNP Q13155
I	327	HIS	-	expression tag	UNP Q13155
I	328	HIS	-	expression tag	UNP Q13155
J	114	MET	-	initiating methionine	UNP Q13155
J	321	LEU	-	expression tag	UNP Q13155
J	322	GLU	-	expression tag	UNP Q13155
J	323	HIS	-	expression tag	UNP Q13155
J	324	HIS	-	expression tag	UNP Q13155
J	325	HIS	-	expression tag	UNP Q13155
J	326	HIS	-	expression tag	UNP Q13155
J	327	HIS	-	expression tag	UNP Q13155
J	328	HIS	-	expression tag	UNP Q13155

- Molecule 3 is a protein called Bifunctional glutamate/proline--tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	157	1224	777	206	237	4	0	0	0
3	F	157	1224	777	206	237	4	0	0	0
3	K	157	1224	777	206	237	4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	157	1224	777	206	237	4	0	0	0

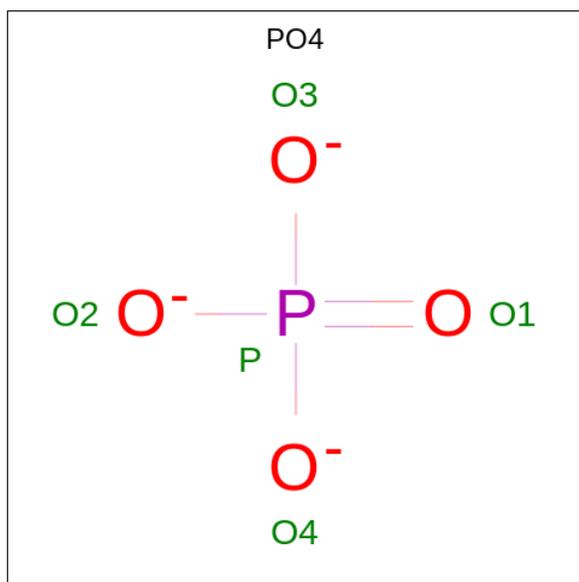
There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	158	LEU	-	expression tag	UNP P07814
E	159	GLU	-	expression tag	UNP P07814
E	160	HIS	-	expression tag	UNP P07814
E	161	HIS	-	expression tag	UNP P07814
E	162	HIS	-	expression tag	UNP P07814
E	163	HIS	-	expression tag	UNP P07814
E	164	HIS	-	expression tag	UNP P07814
E	165	HIS	-	expression tag	UNP P07814
F	158	LEU	-	expression tag	UNP P07814
F	159	GLU	-	expression tag	UNP P07814
F	160	HIS	-	expression tag	UNP P07814
F	161	HIS	-	expression tag	UNP P07814
F	162	HIS	-	expression tag	UNP P07814
F	163	HIS	-	expression tag	UNP P07814
F	164	HIS	-	expression tag	UNP P07814
F	165	HIS	-	expression tag	UNP P07814
K	158	LEU	-	expression tag	UNP P07814
K	159	GLU	-	expression tag	UNP P07814
K	160	HIS	-	expression tag	UNP P07814
K	161	HIS	-	expression tag	UNP P07814
K	162	HIS	-	expression tag	UNP P07814
K	163	HIS	-	expression tag	UNP P07814
K	164	HIS	-	expression tag	UNP P07814
K	165	HIS	-	expression tag	UNP P07814
L	158	LEU	-	expression tag	UNP P07814
L	159	GLU	-	expression tag	UNP P07814
L	160	HIS	-	expression tag	UNP P07814
L	161	HIS	-	expression tag	UNP P07814
L	162	HIS	-	expression tag	UNP P07814
L	163	HIS	-	expression tag	UNP P07814
L	164	HIS	-	expression tag	UNP P07814
L	165	HIS	-	expression tag	UNP P07814

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	H	1	Total Zn 1 1	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	G	1	Total	O	P	0	0
			5	4	1		
5	G	1	Total	O	P	0	0
			5	4	1		
5	G	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		

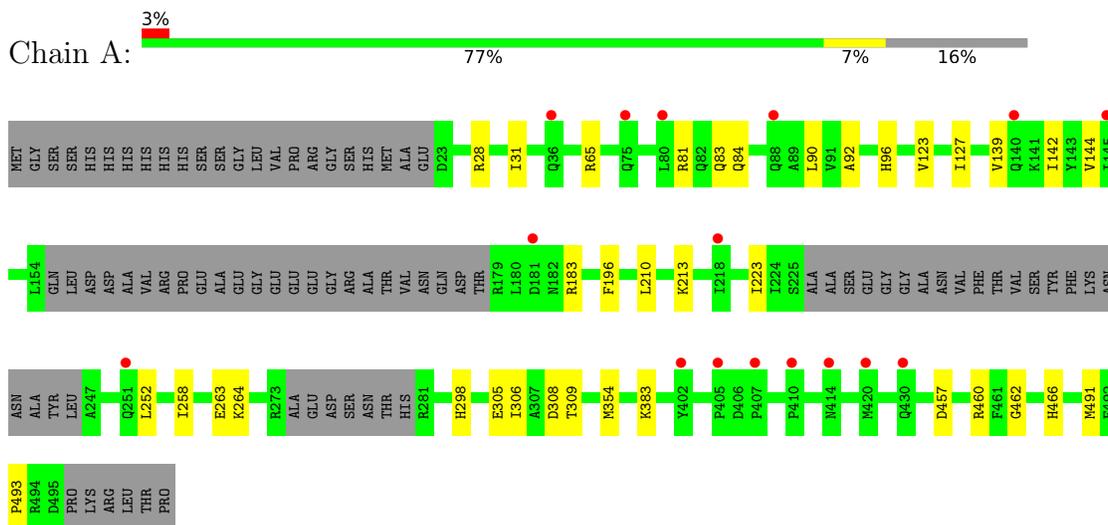
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	O	0	0
			1	1		
6	C	1	Total	O	0	0
			1	1		
6	D	2	Total	O	0	0
			2	2		
6	G	2	Total	O	0	0
			2	2		
6	H	2	Total	O	0	0
			2	2		
6	I	2	Total	O	0	0
			2	2		
6	J	2	Total	O	0	0
			2	2		

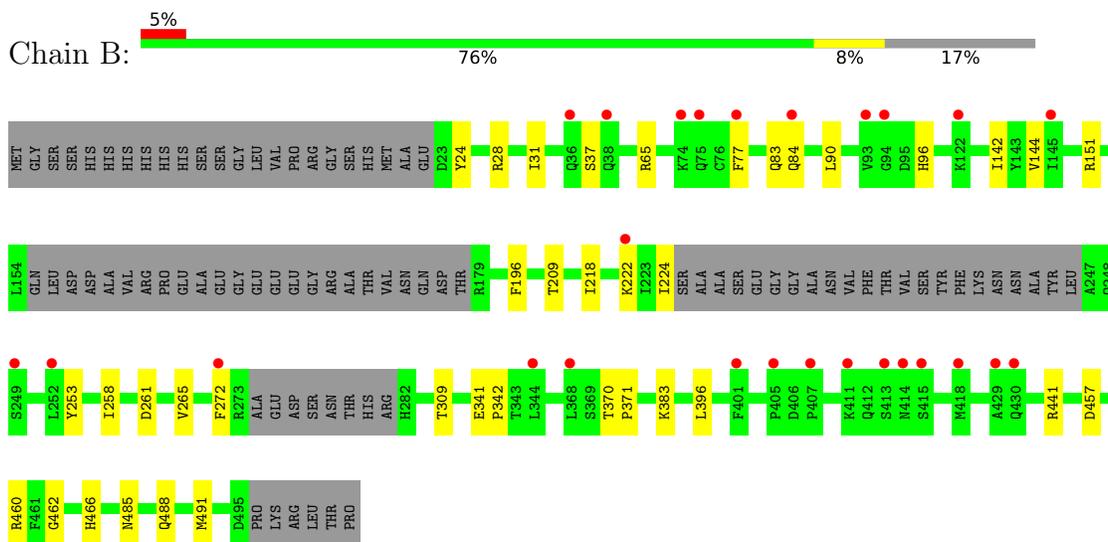
3 Residue-property plots [i](#)

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 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: Aspartate-tRNA ligase, cytoplasmic

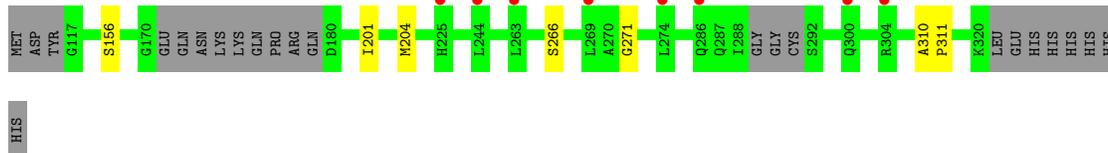
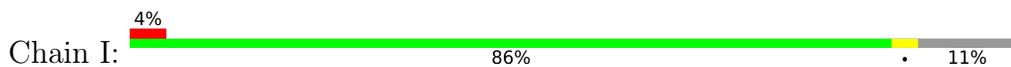


- Molecule 1: Aspartate-tRNA ligase, cytoplasmic

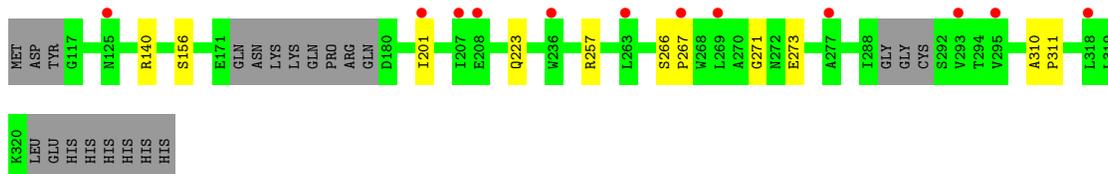
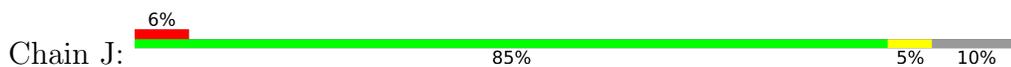


- Molecule 1: Aspartate-tRNA ligase, cytoplasmic

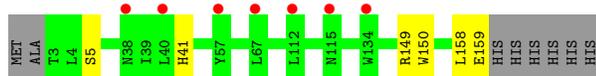




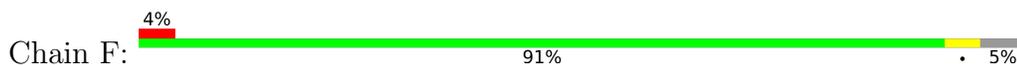
- Molecule 2: Aminoacyl tRNA synthase complex-interacting multifunctional protein 2



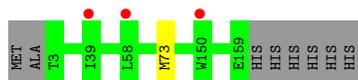
- Molecule 3: Bifunctional glutamate/proline--tRNA ligase



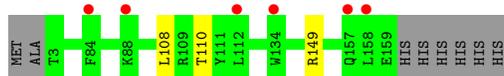
- Molecule 3: Bifunctional glutamate/proline--tRNA ligase



- Molecule 3: Bifunctional glutamate/proline--tRNA ligase



- Molecule 3: Bifunctional glutamate/proline--tRNA ligase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	108.07Å 108.07Å 815.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.60 49.46 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-3.60) 98.8 (49.46-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 3.57Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.237 , 0.275 0.240 , 0.277	Depositor DCC
R_{free} test set	3084 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	113.5	Xtrriage
Anisotropy	0.383	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 98.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.398 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24539	wwPDB-VP
Average B, all atoms (Å ²)	144.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PO4

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	0.65	0/3473	0.71	0/4680
1	B	0.64	0/3456	0.72	0/4658
1	G	0.64	0/3437	0.71	0/4633
1	H	0.65	0/3437	0.71	0/4633
2	C	0.66	0/1531	0.71	0/2076
2	D	0.67	0/1531	0.72	0/2076
2	I	0.67	0/1531	0.70	0/2076
2	J	0.66	0/1540	0.71	0/2088
3	E	0.67	0/1248	0.71	0/1698
3	F	0.67	0/1248	0.70	0/1698
3	K	0.68	0/1248	0.71	0/1698
3	L	0.68	0/1248	0.71	0/1698
All	All	0.66	0/24928	0.71	0/33712

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	3407	0	3419	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3390	0	3401	23	1
1	G	3371	0	3380	27	0
1	H	3371	0	3380	27	0
2	C	1499	0	1539	18	0
2	D	1499	0	1539	10	0
2	I	1499	0	1539	5	0
2	J	1508	0	1545	9	1
3	E	1224	0	1212	3	0
3	F	1224	0	1212	6	0
3	K	1224	0	1212	1	0
3	L	1224	0	1212	3	0
4	A	1	0	0	0	0
4	H	1	0	0	0	0
5	A	35	0	0	0	0
5	B	25	0	0	0	0
5	G	15	0	0	0	0
5	H	10	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
6	G	2	0	0	0	0
6	H	2	0	0	0	0
6	I	2	0	0	0	0
6	J	2	0	0	0	0
All	All	24539	0	24590	135	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.

The worst 5 of 135 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:65:ARG:NH2	1:B:462:GLY:O	1.94	0.99
1:A:383:LYS:HD3	2:C:119:LEU:HD13	1.43	0.97
1:A:383:LYS:HZ1	2:C:119:LEU:HD22	1.29	0.97
1:A:383:LYS:CE	2:C:119:LEU:HD13	1.97	0.94
1:G:494:ARG:HG2	1:H:223:ILE:HD13	1.47	0.93

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:B:24:TYR:OH	2:J:257:ARG:NH1[1_445]	2.04	0.16

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	413/502 (82%)	384 (93%)	29 (7%)	0	100	100
1	B	411/502 (82%)	382 (93%)	28 (7%)	1 (0%)	47	79
1	G	409/502 (82%)	382 (93%)	27 (7%)	0	100	100
1	H	409/502 (82%)	380 (93%)	28 (7%)	1 (0%)	47	79
2	C	186/215 (86%)	178 (96%)	8 (4%)	0	100	100
2	D	186/215 (86%)	177 (95%)	9 (5%)	0	100	100
2	I	186/215 (86%)	177 (95%)	9 (5%)	0	100	100
2	J	187/215 (87%)	179 (96%)	8 (4%)	0	100	100
3	E	155/165 (94%)	150 (97%)	5 (3%)	0	100	100
3	F	155/165 (94%)	150 (97%)	5 (3%)	0	100	100
3	K	155/165 (94%)	150 (97%)	5 (3%)	0	100	100
3	L	155/165 (94%)	150 (97%)	5 (3%)	0	100	100
All	All	3007/3528 (85%)	2839 (94%)	166 (6%)	2 (0%)	51	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	151	ARG
1	H	151	ARG

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	375/440 (85%)	375 (100%)	0	100	100
1	B	373/440 (85%)	373 (100%)	0	100	100
1	G	372/440 (84%)	372 (100%)	0	100	100
1	H	372/440 (84%)	372 (100%)	0	100	100
2	C	168/189 (89%)	168 (100%)	0	100	100
2	D	168/189 (89%)	168 (100%)	0	100	100
2	I	168/189 (89%)	168 (100%)	0	100	100
2	J	169/189 (89%)	169 (100%)	0	100	100
3	E	137/144 (95%)	137 (100%)	0	100	100
3	F	137/144 (95%)	137 (100%)	0	100	100
3	K	137/144 (95%)	137 (100%)	0	100	100
3	L	137/144 (95%)	137 (100%)	0	100	100
All	All	2713/3092 (88%)	2713 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	312	GLN
1	H	193	GLN
2	I	225	HIS
1	H	312	GLN
2	D	287	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	PO4	G	602	-	4,4,4	0.64	0	6,6,6	0.44	0
5	PO4	B	601	-	4,4,4	0.68	0	6,6,6	0.44	0
5	PO4	A	608	-	4,4,4	0.67	0	6,6,6	0.43	0
5	PO4	A	607	-	4,4,4	0.64	0	6,6,6	0.42	0
5	PO4	B	602	-	4,4,4	0.66	0	6,6,6	0.46	0
5	PO4	A	604	-	4,4,4	0.62	0	6,6,6	0.44	0
5	PO4	A	605	-	4,4,4	0.70	0	6,6,6	0.42	0
5	PO4	H	603	-	4,4,4	0.62	0	6,6,6	0.45	0
5	PO4	G	601	-	4,4,4	0.68	0	6,6,6	0.42	0
5	PO4	A	602	-	4,4,4	0.77	0	6,6,6	0.38	0
5	PO4	A	606	-	4,4,4	0.68	0	6,6,6	0.42	0
5	PO4	B	604	-	4,4,4	0.65	0	6,6,6	0.43	0
5	PO4	A	603	-	4,4,4	0.67	0	6,6,6	0.44	0
5	PO4	G	603	-	4,4,4	0.65	0	6,6,6	0.43	0
5	PO4	H	602	-	4,4,4	0.71	0	6,6,6	0.40	0
5	PO4	B	603	-	4,4,4	0.64	0	6,6,6	0.44	0
5	PO4	B	605	-	4,4,4	0.68	0	6,6,6	0.44	0

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	421/502 (83%)	0.51	16 (3%) 40 26	100, 133, 178, 220	0
1	B	419/502 (83%)	0.59	26 (6%) 20 12	99, 134, 175, 219	0
1	G	417/502 (83%)	0.64	30 (7%) 15 9	100, 133, 180, 227	0
1	H	417/502 (83%)	0.54	17 (4%) 37 24	100, 132, 177, 204	0
2	C	192/215 (89%)	0.44	7 (3%) 42 28	115, 156, 181, 196	0
2	D	192/215 (89%)	0.46	12 (6%) 20 11	111, 153, 180, 201	0
2	I	192/215 (89%)	0.59	8 (4%) 36 23	111, 150, 184, 192	0
2	J	193/215 (89%)	0.61	12 (6%) 20 12	110, 152, 186, 202	0
3	E	157/165 (95%)	0.40	7 (4%) 33 21	116, 152, 193, 210	0
3	F	157/165 (95%)	0.39	7 (4%) 33 21	119, 152, 185, 190	0
3	K	157/165 (95%)	0.43	3 (1%) 66 51	116, 155, 184, 196	0
3	L	157/165 (95%)	0.50	6 (3%) 40 26	118, 152, 185, 203	0
All	All	3071/3528 (87%)	0.53	151 (4%) 29 18	99, 142, 182, 227	0

The worst 5 of 151 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	94	GLY	6.6
1	B	93	VAL	6.2
1	H	88	GLN	4.4
1	H	140	GLN	4.3
1	H	75	GLN	4.0

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(Å ²)	Q<0.9
5	PO4	A	605	5/5	0.50	0.49	168,173,182,183	0
5	PO4	A	606	5/5	0.50	0.28	197,199,201,204	0
5	PO4	G	602	5/5	0.56	0.27	185,187,189,190	0
5	PO4	B	605	5/5	0.60	0.24	199,204,204,207	0
5	PO4	B	603	5/5	0.62	0.20	188,189,192,195	0
5	PO4	A	607	5/5	0.65	0.50	191,194,195,200	0
5	PO4	A	604	5/5	0.70	0.26	165,165,168,173	0
5	PO4	A	608	5/5	0.72	0.17	205,211,212,213	0
5	PO4	A	603	5/5	0.75	0.18	189,199,203,206	0
5	PO4	B	602	5/5	0.78	0.66	157,164,166,169	0
5	PO4	B	604	5/5	0.80	0.35	157,157,160,167	0
5	PO4	B	601	5/5	0.82	0.26	138,143,146,146	0
5	PO4	G	601	5/5	0.83	0.25	136,140,142,144	0
5	PO4	G	603	5/5	0.83	0.24	179,180,183,184	0
5	PO4	H	602	5/5	0.85	0.20	135,140,141,142	0
5	PO4	H	603	5/5	0.89	0.25	176,177,180,183	0
5	PO4	A	602	5/5	0.91	0.20	133,135,140,141	0
4	ZN	A	601	1/1	0.96	0.19	136,136,136,136	0
4	ZN	H	601	1/1	0.98	0.17	144,144,144,144	0

6.5 Other polymers [i](#)

There are no such residues in this entry.