



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 20, 2025 – 01:14 pm BST

PDB ID : 9H1T / pdb_00009h1t
Title : Crystal structure of apo-tyrosinase from Priestia megaterium F227Y mutant
Authors : Englund, A.N.B.; Rohr, A.K.
Deposited on : 2024-10-10
Resolution : 2.14 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
Xtriage (Phenix) : 2.0
EDS : **FAILED**
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

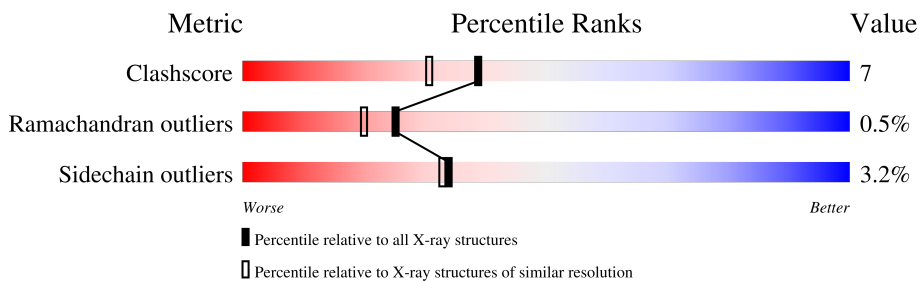
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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))
Clashscore	180529	3585 (2.16-2.12)
Ramachandran outliers	177936	3554 (2.16-2.12)
Sidechain outliers	177891	3553 (2.16-2.12)

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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	303	
1	B	303	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4990 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 Tyrosinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	1	0
			2319	1474	418	419	8			
1	B	287	Total	C	N	O	S	0	0	0
			2348	1492	424	424	8			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	TYR	PHE	engineered mutation	UNP B2ZB02
A	298	HIS	-	expression tag	UNP B2ZB02
A	299	HIS	-	expression tag	UNP B2ZB02
A	300	HIS	-	expression tag	UNP B2ZB02
A	301	HIS	-	expression tag	UNP B2ZB02
A	302	HIS	-	expression tag	UNP B2ZB02
A	303	HIS	-	expression tag	UNP B2ZB02
B	227	TYR	PHE	engineered mutation	UNP B2ZB02
B	298	HIS	-	expression tag	UNP B2ZB02
B	299	HIS	-	expression tag	UNP B2ZB02
B	300	HIS	-	expression tag	UNP B2ZB02
B	301	HIS	-	expression tag	UNP B2ZB02
B	302	HIS	-	expression tag	UNP B2ZB02
B	303	HIS	-	expression tag	UNP B2ZB02

- Molecule 2 is water.

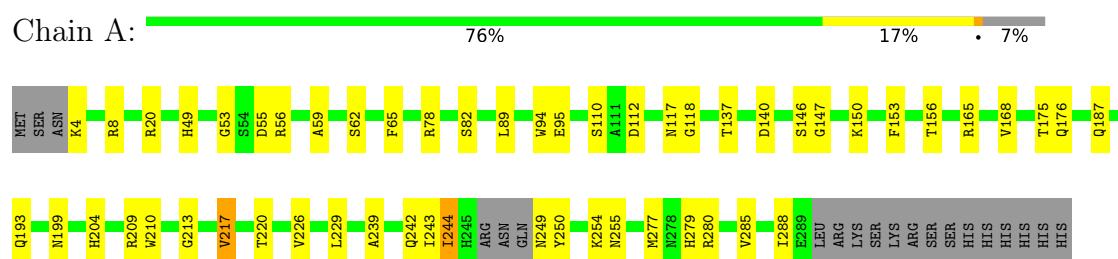
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	103	Total	O	0	0
			103	103		
2	B	220	Total	O	0	0
			220	220		

3 Residue-property plots [i](#)

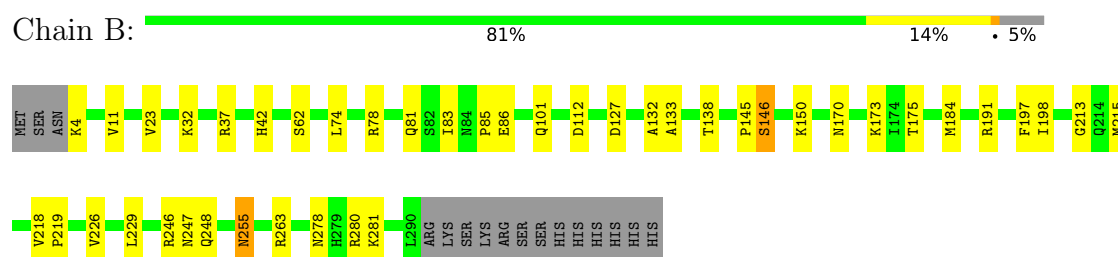
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS failed to run properly.

• Molecule 1: Tyrosinase



• Molecule 1: Tyrosinase



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.89Å 78.63Å 86.59Å 90.00° 103.97° 90.00°	Depositor
Resolution (Å)	40.01 – 2.14	Depositor
% Data completeness (in resolution range)	96.6 (40.01-2.14)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.75 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.204 , 0.283	Depositor
Wilson B-factor (Å ²)	-50.7	Xtriage
Anisotropy	-0.211	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-h-l	Xtriage
Total number of atoms	4990	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% 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	0.30	0/2395	0.52	0/3264
1	B	0.37	0/2425	0.57	0/3305
All	All	0.33	0/4820	0.54	0/6569

There are no bond length outliers.

There are no bond angle outliers.

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	2319	0	2193	31	1
1	B	2348	0	2231	30	0
2	A	103	0	0	5	0
2	B	220	0	0	12	0
All	All	4990	0	4424	61	1

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 7.

All (61) 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:4:LYS:HD3	1:A:280:ARG:HD3	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLN:NE2	2:A:402:HOH:O	2.23	0.69
1:A:110:SER:OG	1:A:112:ASP:OD1	2.11	0.67
1:A:8:ARG:HG2	1:A:89:LEU:O	1.94	0.67
1:A:254:LYS:NZ	1:A:255:ASN:OD1	2.23	0.66
1:B:81:GLN:HG3	1:B:85:PRO:HA	1.76	0.66
1:B:133:ALA:O	2:B:403:HOH:O	2.13	0.65
1:A:56:ARG:HB3	1:A:62:SER:HB2	1.79	0.64
1:A:95:GLU:HG3	1:A:165:ARG:HH21	1.64	0.63
1:A:49:HIS:NE2	2:A:406:HOH:O	2.31	0.62
1:B:255:ASN:ND2	2:B:411:HOH:O	2.31	0.62
1:A:78:ARG:NH2	2:A:401:HOH:O	2.17	0.61
1:B:4:LYS:HG2	1:B:280:ARG:HB3	1.83	0.60
1:A:242:GLN:NE2	1:A:277:MET:O	2.33	0.58
1:A:95:GLU:OE2	1:A:165:ARG:NH2	2.36	0.58
1:B:170:ASN:HA	1:B:173:LYS:HD2	1.86	0.56
1:B:138:THR:OG1	1:B:146:SER:HB2	2.07	0.54
1:A:209[B]:ARG:HH11	1:A:209[B]:ARG:HA	1.74	0.52
1:B:247:ASN:ND2	2:B:414:HOH:O	2.38	0.51
1:A:280:ARG:HH11	1:A:280:ARG:HG2	1.76	0.51
1:B:248:GLN:HG3	2:B:417:HOH:O	2.09	0.50
1:B:145:PRO:O	2:B:404:HOH:O	2.20	0.50
1:A:280:ARG:NH1	1:A:285:VAL:HG23	2.27	0.49
1:A:150:LYS:O	1:A:213:GLY:HA3	2.11	0.49
1:A:217:VAL:HG22	1:A:220:THR:OG1	2.14	0.48
1:B:78:ARG:NH2	2:B:409:HOH:O	2.27	0.48
1:B:198:ILE:HG22	2:B:464:HOH:O	2.15	0.47
1:A:165:ARG:NH1	2:A:414:HOH:O	2.47	0.46
1:B:32:LYS:NZ	1:B:83:ILE:HD11	2.30	0.46
1:B:112:ASP:OD2	2:B:405:HOH:O	2.21	0.46
1:A:59:ALA:O	1:A:65:PHE:HA	2.16	0.46
1:A:156:THR:HG21	1:A:209[B]:ARG:NH2	2.31	0.46
1:B:247:ASN:ND2	2:B:421:HOH:O	2.49	0.46
1:A:209[B]:ARG:HA	1:A:209[B]:ARG:NH1	2.31	0.45
1:A:153:PHE:HA	1:A:210:TRP:O	2.17	0.45
1:B:127:ASP:HA	1:B:132:ALA:HB1	1.99	0.45
1:A:280:ARG:HH12	1:A:285:VAL:HG23	1.82	0.45
1:B:215:MET:HE2	1:B:226:VAL:HG13	1.98	0.45
1:B:247:ASN:OD1	1:B:247:ASN:N	2.39	0.44
1:B:62:SER:O	1:B:191:ARG:HD3	2.17	0.44
1:A:65:PHE:HZ	1:A:204:HIS:CD2	2.36	0.44
1:B:150:LYS:O	1:B:213:GLY:HA3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:VAL:N	1:B:219:PRO:HD2	2.33	0.44
1:B:278:ASN:CG	1:B:281:LYS:HG3	2.42	0.44
1:B:246:ARG:HA	1:B:246:ARG:HD3	1.80	0.43
1:A:249:ASN:HB3	1:A:250:TYR:H	1.54	0.43
1:B:184:MET:HG3	1:B:197:PHE:HB3	2.00	0.42
1:A:137:THR:HG22	2:A:425:HOH:O	2.19	0.42
1:B:42:HIS:HB3	2:B:480:HOH:O	2.18	0.42
1:B:86:GLU:O	1:B:86:GLU:HG3	2.19	0.42
1:B:37:ARG:NH1	2:B:406:HOH:O	2.22	0.42
1:A:239:ALA:HB1	1:A:279:HIS:CE1	2.55	0.42
1:B:198:ILE:HD12	1:B:198:ILE:HA	1.95	0.41
1:A:280:ARG:HH11	1:A:280:ARG:CG	2.34	0.41
1:A:140:ASP:HB3	1:A:146:SER:HB3	2.03	0.41
1:B:263:ARG:HB2	2:B:470:HOH:O	2.19	0.41
1:A:243:ILE:O	1:A:244:ILE:C	2.64	0.41
1:A:117:ASN:OD1	1:A:118:GLY:N	2.52	0.40
1:A:187:GLN:OE1	1:A:187:GLN:HA	2.21	0.40
1:B:74:LEU:HD21	1:B:78:ARG:NH2	2.36	0.40
1:B:175:THR:O	1:B:248:GLN:HG2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ARG:NH2	1:A:53:GLY:O[2_545]	2.08	0.12

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	280/303 (92%)	268 (96%)	9 (3%)	3 (1%)	12 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	285/303 (94%)	276 (97%)	9 (3%)	0	100	100
All	All	565/606 (93%)	544 (96%)	18 (3%)	3 (0%)	25	20

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	ILE
1	A	147	GLY
1	A	244	ILE

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	245/266 (92%)	235 (96%)	10 (4%)	26	23
1	B	249/266 (94%)	243 (98%)	6 (2%)	44	45
All	All	494/532 (93%)	478 (97%)	16 (3%)	34	33

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
1	A	82	SER
1	A	94	TRP
1	A	168	VAL
1	A	175	THR
1	A	176	GLN
1	A	199	ASN
1	A	217	VAL
1	A	226	VAL
1	A	229	LEU
1	B	11	VAL
1	B	23	VAL
1	B	101	GLN

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Mol	Chain	Res	Type
1	B	146	SER
1	B	229	LEU
1	B	255	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	105	GLN
1	A	193	GLN
1	B	13	HIS
1	B	142	GLN
1	B	187	GLN
1	B	199	ASN
1	B	248	GLN
1	B	255	ASN

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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