



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 06:45 PM EDT

PDB ID : 1T1A / pdb_00001t1a
Title : Late intermediate IL1 from time-resolved crystallography of the E46Q mutant of PYP
Authors : Rajagopal, S.; Anderson, S.; Srajer, V.; Schmidt, M.; Pahl, R.; Moffat, K.
Deposited on : 2004-04-15
Resolution : 1.60 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	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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 1.60 Å.

There are no overall percentile quality scores available for this entry.

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

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1974 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.

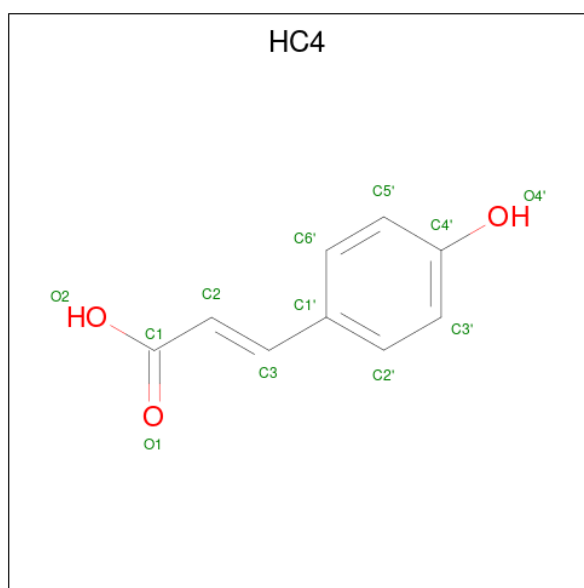
- Molecule 1 is a protein called Photoactive yellow protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	125	Total	C	N	O	S	0	0	0
			976	620	159	191	6			
1	2-A	125	Total	C	N	O	S	0	0	0
			976	620	159	191	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	GLN	GLU	engineered mutation	UNP P16113

- Molecule 2 is 4'-HYDROXYCINNAMIC ACID (CCD ID: HC4) (formula: C₉H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	1-A	1	Total	C	O	0	0
			11	9	2		
2	2-A	1	Total	C	O	0	0
			11	9	2		

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

3 Data and refinement statistics

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

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	66.92Å 66.92Å 41.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.60	Depositor
% Data completeness (in resolution range)	100.0 (30.00-1.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.313 , 0.331	Depositor
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.038	Xtriage
L-test for twinning ¹	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.009 for h,-h-k,-l	Xtriage
Total number of atoms	1974	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 8.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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](#)

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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](#)

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
2	HC4	2-A	169	1	11,11,12	1.70	4 (36%)	13,13,15	0.96	1 (7%)
2	HC4	1-A	169	1	11,11,12	1.84	4 (36%)	13,13,15	1.56	2 (15%)

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
2	HC4	2-A	169	1	-	1/4/4/5	0/1/1/1
2	HC4	1-A	169	1	-	2/4/4/5	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2-A	169	HC4	O4'-C4'	-3.05	1.30	1.37
2	1-A	169	HC4	C3'-C4'	2.87	1.44	1.39
2	1-A	169	HC4	C2-C1	-2.66	1.37	1.44
2	1-A	169	HC4	C3'-C2'	-2.61	1.34	1.38
2	1-A	169	HC4	C6'-C5'	-2.53	1.34	1.38
2	2-A	169	HC4	O1-C1	2.35	1.29	1.22
2	2-A	169	HC4	C3'-C2'	2.24	1.42	1.38
2	2-A	169	HC4	C5'-C4'	2.21	1.43	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-A	169	HC4	C1'-C3-C2	3.85	133.76	127.11
2	2-A	169	HC4	C5'-C6'-C1'	2.28	124.17	121.22
2	1-A	169	HC4	C5'-C4'-C3'	-2.14	116.36	119.77

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1-A	169	HC4	O1-C1-C2-C3
2	1-A	169	HC4	C1-C2-C3-C1'

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Mol	Chain	Res	Type	Atoms
2	2-A	169	HC4	O1-C1-C2-C3

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

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

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

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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