



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 08:54 PM GMT

PDB ID : 1B7Y
Title : PHENYLALANYL TRNA SYNTHETASE COMPLEXED WITH PHENYL
ALANINYL-ADENYLATE
Authors : Reshetnikova, L.; Moor, N.; Lavrik, O.; Vassylyev, D.G.
Deposited on : 1999-01-26
Resolution : 2.50 Å (reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

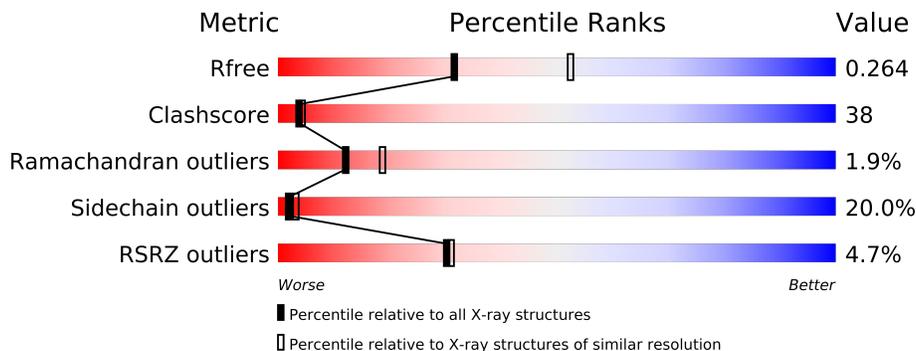
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	350	
2	B	785	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	A	1001	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8439 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PROTEIN (PHENYLALANYL-TRNA SYNTHETASE).

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

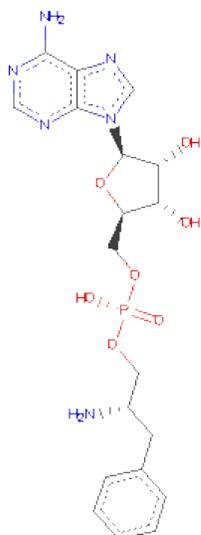
- Molecule 2 is a protein called PROTEIN (PHENYLALANYL-TRNA SYNTHETASE).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is ADENOSINE-5'-[PHENYLALANINOL-PHOSPHATE] (three-letter code: FYA) (formula: C₁₉H₂₅N₆O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	33	19	6	7	1	0	0

- Molecule 5 is water.

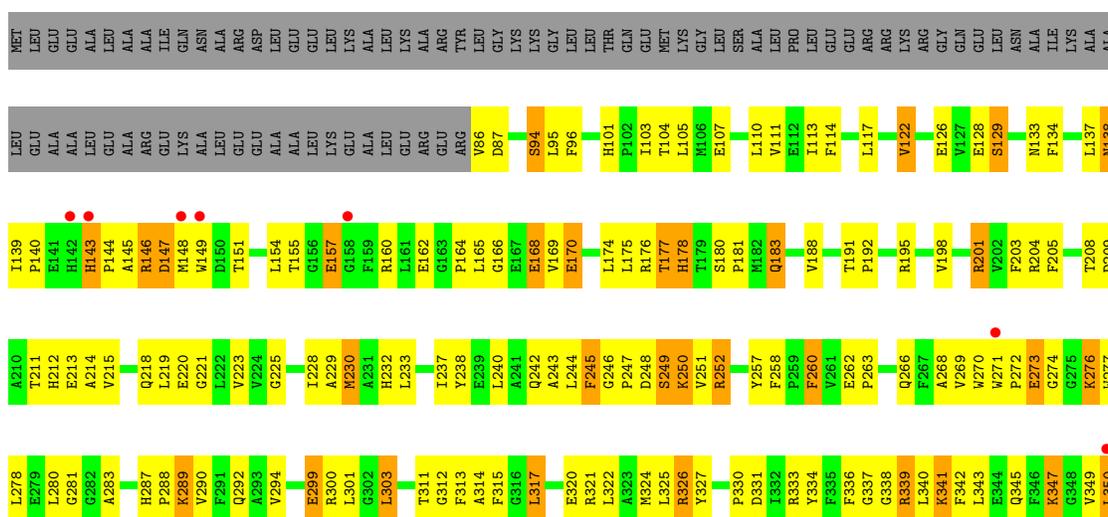
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	48	Total	O	0	0
			48	48		
5	B	191	Total	O	0	0
			191	191		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

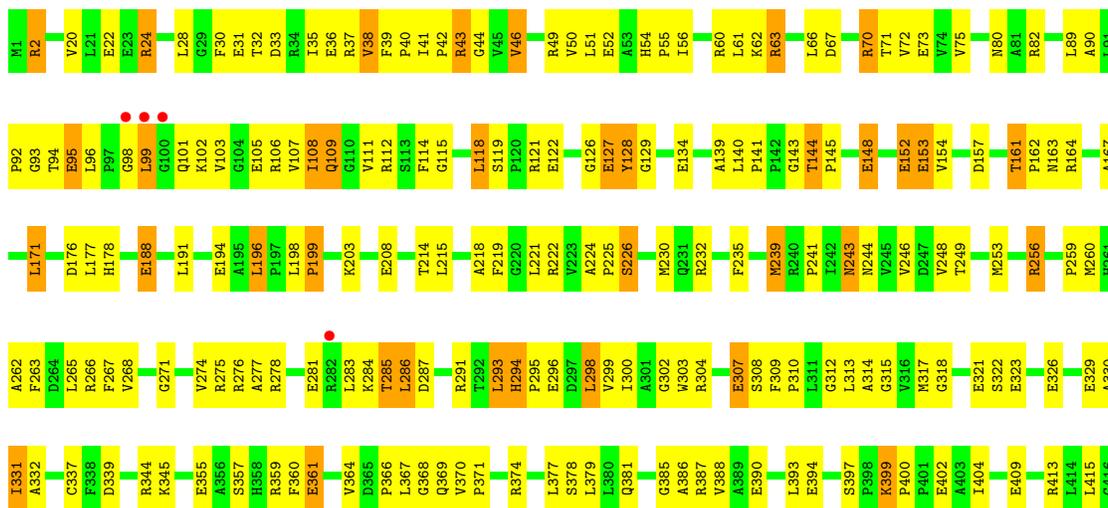
- Molecule 1: PROTEIN (PHENYLALANYL-TRNA SYNTHETASE)

Chain A:



- Molecule 2: PROTEIN (PHENYLALANYL-TRNA SYNTHETASE)

Chain B:



GLY	E716	G690	E581	D517	T417
LEU	A717	F651	E582	F518	L427
ARG	A718	L652	T583	E519	L428
GLY			H584	D520	K429
LEU	Y721	H656	G587	A521	R430
ASP	L722	P657	L588	R522	E438
THR	E723	E658	L589	R523	
PRO	S724	I659	F590	F524	
		A660	G591	R525	
	L727	Q661	E592	F526	T441
	F728	E662	G593	D527	
	D729	L663	G594	P528	P446
	L730	E664	G595	P529	P447
	Y731	L665	L596	R530	S446
	Q732	P666	P597	H449	H449
	G733	V668	W598	L531	R450
	P734	H669	A599	L532	L451
	P735	L670	K600	L533	L452
	L736	F671	E601	L534	
	F737	E672	R602	N535	D458
	E738	L673	R603	L459	L459
	G739	R674	L603	V460	V460
	H740	L675	S604	E461	E461
	K741	P676	L608	E540	E462
	S742		L609	K541	
	L743	R680	K510	A542	R465
	A744	P681	L613	A543	L466
	F745	L682	E614	L544	Q467
	H746	Q685	A615	R545	
	L747		L616	T546	P473
	R748	S688	F617	H547	
	F749	R689	A618	L548	D484
	R750	H690	G621	F549	V485
	H751	P691	L622	P550	R486
	P752	A692	G623	G551	G487
	K753	A693	F624	V552	V488
	R754	F694	Q629	R553	F489
	T755	R695	A630	R554	A490
	L756	D696	F631	V556	P491
	R757	L697	P632	K557	
	D758	A698	F633	K494	
	E759	V699	L634	R497	L498
	E760	V700	H635	L498	L498
	V761	P701	P636	R499	R499
	E762	A703	G637	E500	E500
	E763	P702	V638	V501	V501
	A764	P704	S639		
	V765	T705	V642	L505	L505
	S766	P706	L643	G506	G506
	R767	G707	E572	F507	F507
	V768	E708	V573	Q508	Q508
	A769	V709	V644	E509	E509
	E770	E710	E645	V510	V510
	A771	E711	G646	Y511	Y511
	L772	L712	E648	T512	T512
	R773	L713	V649	V513	V513
	A774	V714		S514	S514
	R775	R715		F515	F515
	GLY			M516	M516
	PHE				

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.50Å 174.50Å 140.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.50 47.41 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.7 (50.00-2.50) 95.7 (47.41-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	15112.19 (at 2.51Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.230 , 0.267 0.229 , 0.264	Depositor DCC
R_{free} test set	4107 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.6	EDS
Estimated twinning fraction	0.056 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 81641 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8439	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: MG, FYA

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	0.54	0/2180	0.76	0/2957
2	B	0.53	0/6205	0.79	4/8436 (0.0%)
All	All	0.53	0/8385	0.78	4/11393 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	115	GLY	N-CA-C	-5.83	98.54	113.10
2	B	601	GLU	CB-CA-C	-5.59	99.22	110.40
2	B	128	TYR	N-CA-C	5.35	125.44	111.00
2	B	570	LEU	CA-CB-CG	5.28	127.44	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2112	0	2062	164	0
2	B	6054	0	6109	495	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	33	0	24	4	0
5	A	48	0	0	4	0
5	B	191	0	0	6	0
All	All	8439	0	8195	626	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 38.

The worst 5 of 626 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:262:GLU:HG2	5:A:1015:HOH:O	1.45	1.16
2:B:600:LYS:HG2	2:B:601:GLU:H	1.04	1.14
2:B:75:VAL:HG11	2:B:108:ILE:HG21	1.31	1.12
2:B:285:THR:HG21	2:B:291:ARG:HE	1.20	1.02
2:B:294:HIS:CD2	2:B:296:GLU:H	1.79	1.00

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	263/350 (75%)	244 (93%)	14 (5%)	5 (2%)	12	19
2	B	773/785 (98%)	695 (90%)	63 (8%)	15 (2%)	12	19
All	All	1036/1135 (91%)	939 (91%)	77 (7%)	20 (2%)	12	19

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
2	B	488	VAL
2	B	664	GLU
1	A	338	GLY
2	B	708	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%)	176 (83%)	37 (17%)	3 5
2	B	623/630 (99%)	493 (79%)	130 (21%)	1 2
All	All	836/907 (92%)	669 (80%)	167 (20%)	2 3

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	243	ASN
2	B	361	GLU
2	B	716	GLU
2	B	283	LEU
2	B	307	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	54	HIS
2	B	212	HIS
2	B	656	HIS
2	B	109	GLN
2	B	178	HIS

5.3.3 RNA [i](#)

There are no RNA chains 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 carbohydrates 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	FYA	A	1002	-	36,36,36	1.07	2 (5%)	52,52,52	1.24	3 (5%)

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	FYA	A	1002	-	-	0/20/36/36	0/2/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	FYA	O3P-C	-4.15	1.27	1.44
4	A	1002	FYA	O4'-C1'	2.22	1.44	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	FYA	O3P-C-CA	6.91	120.84	108.69
4	A	1002	FYA	C3'-C2'-C1'	2.70	105.13	100.91
4	A	1002	FYA	C8-N9-C4	-2.15	105.25	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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

6.1 Protein, DNA and RNA chains

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%)	0.18	7 (2%) 53 55	27, 54, 103, 129	0
2	B	775/785 (98%)	0.16	42 (5%) 25 25	21, 59, 108, 128	0
All	All	1040/1135 (91%)	0.17	49 (4%) 30 31	21, 58, 107, 129	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	TRP	6.6
2	B	753	LYS	5.9
1	A	142	HIS	4.9
1	A	350	LEU	4.9
2	B	689	ARG	4.6

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	A	1001	1/1	0.27	9.41	42,42,42,42	0
4	FYA	A	1002	33/33	0.15	-0.11	40,65,73,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.