



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 01:29 PM UTC

PDB ID : 6AT7 / pdb_00006at7
Title : Phenylalanine Ammonia-Lyase (PAL) from Sorghum bicolor
Authors : Jun, S.Y.; Kang, C.
Deposited on : 2017-08-28
Resolution : 2.49 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	:	FAILED
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

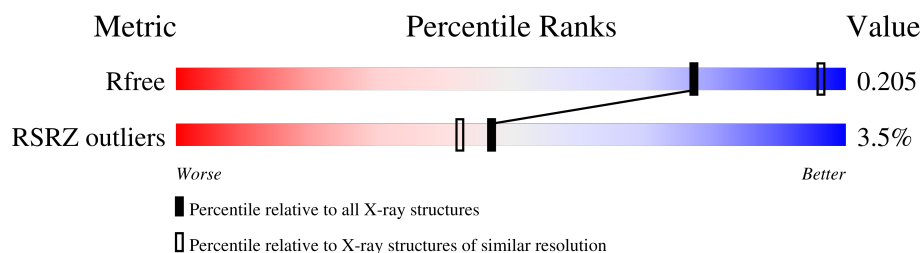
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	5829 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 20689 atoms, of which 10059 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.

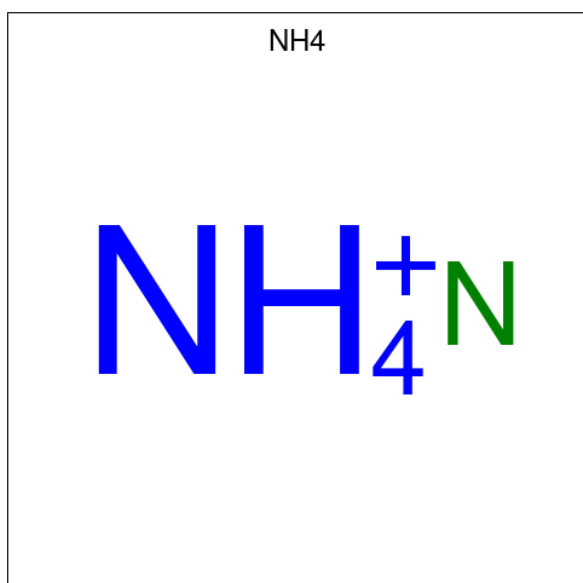
- Molecule 1 is a protein called Phenylalanine ammonia-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	692	Total	C	H	N	O	S	0	0	0
			10273	3245	5109	907	992	20			
1	B	672	Total	C	H	N	O	S	0	0	0
			9960	3152	4942	881	965	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	chromophore	UNP C5XXT8
A	?	-	SER	chromophore	UNP C5XXT8
A	190	MDO	GLY	chromophore	UNP C5XXT8
B	?	-	ALA	chromophore	UNP C5XXT8
B	?	-	SER	chromophore	UNP C5XXT8
B	190	MDO	GLY	chromophore	UNP C5XXT8

- Molecule 2 is AMMONIUM ION (CCD ID: NH4) (formula: H₄N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	H	N	0	0
			5	4	1		
2	B	1	Total	H	N	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	212	Total	O	0	0
			212	212		
3	B	234	Total	O	0	0
			234	234		

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	126.30Å 126.30Å 337.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.66 – 2.49 44.66 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.66-2.49) 99.8 (44.66-2.49)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.78 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.160 , 0.202 0.163 , 0.205	Depositor DCC
R_{free} test set	2000 reflections (4.16%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20689	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	MDO	A	190	1	11,13,14	3.50	6 (54%)	15,18,20	2.53	5 (33%)
1	MDO	B	190	1	11,13,14	3.63	6 (54%)	15,18,20	2.70	5 (33%)

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
1	MDO	A	190	1	-	0/4/23/24	0/1/1/1
1	MDO	B	190	1	-	0/4/23/24	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	190	MDO	C1-N2	7.47	1.43	1.32
1	A	190	MDO	C1-N2	7.06	1.42	1.32
1	B	190	MDO	CA2-C2	5.71	1.54	1.43
1	A	190	MDO	CA2-C2	5.63	1.54	1.43
1	B	190	MDO	C1-N3	5.26	1.46	1.37
1	A	190	MDO	C1-N3	5.20	1.46	1.37
1	B	190	MDO	C2-N3	3.34	1.47	1.40
1	A	190	MDO	C2-N3	3.17	1.47	1.40
1	B	190	MDO	CA2-N2	2.65	1.43	1.39
1	B	190	MDO	O2-C2	-2.32	1.18	1.23
1	A	190	MDO	O2-C2	-2.31	1.18	1.23
1	A	190	MDO	CA2-N2	2.30	1.43	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	MDO	O2-C2-CA2	-5.11	127.76	131.02
1	A	190	MDO	O2-C2-CA2	-4.91	127.89	131.02
1	B	190	MDO	CA2-N2-C1	4.90	109.78	105.39
1	A	190	MDO	CA2-N2-C1	4.58	109.49	105.39
1	B	190	MDO	CA2-C2-N3	4.57	107.34	103.50
1	A	190	MDO	CA2-C2-N3	4.18	107.01	103.50
1	B	190	MDO	C2-CA2-N2	-4.15	105.97	108.95
1	A	190	MDO	C2-N3-C1	-3.86	106.28	108.07
1	B	190	MDO	C2-N3-C1	-3.76	106.33	108.07
1	A	190	MDO	C2-CA2-N2	-3.57	106.39	108.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are modelled with single atom - leaving 0 for Mogul analysis.

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.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 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	691/702 (98%)	-0.32	25 (3%)	46 41	19, 37, 107, 179	0
1	B	671/702 (95%)	-0.39	22 (3%)	49 45	19, 35, 85, 131	0
All	All	1362/1404 (97%)	-0.36	47 (3%)	47 42	19, 36, 96, 179	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	THR	5.2
1	B	328	ASP	4.7
1	B	605	THR	4.2
1	B	593	ASP	4.0
1	A	104	GLY	3.8
1	B	327	LEU	3.8
1	B	536	THR	3.7
1	B	592	GLY	3.4
1	A	545	SER	3.4
1	B	326	GLU	3.4
1	A	543	LEU	3.3
1	A	332	LYS	3.3
1	B	321	ALA	3.2
1	B	323	LYS	3.1
1	B	333	PRO	3.1
1	A	333	PRO	3.1
1	B	702	VAL	3.1
1	A	542	ASP	3.0
1	B	325	ASN	2.9
1	A	594	ALA	2.9
1	A	96	TYR	2.9
1	B	331	LEU	2.9
1	A	536	THR	2.8
1	A	544	SER	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	548	PHE	2.7
1	B	110	THR	2.7
1	A	327	LEU	2.6
1	A	540	SER	2.6
1	A	331	LEU	2.6
1	A	593	ASP	2.5
1	B	324	VAL	2.5
1	A	106	SER	2.5
1	A	102	PHE	2.4
1	A	103	GLY	2.4
1	B	600	VAL	2.3
1	B	595	GLU	2.2
1	A	330	LEU	2.2
1	A	107	HIS	2.2
1	A	546	ALA	2.2
1	B	334	LYS	2.2
1	A	99	THR	2.1
1	A	539	PRO	2.1
1	B	332	LYS	2.1
1	B	99	THR	2.1
1	B	322	LYS	2.1
1	A	595	GLU	2.1
1	B	606	LYS	2.1

5.2 Non-standard residues in protein, DNA, RNA chains [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
1	MDO	B	190	13/14	0.80	0.13	24,30,33,37	0
1	MDO	A	190	13/14	0.87	0.12	24,31,37,42	0

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 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
2	NH4	B	801	1/1	0.61	0.22	46,55,55,55	0
2	NH4	A	801	1/1	0.70	0.23	52,62,62,62	0

5.5 Other polymers [i](#)

There are no such residues in this entry.