



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:30 PM UTC

PDB ID : 6G4F / pdb_00006g4f
Title : Crystal structure of the omega TRANSAMINASE FROM PSEUDOMONAS
Jessenii in complex with PMP
Authors : Rozeboom, H.J.; Janssen, D.B.
Deposited on : 2018-03-27
Resolution : 2.50 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 : 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

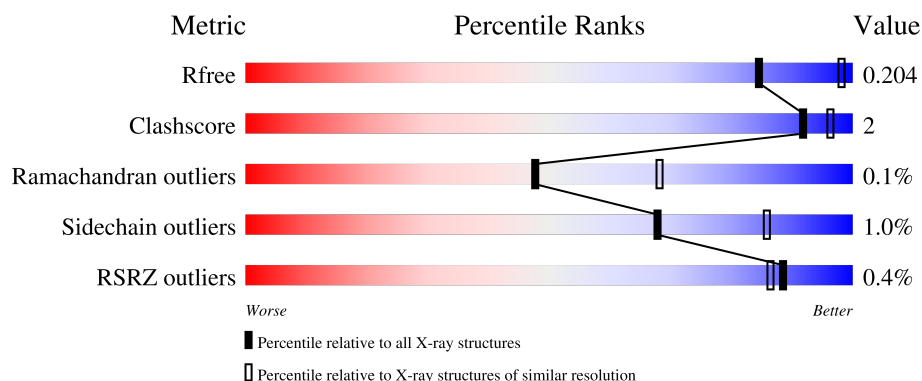
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	464	92% 5%
1	B	464	92% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7275 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.

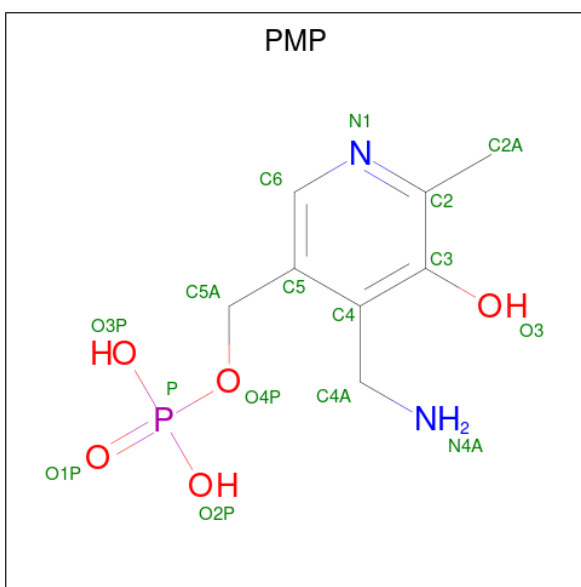
- Molecule 1 is a protein called Aspartate aminotransferase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	1	0
			3470	2217	599	637	17			
1	B	453	Total	C	N	O	S	0	1	0
			3480	2224	601	638	17			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	PRO	-	expression tag	UNP A0A2D8IND4
A	457	GLY	-	expression tag	UNP A0A2D8IND4
A	458	GLY	-	expression tag	UNP A0A2D8IND4
A	459	HIS	-	expression tag	UNP A0A2D8IND4
A	460	HIS	-	expression tag	UNP A0A2D8IND4
A	461	HIS	-	expression tag	UNP A0A2D8IND4
A	462	HIS	-	expression tag	UNP A0A2D8IND4
A	463	HIS	-	expression tag	UNP A0A2D8IND4
A	464	HIS	-	expression tag	UNP A0A2D8IND4
B	456	PRO	-	expression tag	UNP A0A2D8IND4
B	457	GLY	-	expression tag	UNP A0A2D8IND4
B	458	GLY	-	expression tag	UNP A0A2D8IND4
B	459	HIS	-	expression tag	UNP A0A2D8IND4
B	460	HIS	-	expression tag	UNP A0A2D8IND4
B	461	HIS	-	expression tag	UNP A0A2D8IND4
B	462	HIS	-	expression tag	UNP A0A2D8IND4
B	463	HIS	-	expression tag	UNP A0A2D8IND4
B	464	HIS	-	expression tag	UNP A0A2D8IND4

- Molecule 2 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (CCD ID: PMP) (formula: C₈H₁₃N₂O₅P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



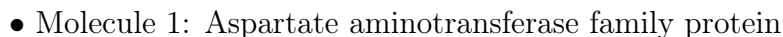
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	127	Total	O	0	0
			127	127		
5	B	161	Total	O	0	0
			161	161		

i

- Molecule 1: Aspartate aminotransferase family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	97.56Å 97.56Å 119.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.90 – 2.50 50.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.90-2.50) 99.9 (50.90-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.160 , 0.203 0.167 , 0.204	Depositor DCC
R_{free} test set	1979 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 27.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7275	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: PMP, PLP, GOL

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	0.64	0/3552	0.80	0/4814
1	B	0.66	0/3562	0.81	2/4827 (0.0%)
All	All	0.65	0/7114	0.80	2/9641 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	LYS	CB-CG-CD	5.44	123.82	111.30
1	B	287	LYS	CB-CA-C	5.05	120.47	110.42

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	3470	0	3447	9	0
1	B	3480	0	3457	13	0
2	A	16	0	10	0	0
3	A	6	0	8	0	0
4	B	15	0	6	0	0
5	A	127	0	0	1	0
5	B	161	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7275	0	6928	22	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 2.

All (22) 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:B:249:ARG:NH2	1:B:279:GLN:O	2.37	0.58
1:A:249:ARG:NH2	1:A:279:GLN:O	2.37	0.57
1:A:303:ALA:HB3	1:A:304:PRO:HD3	1.91	0.52
1:B:303:ALA:HB3	1:B:304:PRO:HD3	1.92	0.51
1:B:112:VAL:HG22	1:B:300:LEU:HD22	1.95	0.48
1:B:260:VAL:HG12	1:B:287:LYS:HD2	1.98	0.46
1:A:327:GLY:O	1:A:328:HIS:C	2.59	0.45
1:A:154:ILE:HA	1:A:159:ALA:HB2	1.97	0.44
1:A:432:ASN:OD1	1:A:432:ASN:C	2.61	0.44
1:B:59:SER:HB2	1:B:292:SER:OG	2.18	0.43
1:A:92:ARG:HB3	1:A:93:PRO:HD3	1.99	0.42
1:B:154:ILE:HA	1:B:159:ALA:HB2	2.00	0.42
1:A:146:SER:O	1:A:180:HIS:HA	2.20	0.42
1:B:164:LEU:HB2	1:B:167:ASN:HD22	1.85	0.42
1:B:146:SER:O	1:B:180:HIS:HA	2.20	0.41
1:B:8:LEU:HB3	1:B:9:PRO:HD3	2.03	0.41
1:B:432:ASN:OD1	1:B:432:ASN:C	2.64	0.41
1:B:327:GLY:O	1:B:328:HIS:C	2.63	0.41
1:B:92:ARG:HB3	1:B:93:PRO:HD3	2.03	0.40
1:A:127:LYS:NZ	5:A:607:HOH:O	2.50	0.40
1:B:135:ALA:HB2	1:B:312:GLN:HB2	2.03	0.40
1:A:59:SER:HB2	1:A:292[B]:SER:OG	2.21	0.40

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	450/464 (97%)	431 (96%)	18 (4%)	1 (0%)	43	63
1	B	452/464 (97%)	433 (96%)	19 (4%)	0	100	100
All	All	902/928 (97%)	864 (96%)	37 (4%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	396	GLN

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	361/371 (97%)	356 (99%)	5 (1%)	59	81
1	B	361/371 (97%)	359 (99%)	2 (1%)	78	91
All	All	722/742 (97%)	715 (99%)	7 (1%)	68	86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	349	GLU
1	A	356	GLN
1	A	359	ARG
1	A	452	GLN
1	B	312	GLN
1	B	452	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	180	HIS
1	A	410	GLN
1	A	452	GLN
1	B	167	ASN
1	B	180	HIS
1	B	356	GLN
1	B	452	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 ligands 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	$\# Z > 2$
3	GOL	A	502	-	5,5,5	0.31	0	5,5,5	0.39	0
2	PMP	A	501	-	16,16,16	2.60	3 (18%)	22,23,23	1.61	6 (27%)
4	PLP	B	501	1	15,15,16	3.19	3 (20%)	21,22,23	2.75	4 (19%)

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
3	GOL	A	502	-	-	2/4/4/4	-
2	PMP	A	501	-	-	4/8/8/8	0/1/1/1
4	PLP	B	501	1	-	0/6/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	PLP	C5-C4	9.54	1.51	1.40
2	A	501	PMP	C3-C2	6.60	1.47	1.41
4	B	501	PLP	C3-C2	6.11	1.47	1.41
2	A	501	PMP	C5-C4	5.61	1.48	1.40
2	A	501	PMP	C3-C4	5.34	1.47	1.40
4	B	501	PLP	C3-C4	3.61	1.47	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	PLP	C4A-C4-C5	8.45	129.65	120.94
4	B	501	PLP	C6-C5-C4	4.81	122.04	118.10
4	B	501	PLP	C3-C4-C5	-4.74	112.90	118.59
4	B	501	PLP	C5A-C5-C6	-3.95	112.92	119.36
2	A	501	PMP	C4A-C4-C3	2.65	124.71	120.22
2	A	501	PMP	O4P-P-O1P	-2.64	99.32	106.44
2	A	501	PMP	C3-C4-C5	-2.58	116.39	118.73
2	A	501	PMP	C6-N1-C2	2.38	123.51	119.20
2	A	501	PMP	C6-C5-C4	2.33	119.82	118.06
2	A	501	PMP	O2P-P-O1P	2.06	118.87	110.83

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PMP	C5A-O4P-P-O1P
2	A	501	PMP	C5A-O4P-P-O3P
3	A	502	GOL	C1-C2-C3-O3
3	A	502	GOL	O2-C2-C3-O3
2	A	501	PMP	C3-C4-C4A-N4A
2	A	501	PMP	C5A-O4P-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	451/464 (97%)	-0.31	3 (0%) 84 81	13, 38, 61, 97	1 (0%)
1	B	453/464 (97%)	-0.45	1 (0%) 91 89	15, 34, 52, 72	1 (0%)
All	All	904/928 (97%)	-0.38	4 (0%) 88 86	13, 36, 57, 97	2 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	456	PRO	4.4
1	A	6	SER	2.6
1	A	364	HIS	2.3
1	B	458	GLY	2.2

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](#)

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
3	GOL	A	502	6/6	0.88	0.14	62,63,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PLP	B	501	15/16	0.97	0.07	25,28,32,32	0
2	PMP	A	501	16/16	0.98	0.05	26,27,28,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.