



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:13 PM UTC

PDB ID : 4P71 / pdb_00004p71
Title : Apo PheRS from *P. aeuriginosa*
Authors : Ferguson, A.D.
Deposited on : 2014-03-25
Resolution : 2.79 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	:	4-5-2 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

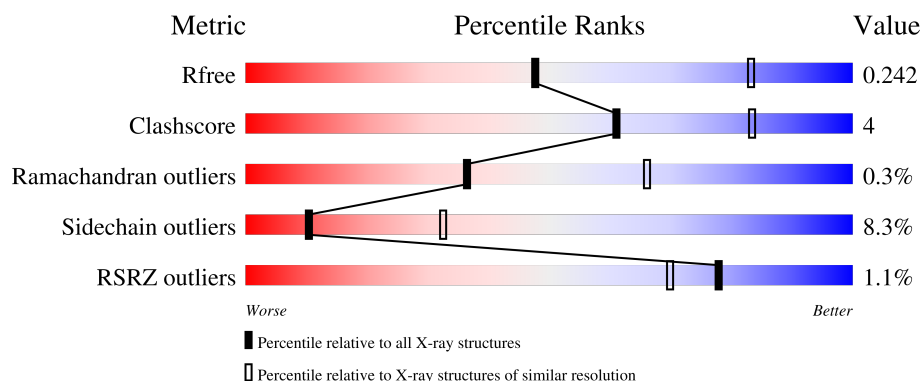
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	792	82% 16% .
1	B	792	83% 14% .
2	C	338	59% 11% . 29%
2	D	338	3% 59% 11% .. 28%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16150 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 Phenylalanine-tRNA ligase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	791	Total	C	N	O	S	0	0	0
			6103	3854	1087	1141	21			
1	B	791	Total	C	N	O	S	0	0	0
			6103	3854	1087	1141	21			

- Molecule 2 is a protein called Phenylalanine-tRNA ligase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	239	Total	C	N	O	S	0	0	0
			1923	1218	340	351	14			
2	D	243	Total	C	N	O	S	0	0	0
			1952	1238	344	355	15			

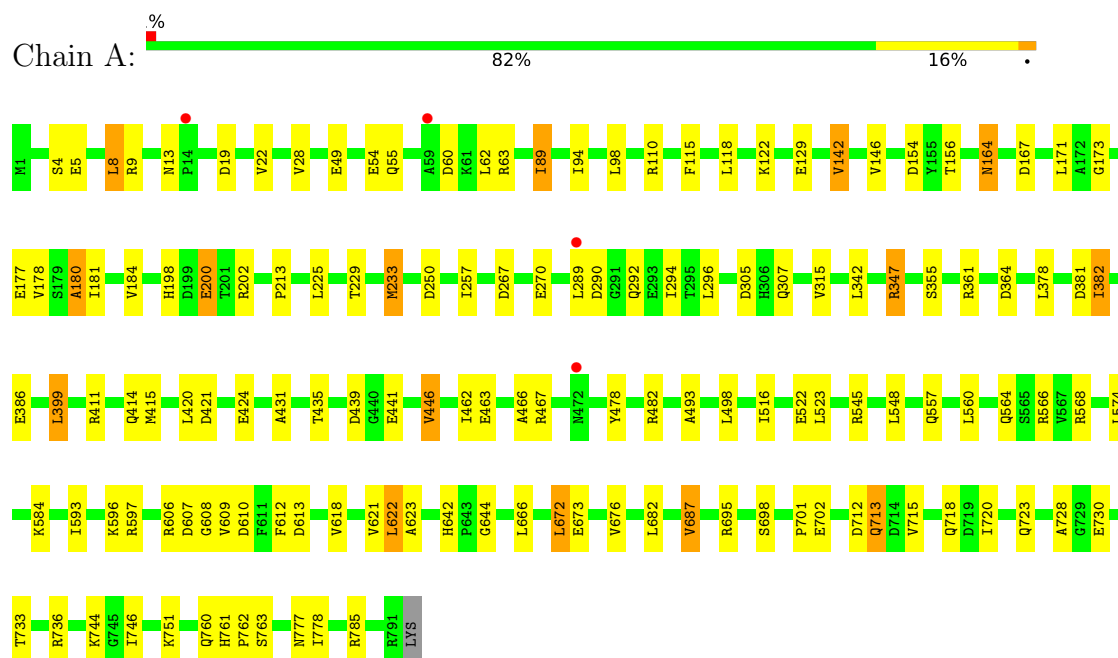
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total	O	0	0
			22	22		
3	B	37	Total	O	0	0
			37	37		
3	C	5	Total	O	0	0
			5	5		
3	D	5	Total	O	0	0
			5	5		

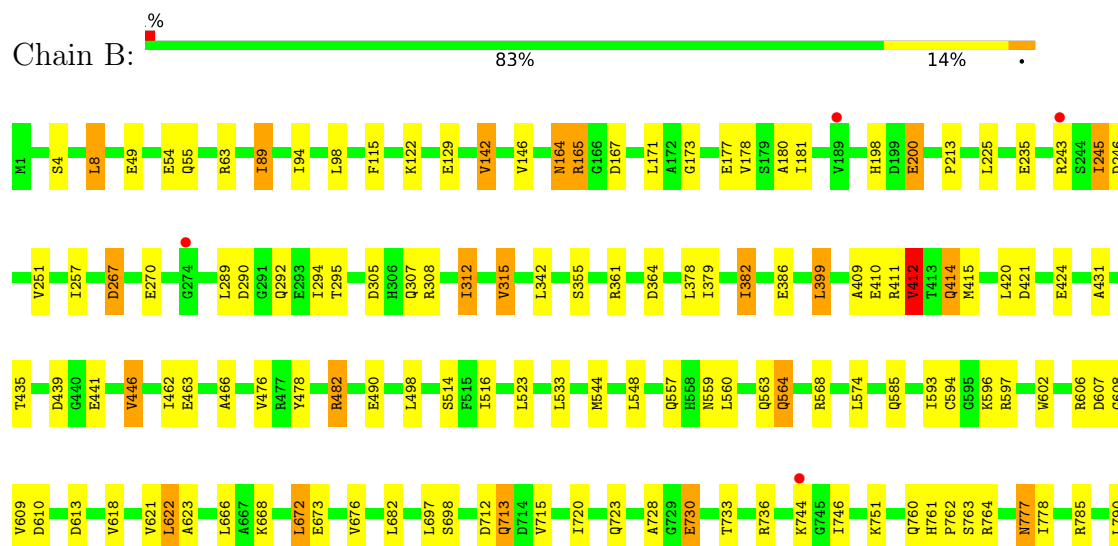
3 Residue-property plots

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: Phenylalanine-tRNA ligase beta subunit



• Molecule 1: Phenylalanine-tRNA ligase beta subunit



T122	T123	S124	P125	M126	G132	V139	G146	R153	K158	G159	L160	S167	F171	P174	E177	V178	D179	I180	V183	C184	SER	GLY	ASN	GLY	CYS	ARG	VAL	CYS	G195	T196	G197	M202	F227	G228	R245	D249	L252	Q257	F258	R259																
ASN	VAL	ALA	LYS	LYS	VAL	GLN	VAL	ASN	ALA	ARG	LYS	THR	GLU	LEU	GLU	GLY	ALA	ALA	LEU	ALA	ALA	ARG	L8	A9	E11	R12	I13	D14	V15	T16	L17	P18		H28	P29	V30		V48	H70	F71	A72		N82	A83	N84		H90		G112	D118	S119	D120				
MET	GLU	ASN	LEU	ASP	ALA	LEU	VAL	GLN	ALA	GLU	VAL	HIS	THR	GLU	GLU	ASP	VAL	ASN	ALA	LEU	GLU	GLN	ILE	ARG	VAL	HIS	TYR	LEU	GLY	LYS	LYS	GLY	GLU	LEU	THR	GLN	VAL	MET	LYS	THR	LYS	LEU	GLY	ASP	LEU	PRO	ALA	GLU	GLU	ARG	PRO	LYS	VAL	GLY	ALA	LEU

4 Data and refinement statistics

Property	Value
Space group	C 1 2 1
Cell constants a, b, c, α , β , γ	112.78Å 219.08Å 107.13Å 90.00° 101.91° 90.00°
Resolution (Å)	39.00 – 2.79 39.00 – 2.79
% Data completeness (in resolution range)	99.0 (39.00-2.79) 99.0 (39.00-2.79)
R_{merge}	0.07
R_{sym}	(Not available)
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.81Å)
Refinement program	BUSTER 2.11.5, ROVERSI, SHARFF, SMART, VONRHEIN, MATTH
R, R_{free}	0.191 , 0.227 0.203 , 0.242
R_{free} test set	3162 reflections (5.06%)
Wilson B-factor (Å ²)	51.4
Anisotropy	0.810
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.4
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$
Estimated twinning fraction	No twinning to report.
F_o, F_c correlation	0.95
Total number of atoms	16150
Average B, all atoms (Å ²)	64.0

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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	0.80	1/6221 (0.0%)	1.30	20/8450 (0.2%)
1	B	0.80	0/6221	1.30	17/8450 (0.2%)
2	C	0.82	1/1972 (0.1%)	1.36	10/2664 (0.4%)
2	D	0.84	2/2001 (0.1%)	1.39	13/2704 (0.5%)
All	All	0.80	4/16415 (0.0%)	1.32	60/22268 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	126	MET	SD-CE	-8.62	1.58	1.79
1	A	233	MET	SD-CE	-8.37	1.58	1.79
2	C	15	VAL	CA-C	5.50	1.59	1.52
2	D	15	VAL	C-N	5.34	1.41	1.33

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	15	VAL	CA-C-N	9.80	142.25	126.86
2	D	15	VAL	C-N-CA	9.80	142.25	126.86
2	C	15	VAL	CA-C-N	9.35	137.78	122.73
2	C	15	VAL	C-N-CA	9.35	137.78	122.73
2	D	171	PHE	CA-CB-CG	8.01	121.81	113.80

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	6103	0	6136	56	0
1	B	6103	0	6136	60	0
2	C	1923	0	1846	16	0
2	D	1952	0	1882	24	0
3	A	22	0	0	0	0
3	B	37	0	0	1	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
All	All	16150	0	16000	133	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 4.

The worst 5 of 133 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:D:15:VAL:HG22	2:D:16:THR:H	1.25	1.01
2:C:15:VAL:HG12	2:C:16:THR:H	1.40	0.86
1:A:198:HIS:HD2	1:A:200:GLU:H	1.31	0.77
1:B:198:HIS:HD2	1:B:200:GLU:H	1.32	0.76
1:B:559:ASN:HD21	2:D:252:LEU:H	1.31	0.76

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	789/792 (100%)	768 (97%)	21 (3%)	0	100	100
1	B	789/792 (100%)	766 (97%)	23 (3%)	0	100	100
2	C	235/338 (70%)	224 (95%)	9 (4%)	2 (1%)	14	41
2	D	239/338 (71%)	223 (93%)	12 (5%)	4 (2%)	7	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2052/2260 (91%)	1981 (96%)	65 (3%)	6 (0%)	36 66

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	15	VAL
2	C	118	ASP
2	D	118	ASP
2	D	10	ALA
2	D	120	ASP

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	645/646 (100%)	588 (91%)	57 (9%)	9 29
1	B	645/646 (100%)	583 (90%)	62 (10%)	8 26
2	C	207/287 (72%)	195 (94%)	12 (6%)	18 49
2	D	211/287 (74%)	201 (95%)	10 (5%)	23 57
All	All	1708/1866 (92%)	1567 (92%)	141 (8%)	10 32

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	764	ARG
2	C	11	GLU
2	C	249	ASP
1	A	676	VAL
1	A	673	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	22	GLN
2	D	181	GLN
2	C	28	HIS
2	D	70	HIS
2	D	257	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 [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	791/792 (99%)	-0.11	4 (0%) 87 82	38, 61, 92, 119	0
1	B	791/792 (99%)	-0.16	4 (0%) 87 82	41, 61, 94, 119	0
2	C	239/338 (70%)	-0.05	5 (2%) 63 54	45, 61, 89, 109	0
2	D	243/338 (71%)	0.08	10 (4%) 41 33	41, 60, 97, 134	0
All	All	2064/2260 (91%)	-0.10	23 (1%) 78 70	38, 61, 94, 134	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	8	LEU	4.8
2	D	15	VAL	4.7
2	C	182	CYS	3.5
2	C	15	VAL	3.4
2	C	196	THR	3.2

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.