



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:52 AM UTC

PDB ID : 6TAI / pdb_00006tai
Title : Crystal structure of Escherichia coli Orotate Phosphoribosyltransferase with an empty active site at 1.55 Angstrom resolution
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Deposited on : 2019-10-29
Resolution : 1.55 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

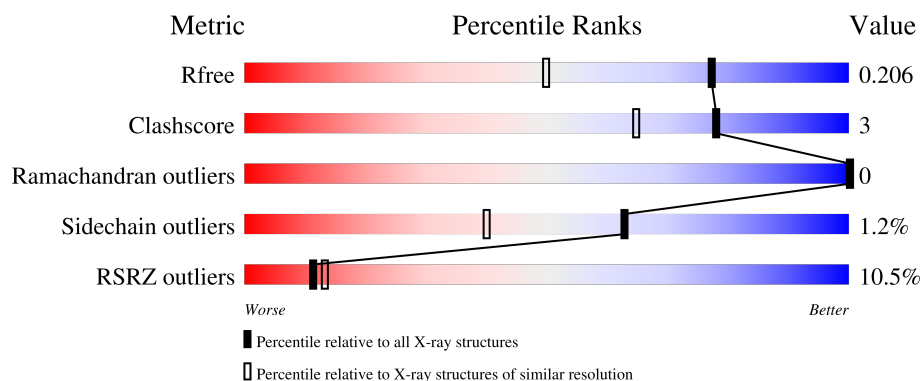
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	AAA	213	14% 91% 7%
1	BBB	213	6% 88% 7%

2 Entry composition [i](#)

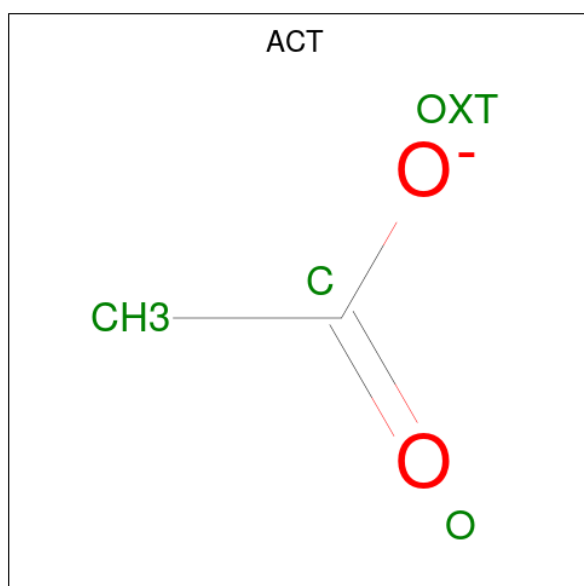
There are 4 unique types of molecules in this entry. The entry contains 6659 atoms, of which 3228 are hydrogens and 0 are deuteriums.

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 Orotate phosphoribosyltransferase.

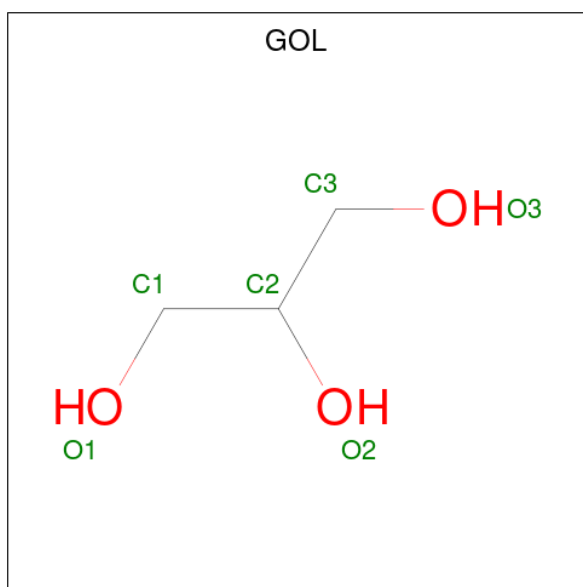
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	207	Total	C	H	N	O	S	58	1	0
			3186	1026	1584	266	304	6			
1	BBB	204	Total	C	H	N	O	S	56	4	0
			3256	1038	1633	273	305	7			

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	H	O	0	0
			7	2	3	2		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	BBB	1	Total	C	H	O	2	0
			14	3	8	3		

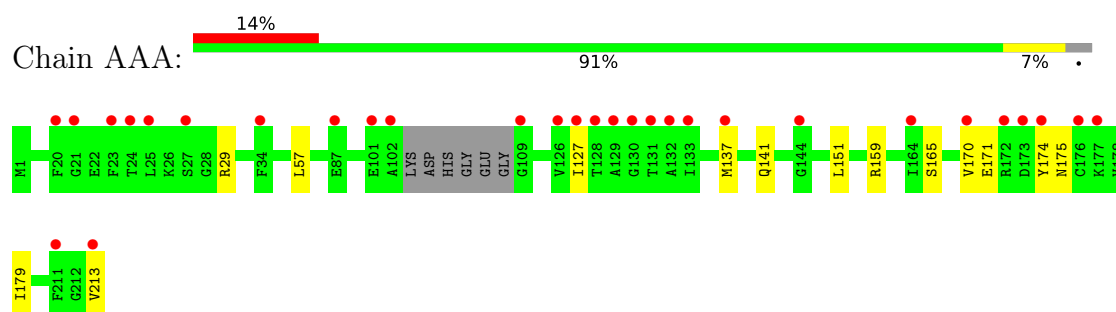
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	86	Total	O	0	1
			87	87		
4	BBB	109	Total	O	0	0
			109	109		

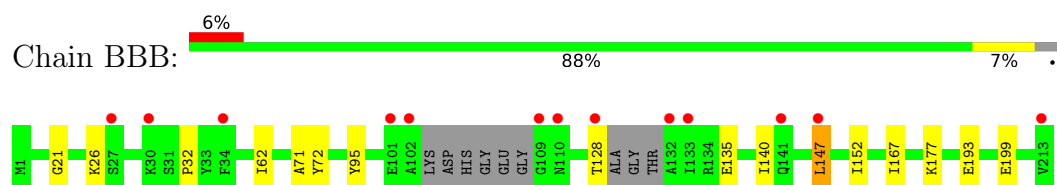
3 Residue-property plots [i](#)

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: Orotate phosphoribosyltransferase



- Molecule 1: Orotate phosphoribosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	75.46Å 131.75Å 39.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.48 – 1.55 65.48 – 1.55	Depositor EDS
% Data completeness (in resolution range)	98.8 (65.48-1.55) 98.8 (65.48-1.55)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 1.55Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.177 , 0.204 0.180 , 0.206	Depositor DCC
R_{free} test set	2807 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6659	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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: GOL, ACT

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	AAA	0.19	0/1629	0.40	0/2199
1	BBB	0.21	0/1649	0.41	0/2220
All	All	0.20	0/3278	0.41	0/4419

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	AAA	1602	1584	1586	8	0
1	BBB	1623	1633	1625	10	0
2	AAA	4	3	3	0	0
3	BBB	6	8	8	0	0
4	AAA	87	0	0	0	0
4	BBB	109	0	0	4	0
All	All	3431	3228	3222	18	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 (18) 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:BBB:135:GLU:OE2	4:BBB:401:HOH:O	2.16	0.59
1:AAA:165:SER:HB3	1:AAA:213:VAL:HG21	1.84	0.59
1:BBB:26:LYS:HE3	1:BBB:128:THR:HG21	1.90	0.53
1:BBB:152[A]:ILE:HD11	1:BBB:167:ILE:HD11	1.92	0.52
1:AAA:171:GLU:O	1:AAA:175:ASN:N	2.44	0.51
1:BBB:128:THR:HG22	4:BBB:485:HOH:O	2.14	0.48
1:BBB:193:GLU:OE2	4:BBB:402:HOH:O	2.20	0.48
1:AAA:159:ARG:HG2	1:AAA:213:VAL:HG12	1.96	0.47
1:BBB:21:GLY:O	1:BBB:32:PRO:HA	2.15	0.47
1:AAA:151:LEU:HD13	1:AAA:179:ILE:HG13	1.98	0.46
1:BBB:71:ALA:HA	1:BBB:72:TYR:HA	1.79	0.45
1:AAA:127:ILE:HD12	1:AAA:170:VAL:HG21	2.00	0.44
1:AAA:213:VAL:O	1:AAA:213:VAL:HG23	2.17	0.43
1:AAA:137:MET:HE1	1:AAA:174:TYR:CG	2.53	0.43
1:BBB:140:ILE:HG21	1:BBB:147:LEU:HD22	2.01	0.43
1:AAA:57:LEU:HG	1:AAA:151:LEU:HD22	2.01	0.42
1:BBB:199:GLU:HB3	4:BBB:456:HOH:O	2.20	0.41
1:BBB:62:ILE:HD11	1:BBB:177:LYS:HD3	2.03	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	AAA	204/213 (96%)	202 (99%)	2 (1%)	0	100	100
1	BBB	202/213 (95%)	201 (100%)	1 (0%)	0	100	100
All	All	406/426 (95%)	403 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	163/171 (95%)	161 (99%)	2 (1%)	63	40
1	BBB	169/171 (99%)	167 (99%)	2 (1%)	63	40
All	All	332/342 (97%)	328 (99%)	4 (1%)	63	40

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	29	ARG
1	AAA	141	GLN
1	BBB	95	TYR
1	BBB	147	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

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	ACT	AAA	301	-	3,3,3	1.16	0	3,3,3	1.58	0
3	GOL	BBB	301	-	5,5,5	0.79	0	5,5,5	1.04	0

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	BBB	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	BBB	301	GOL	C1-C2-C3-O3
3	BBB	301	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	AAA	207/213 (97%)	0.68	30 (14%) 6 6	14, 41, 90, 127	1 (0%)
1	BBB	204/213 (95%)	0.39	13 (6%) 25 30	11, 34, 80, 128	4 (1%)
All	All	411/426 (96%)	0.54	43 (10%) 11 13	11, 37, 88, 128	5 (1%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	34	PHE	6.6
1	AAA	174	TYR	5.7
1	AAA	102	ALA	5.5
1	BBB	102	ALA	5.0
1	AAA	213	VAL	4.4
1	BBB	128	THR	4.2
1	AAA	129	ALA	4.1
1	BBB	132	ALA	4.0
1	AAA	27	SER	3.8
1	AAA	21	GLY	3.7
1	BBB	133	ILE	3.6
1	AAA	127	ILE	3.6
1	BBB	147	LEU	3.3
1	AAA	131	THR	3.0
1	AAA	172	ARG	3.0
1	AAA	132	ALA	2.9
1	BBB	101	GLU	2.8
1	AAA	176	CYS	2.8
1	AAA	173	ASP	2.8
1	AAA	20	PHE	2.8
1	AAA	133	ILE	2.8
1	BBB	27	SER	2.7
1	AAA	128	THR	2.7
1	AAA	25	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	BBB	141	GLN	2.6
1	BBB	30	LYS	2.6
1	AAA	126	VAL	2.5
1	AAA	101	GLU	2.4
1	AAA	130	GLY	2.4
1	AAA	164	ILE	2.4
1	AAA	144	GLY	2.3
1	BBB	109	GLY	2.3
1	AAA	137	MET	2.3
1	AAA	211	PHE	2.3
1	AAA	23	PHE	2.2
1	AAA	24	THR	2.2
1	AAA	34	PHE	2.2
1	AAA	170	VAL	2.2
1	AAA	109	GLY	2.1
1	AAA	87	GLU	2.1
1	BBB	110	ASN	2.1
1	AAA	177	LYS	2.0
1	BBB	213	VAL	2.0

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($\text{\AA}^2$)	Q<0.9
2	ACT	AAA	301	4/4	0.78	0.15	52,56,66,66	0
3	GOL	BBB	301	6/6	0.83	0.13	44,68,83,92	2

6.5 Other polymers [i](#)

There are no such residues in this entry.