



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:56 AM UTC

PDB ID : 7E05 / pdb_00007e05
Title : Trans-3/4-proline-hydroxylase H11 apo structure
Authors : Gong, W.G.; Yang, L.Y.
Deposited on : 2021-01-27
Resolution : 1.88 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	:	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

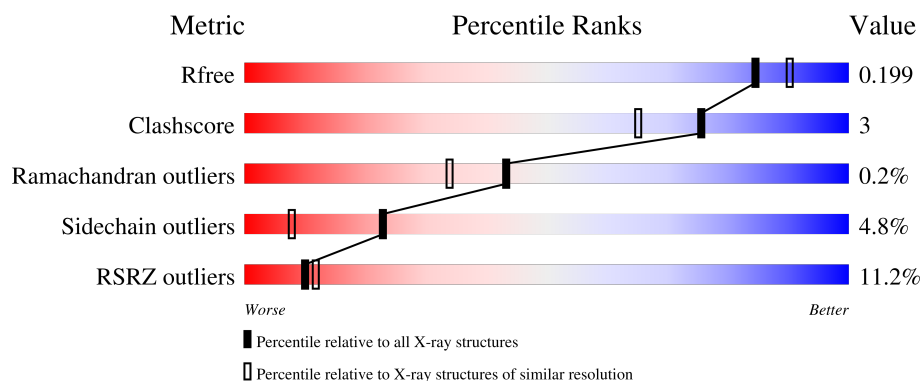
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	268	10% 89% 9% ..
1	B	268	12% 83% 13% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4756 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 Phytanoyl-CoA dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	1	0
			2101	1333	373	389	6			
1	B	262	Total	C	N	O	S	0	2	0
			2102	1333	375	388	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLN	-	expression tag	UNP S5TUM1
A	0	ILE	-	expression tag	UNP S5TUM1
B	-1	GLN	-	expression tag	UNP S5TUM1
B	0	ILE	-	expression tag	UNP S5TUM1

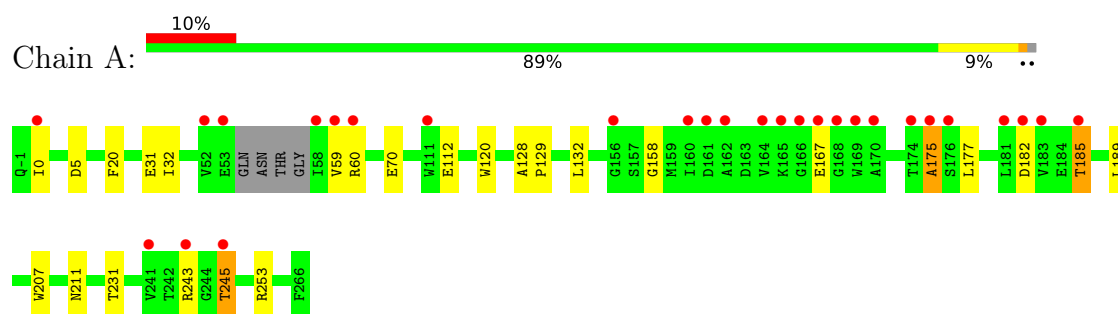
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	284	Total	O	0	0
			284	284		
2	B	269	Total	O	0	0
			269	269		

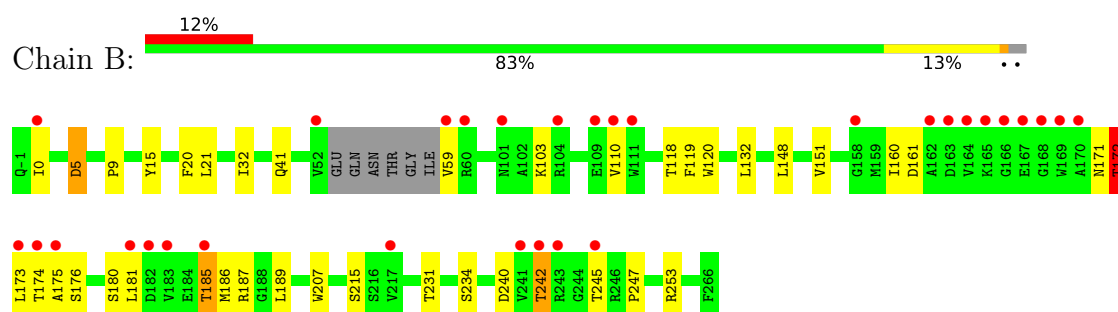
3 Residue-property plots [i](#)

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 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: Phytanoyl-CoA dioxygenase



- Molecule 1: Phytanoyl-CoA dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.50Å 106.50Å 143.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.78 – 1.88 42.78 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.78-1.88) 99.8 (42.78-1.88)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 1.88Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.171 , 0.211 (Not available) , 0.199	Depositor DCC
R_{free} test set	3381 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtrriage
Anisotropy	0.045	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4756	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.8559e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	1.45	5/2156 (0.2%)	1.19	1/2929 (0.0%)
1	B	1.46	7/2157 (0.3%)	1.25	5/2929 (0.2%)
All	All	1.45	12/4313 (0.3%)	1.22	6/5858 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	129	PRO	N-CA	7.26	1.52	1.47
1	A	128	ALA	N-CA	-7.04	1.39	1.45
1	B	118	THR	CA-C	-7.04	1.43	1.52
1	A	32	ILE	CA-C	-6.29	1.44	1.52
1	A	245	THR	N-CA	6.20	1.52	1.46
1	B	32	ILE	CA-C	-5.92	1.45	1.52
1	A	31	GLU	C-O	-5.80	1.17	1.24
1	B	247	PRO	N-CA	-5.51	1.40	1.47
1	B	15	TYR	N-CA	-5.50	1.39	1.46
1	B	9	PRO	C-O	5.48	1.30	1.24
1	B	119	PHE	N-CA	-5.25	1.40	1.46
1	B	21	LEU	N-CA	-5.13	1.40	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	SER	CA-CB-OG	-6.87	97.37	111.10
1	B	176	SER	N-CA-C	6.00	118.56	108.23
1	B	172	THR	N-CA-C	-5.50	106.34	113.16
1	B	175	ALA	O-C-N	5.20	127.49	122.09
1	A	243	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	B	242	THR	N-CA-C	5.06	117.19	111.02

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	2101	0	2028	9	0
1	B	2102	0	2036	16	0
2	A	284	0	0	2	0
2	B	269	0	0	3	0
All	All	4756	0	4064	25	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 3.

All (25) 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:181:LEU:HD13	1:B:186:MET:HE3	1.70	0.72
1:A:158:GLY:C	1:A:211:ASN:HD21	2.02	0.68
1:A:182:ASP:HB3	1:A:185:THR:OG1	1.95	0.66
1:B:171:ASN:OD1	1:B:173:LEU:N	2.28	0.63
1:B:253:ARG:NH1	2:B:303:HOH:O	2.32	0.63
1:A:112:GLU:OE1	1:A:175:ALA:O	2.19	0.60
1:B:59:VAL:HG23	1:B:59:VAL:O	2.02	0.59
1:B:172:THR:HG21	2:B:389:HOH:O	2.04	0.57
1:B:240:ASP:OD1	1:B:242:THR:HB	2.06	0.56
1:B:160:ILE:HG21	1:B:185:THR:HG21	1.87	0.56
1:A:59:VAL:O	1:A:59:VAL:HG23	2.05	0.55
1:B:181:LEU:HD13	1:B:186:MET:CE	2.36	0.53
1:B:160:ILE:CG2	1:B:185:THR:HG21	2.39	0.53
1:A:132:LEU:C	1:A:132:LEU:HD12	2.35	0.52
1:A:0:ILE:HG23	2:A:831:HOH:O	2.16	0.46
1:B:132:LEU:C	1:B:132:LEU:HD12	2.42	0.44
1:B:120:TRP:CH2	1:B:231:THR:HG21	2.53	0.43
1:B:5:ASP:CG	2:B:412:HOH:O	2.61	0.43
1:B:20:PHE:HA	1:B:207:TRP:O	2.19	0.43
1:A:20:PHE:HA	1:A:207:TRP:O	2.19	0.43
1:B:181:LEU:CD1	1:B:186:MET:HE3	2.45	0.43
1:B:151:VAL:HG11	1:B:189:LEU:HD22	2.02	0.41
1:A:253:ARG:NH2	2:A:816:HOH:O	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:MET:O	1:B:187:ARG:C	2.63	0.40
1:A:120:TRP:CH2	1:A:231:THR:HG21	2.57	0.40

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	261/268 (97%)	255 (98%)	5 (2%)	1 (0%)	30	18
1	B	260/268 (97%)	256 (98%)	4 (2%)	0	100	100
All	All	521/536 (97%)	511 (98%)	9 (2%)	1 (0%)	43	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	ALA

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	221/225 (98%)	213 (96%)	8 (4%)	31	14
1	B	222/225 (99%)	209 (94%)	13 (6%)	18	5
All	All	443/450 (98%)	422 (95%)	21 (5%)	23	8

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	60	ARG
1	A	70	GLU
1	A	167	GLU
1	A	177	LEU
1	A	185	THR
1	A	189	LEU
1	A	245	THR
1	B	0	ILE
1	B	5	ASP
1	B	41	GLN
1	B	103	LYS
1	B	110	VAL
1	B	148	LEU
1	B	161	ASP
1	B	172	THR
1	B	174	THR
1	B	180	SER
1	B	185	THR
1	B	234	SER
1	B	245	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	97	GLN
1	A	101	ASN
1	A	211	ASN
1	B	97	GLN
1	B	193	ASN

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 [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 [i](#)

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	264/268 (98%)	0.37	28 (10%)	11 13	10, 24, 73, 124	1 (0%)
1	B	262/268 (97%)	0.41	31 (11%)	9 10	10, 25, 68, 105	2 (0%)
All	All	526/536 (98%)	0.39	59 (11%)	10 12	10, 25, 72, 124	3 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	ALA	7.2
1	B	52	VAL	6.7
1	A	58	ILE	6.5
1	B	59	VAL	6.1
1	B	175	ALA	6.0
1	A	169	TRP	5.8
1	A	53	GLU	5.7
1	A	164	VAL	5.4
1	B	183	VAL	5.2
1	A	183	VAL	5.0
1	A	166	GLY	5.0
1	B	174	THR	4.8
1	A	160	ILE	4.2
1	A	170	ALA	4.1
1	A	243	ARG	4.1
1	B	245	THR	4.1
1	A	0	ILE	4.0
1	A	59	VAL	3.8
1	A	174	THR	3.8
1	B	60	ARG	3.7
1	B	0	ILE	3.7
1	A	162	ALA	3.5
1	A	176	SER	3.5
1	A	52	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	60	ARG	3.2
1	A	168	GLY	3.2
1	A	185	THR	3.1
1	B	169	TRP	3.1
1	B	165	LYS	3.1
1	A	241	VAL	3.0
1	B	162	ALA	3.0
1	B	110	VAL	3.0
1	A	111	TRP	3.0
1	A	165	LYS	2.9
1	B	185	THR	2.8
1	A	182	ASP	2.8
1	B	167	GLU	2.8
1	B	164	VAL	2.8
1	A	161	ASP	2.8
1	B	163	ASP	2.7
1	B	242	THR	2.7
1	B	166	GLY	2.6
1	A	245	THR	2.6
1	B	182	ASP	2.5
1	B	168	GLY	2.5
1	B	217	VAL	2.5
1	B	173	LEU	2.5
1	B	241	VAL	2.5
1	A	181	LEU	2.5
1	B	104	ARG	2.5
1	B	243	ARG	2.4
1	B	101	ASN	2.4
1	A	156	GLY	2.3
1	B	181	LEU	2.3
1	B	111	TRP	2.2
1	A	167	GLU	2.2
1	B	170	ALA	2.2
1	B	158	GLY	2.1
1	B	109	GLU	2.0

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.