



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:37 PM UTC

PDB ID : 1B70 / pdb_00001b70
Title : PHENYLALANYL TRNA SYNTHETASE COMPLEXED WITH PHENYLALANINE
Authors : Reshetnikova, L.; Moor, N.; Lavrik, O.; Vassilyev, D.G.
Deposited on : 1999-01-26
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 ⓘ 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

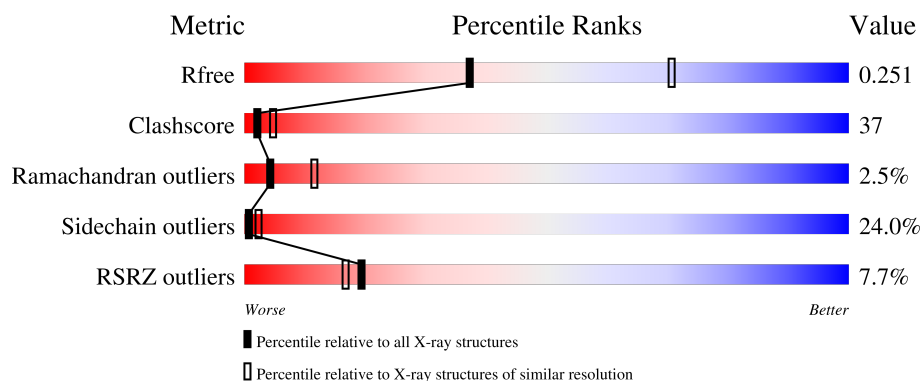
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. 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	350	5% 31% 33% 11% 24%
2	B	785	8% 39% 43% 15%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8313 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 PHENYLALANYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2112	1382	359	364	7			

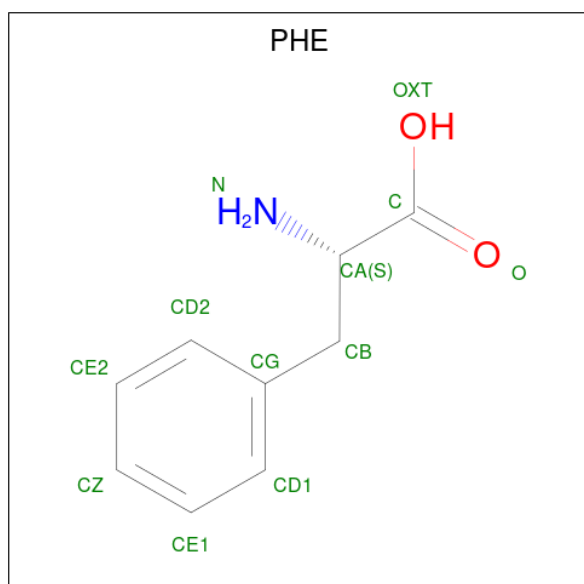
- Molecule 2 is a protein called PHENYLALANYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	775	Total	C	N	O	S	0	0	0
			6054	3879	1078	1087	10			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHENYLALANINE (CCD ID: PHE) (formula: C₉H₁₁NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			12	9	1	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	28	Total	O	0	0
			28	28		
5	B	106	Total	O	0	0
			106	106		

L743	A683	E614	G551	I485	G385	R304	A233
A744	F684	F617	L552	R486	A386	E307	L294
F745	Q685		V553	G487	R387		F235
H746	D686		R554	V488	S308		
L747	P687		V555	E489	F309		M239
R748	S688		L556	A490	P310		R240
F749	R689		R557	P491	A389		P241
H750	H690		E558	K494	E390		I242
H751	F691		N559	R497	L393		N243
P752	A692		L560	R499	E394		N244
K753	A693		D561	E500			V245
R754	F694		L562	R499	S397		V246
T755	R695		D563	E500	I404		D247
L756	E696		R564	V501	P405		V248
R757	L697		P565	V501	F406		T249
D758	A698		E566		R407		N250
E759	V699		R567	L505			
E760	V700			G506	P420		M253
V761	V701		L570	F507	E421		L254
E762	P702		F571	Q508	A422		E255
E763	A703		E572	Q509	E423		R256
A764	G640		V573	V510	T328		A257
V765	R641		G574	V511	E329		Q258
S766	V705		G574	T512	A330		P259
S766	L643		R575	Y513	I331		
R767	V644		V576	S514	A332		A262
V768	E645			F515	L333		F263
A769	G646		E579	M516	E334		D264
E770	E647		R580	D517	V335		L265
A771	E648		E581	P518	A336		
L772	V649		E582	P519			V268
R773	G650		T583	E520	D339		
A774	F651		H584	D520	F340		R275
R775	L652		L585	A521	V341		R276
GLY	G653		A586	R522	P447		A277
PHE	A717		G587	R523	K345		R278
GLY	H656		L588	F524	S448		
LEU	P657		L589	R525	H449		
ARG	E658		F590	L526	R450		
GLY	I659		G591	D527	L451		
LEU	A660		E592	P528	D452		
ASP	Q661		G593	P529	L453		
THR	E662		V594	R530	R454		
PRD	L725		G595	L531			
	A726		L596	L532	D458		
	L727		P597	L533	L459		
	F728		W598	L534	A356		
	D729		A599	N535	S357		
	L730		K600	P536	H358		
	Y731		R601	L537	R359		
	Q732		R602	A538	F360		
	G733		L603	K541	E361		
	P734		G605	A542	V364		
	P735		S604		D365		
	L736				E296		
	P737		L608	R545	D297		
	E738		L609	T546	P366		
	G739		K610	H547	Q369		
	H740		G611	H548			
	K741		P681	F549	R374		
	S742		L682	P550	Q381		

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.00Å 174.00Å 140.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.4 (50.00-2.70) 88.8 (50.00-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3001.55 (at 2.69Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.224 , 0.256 0.223 , 0.251	Depositor DCC
R_{free} test set	3018 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 82.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8313	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: MG

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	0.59	0/2180	1.07	17/2957 (0.6%)
2	B	0.58	0/6205	1.14	64/8436 (0.8%)
All	All	0.58	0/8385	1.12	81/11393 (0.7%)

There are no bond length outliers.

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	774	ALA	N-CA-C	-9.77	101.29	113.01
2	B	601	GLU	N-CA-C	8.93	122.13	110.43
2	B	665	LEU	N-CA-C	8.65	121.63	110.39
2	B	195	ALA	N-CA-C	8.39	120.42	111.28
2	B	665	LEU	CA-C-N	8.24	128.87	120.38

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	2112	0	2062	156	0
2	B	6054	0	6109	478	0
3	A	1	0	0	0	0
4	A	12	0	8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	28	0	0	0	0
5	B	106	0	0	2	0
All	All	8313	0	8179	612	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 37.

The worst 5 of 612 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:165:LEU:HD12	1:A:301:LEU:HD13	1.35	1.08
2:B:285:THR:HG21	2:B:291:ARG:HE	1.25	0.99
2:B:614:GLU:HG2	2:B:624:PHE:HE1	1.24	0.97
2:B:75:VAL:HG11	2:B:108:ILE:HG21	1.45	0.97
2:B:707:TYR:HE1	2:B:711:GLU:HB2	1.30	0.93

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	263/350 (75%)	243 (92%)	13 (5%)	7 (3%)	4	10
2	B	773/785 (98%)	684 (88%)	70 (9%)	19 (2%)	4	11
All	All	1036/1135 (91%)	927 (90%)	83 (8%)	26 (2%)	4	11

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
2	B	488	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	664	GLU
1	A	94	SER
1	A	338	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	213/277 (77%)	164 (77%)	49 (23%)	1	2
2	B	623/630 (99%)	471 (76%)	152 (24%)	1	2
All	All	836/907 (92%)	635 (76%)	201 (24%)	1	2

5 of 201 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	397	SER
2	B	563	ASP
2	B	770	GLU
2	B	450	ARG
2	B	512	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	261	HIS
2	B	656	HIS
2	B	669	HIS
2	B	350	HIS
2	B	101	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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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$
4	PHE	A	352	-	11,12,12	1.94	1 (9%)	11,15,15	1.06	1 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PHE	A	352	-	-	5/8/8/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	352	PHE	OXT-C	-5.96	1.11	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	352	PHE	OXT-C-O	-2.92	117.45	124.08

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	352	PHE	C-CA-CB-CG
4	A	352	PHE	O-C-CA-CB
4	A	352	PHE	OXT-C-CA-CB
4	A	352	PHE	N-CA-CB-CG
4	A	352	PHE	OXT-C-CA-N

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	265/350 (75%)	0.40	16 (6%)	27 24	30, 62, 101, 121	0
2	B	775/785 (98%)	0.49	64 (8%)	17 14	28, 66, 115, 130	0
All	All	1040/1135 (91%)	0.47	80 (7%)	19 17	28, 65, 114, 130	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	LEU	5.3
1	A	221	GLY	5.1
1	A	143	HIS	4.8
2	B	647	GLU	4.4
2	B	738	GLU	3.8

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](#)

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($\text{\AA}^2$)	Q<0.9
3	MG	A	351	1/1	0.88	0.11	36,36,36,36	0
4	PHE	A	352	12/12	0.91	0.15	58,64,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.