



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 07:08 PM UTC

PDB ID : 4H6D / pdb_00004h6d
Title : Crystal structure of PLP-soaked HMP synthase Thi5 from *S. cerevisiae*
Authors : Coquille, S.C.; Roux, C.; Fitzpatrick, T.; Thore, S.
Deposited on : 2012-09-19
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

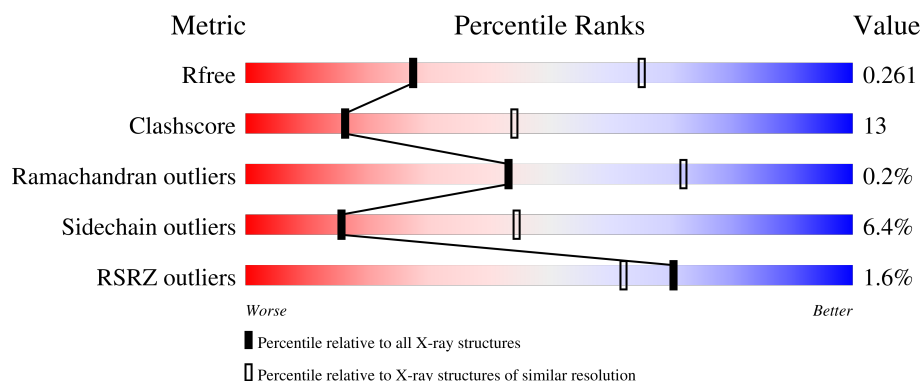
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



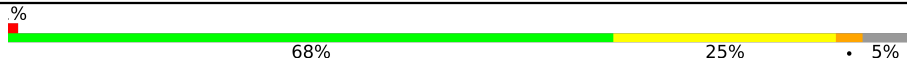
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	346	
1	B	346	
1	C	346	
1	D	346	
1	E	346	

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Mol	Chain	Length	Quality of chain
1	F	346	 68% 25% • 5%
1	G	346	 64% 29% • •
1	H	346	 3% 66% 27% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLP	A	400	-	-	X	-
2	PLP	E	400	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20876 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 Pyrimidine precursor biosynthesis enzyme THI5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	330	Total	C	N	O	S	0	0	0
			2643	1706	435	485	17			
1	A	314	Total	C	N	O	S	0	0	0
			2505	1624	407	458	16			
1	B	329	Total	C	N	O	S	0	0	0
			2634	1700	433	484	17			
1	C	335	Total	C	N	O	S	0	0	0
			2674	1726	440	490	18			
1	D	333	Total	C	N	O	S	0	0	0
			2662	1718	438	488	18			
1	E	302	Total	C	N	O	S	0	0	0
			2417	1566	392	444	15			
1	G	331	Total	C	N	O	S	0	0	0
			2651	1712	436	486	17			
1	H	328	Total	C	N	O	S	0	0	0
			2630	1697	433	483	17			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	101	LYS	GLU	engineered mutation	UNP P43534
F	102	SER	ASP	engineered mutation	UNP P43534
F	317	THR	GLN	engineered mutation	UNP P43534
F	341	HIS	-	expression tag	UNP P43534
F	342	HIS	-	expression tag	UNP P43534
F	343	HIS	-	expression tag	UNP P43534
F	344	HIS	-	expression tag	UNP P43534
F	345	HIS	-	expression tag	UNP P43534
F	346	HIS	-	expression tag	UNP P43534
A	101	LYS	GLU	engineered mutation	UNP P43534
A	102	SER	ASP	engineered mutation	UNP P43534
A	317	THR	GLN	engineered mutation	UNP P43534
A	341	HIS	-	expression tag	UNP P43534

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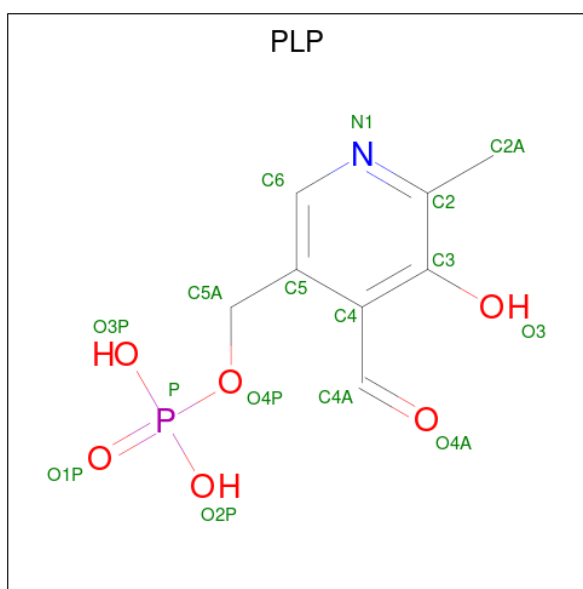
Chain	Residue	Modelled	Actual	Comment	Reference
A	342	HIS	-	expression tag	UNP P43534
A	343	HIS	-	expression tag	UNP P43534
A	344	HIS	-	expression tag	UNP P43534
A	345	HIS	-	expression tag	UNP P43534
A	346	HIS	-	expression tag	UNP P43534
B	101	LYS	GLU	engineered mutation	UNP P43534
B	102	SER	ASP	engineered mutation	UNP P43534
B	317	THR	GLN	engineered mutation	UNP P43534
B	341	HIS	-	expression tag	UNP P43534
B	342	HIS	-	expression tag	UNP P43534
B	343	HIS	-	expression tag	UNP P43534
B	344	HIS	-	expression tag	UNP P43534
B	345	HIS	-	expression tag	UNP P43534
B	346	HIS	-	expression tag	UNP P43534
C	101	LYS	GLU	engineered mutation	UNP P43534
C	102	SER	ASP	engineered mutation	UNP P43534
C	317	THR	GLN	engineered mutation	UNP P43534
C	341	HIS	-	expression tag	UNP P43534
C	342	HIS	-	expression tag	UNP P43534
C	343	HIS	-	expression tag	UNP P43534
C	344	HIS	-	expression tag	UNP P43534
C	345	HIS	-	expression tag	UNP P43534
C	346	HIS	-	expression tag	UNP P43534
D	101	LYS	GLU	engineered mutation	UNP P43534
D	102	SER	ASP	engineered mutation	UNP P43534
D	317	THR	GLN	engineered mutation	UNP P43534
D	341	HIS	-	expression tag	UNP P43534
D	342	HIS	-	expression tag	UNP P43534
D	343	HIS	-	expression tag	UNP P43534
D	344	HIS	-	expression tag	UNP P43534
D	345	HIS	-	expression tag	UNP P43534
D	346	HIS	-	expression tag	UNP P43534
E	101	LYS	GLU	engineered mutation	UNP P43534
E	102	SER	ASP	engineered mutation	UNP P43534
E	317	THR	GLN	engineered mutation	UNP P43534
E	341	HIS	-	expression tag	UNP P43534
E	342	HIS	-	expression tag	UNP P43534
E	343	HIS	-	expression tag	UNP P43534
E	344	HIS	-	expression tag	UNP P43534
E	345	HIS	-	expression tag	UNP P43534
E	346	HIS	-	expression tag	UNP P43534
G	101	LYS	GLU	engineered mutation	UNP P43534

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Chain	Residue	Modelled	Actual	Comment	Reference
G	102	SER	ASP	engineered mutation	UNP P43534
G	317	THR	GLN	engineered mutation	UNP P43534
G	341	HIS	-	expression tag	UNP P43534
G	342	HIS	-	expression tag	UNP P43534
G	343	HIS	-	expression tag	UNP P43534
G	344	HIS	-	expression tag	UNP P43534
G	345	HIS	-	expression tag	UNP P43534
G	346	HIS	-	expression tag	UNP P43534
H	101	LYS	GLU	engineered mutation	UNP P43534
H	102	SER	ASP	engineered mutation	UNP P43534
H	317	THR	GLN	engineered mutation	UNP P43534
H	341	HIS	-	expression tag	UNP P43534
H	342	HIS	-	expression tag	UNP P43534
H	343	HIS	-	expression tag	UNP P43534
H	344	HIS	-	expression tag	UNP P43534
H	345	HIS	-	expression tag	UNP P43534
H	346	HIS	-	expression tag	UNP P43534

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



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

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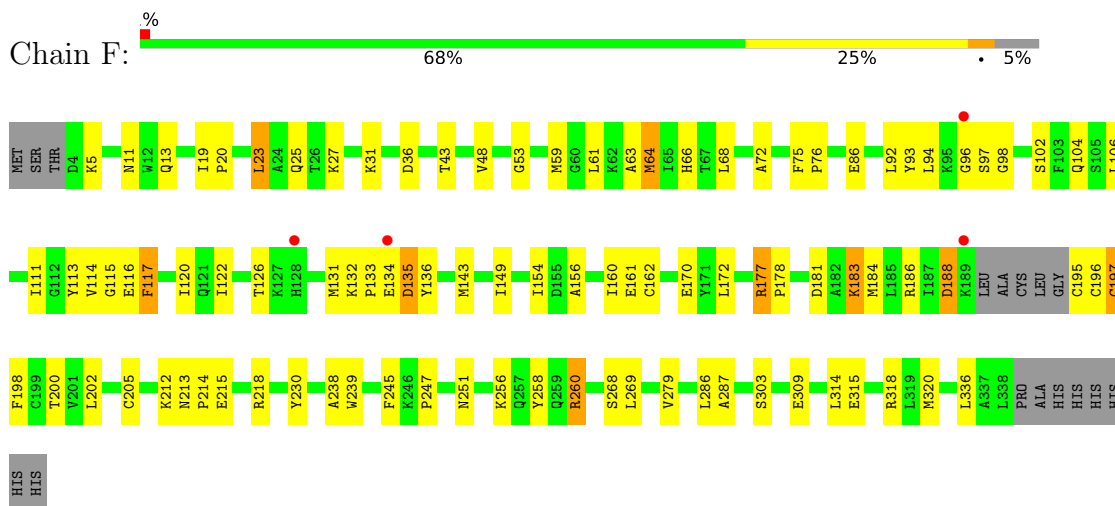
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

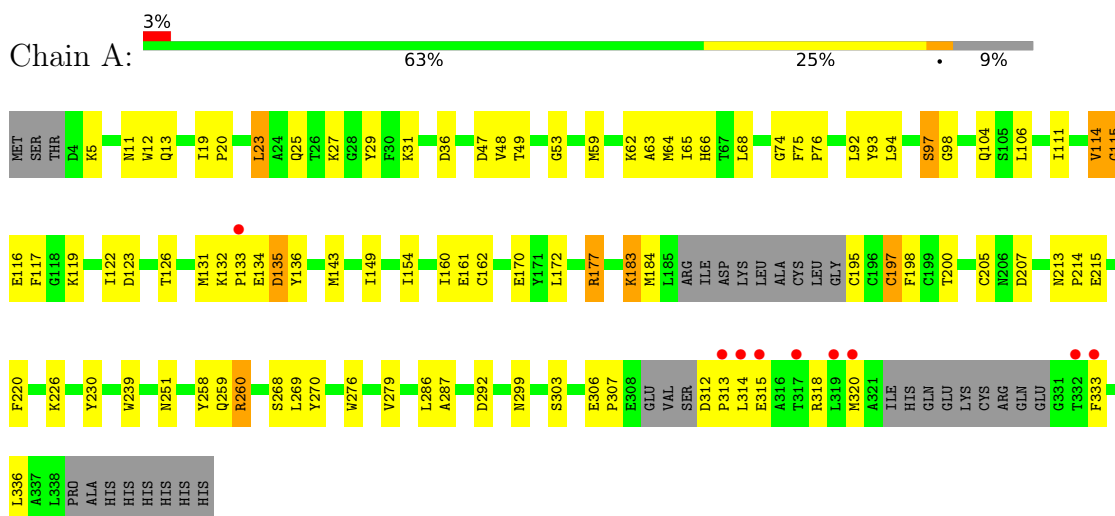
3 Residue-property plots

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: Pyrimidine precursor biosynthesis enzyme THI5

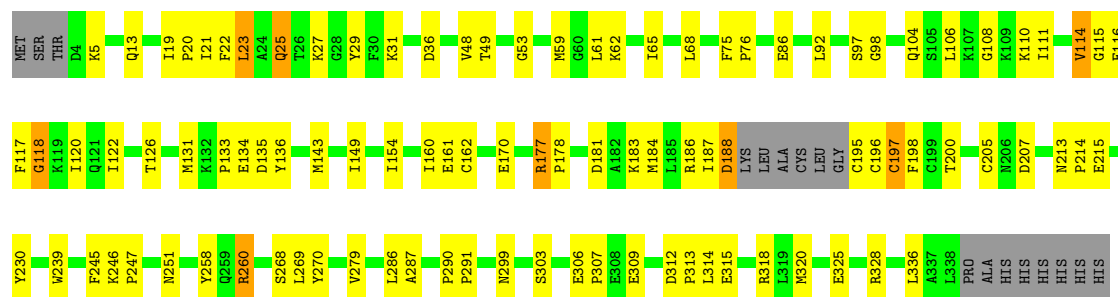


- Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5

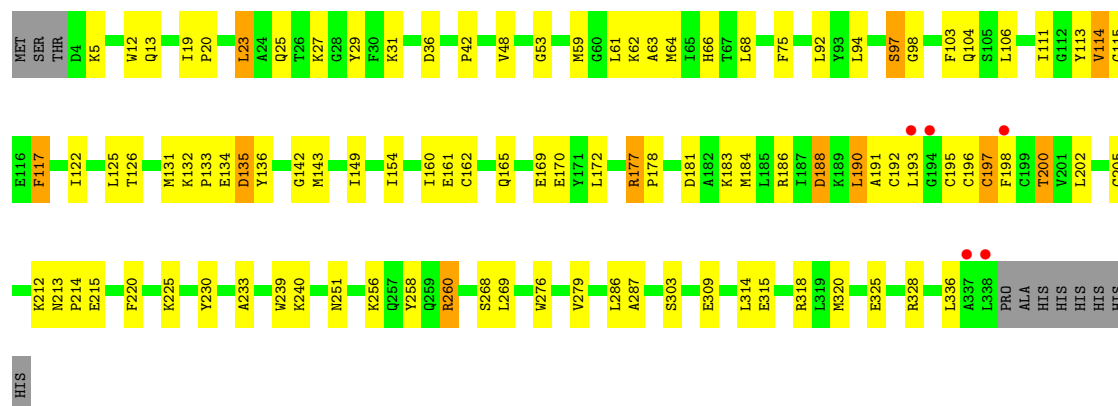


- Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5

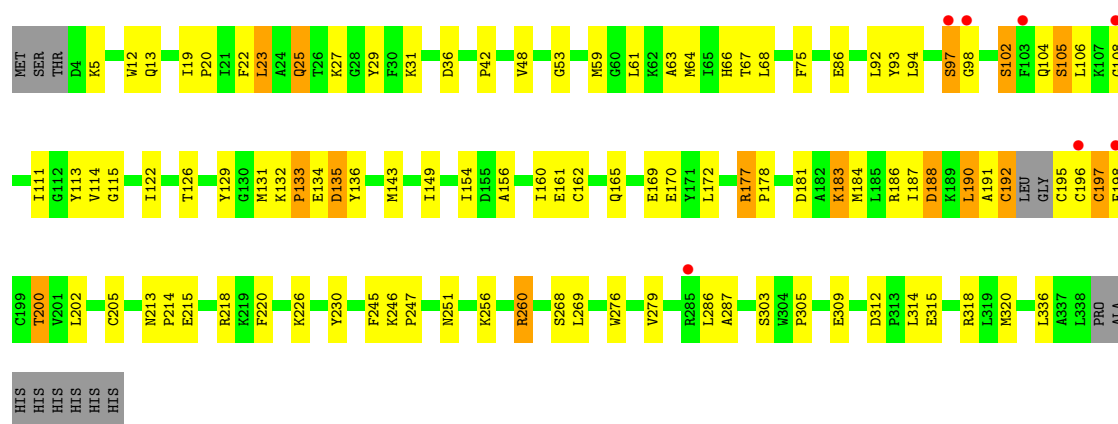




• Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5

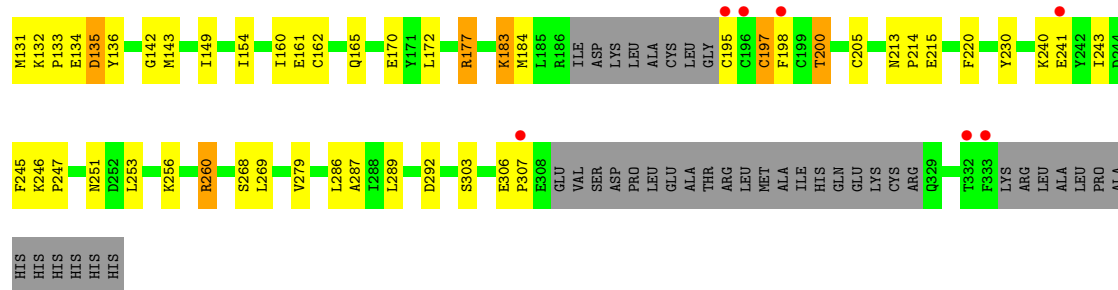


• Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5



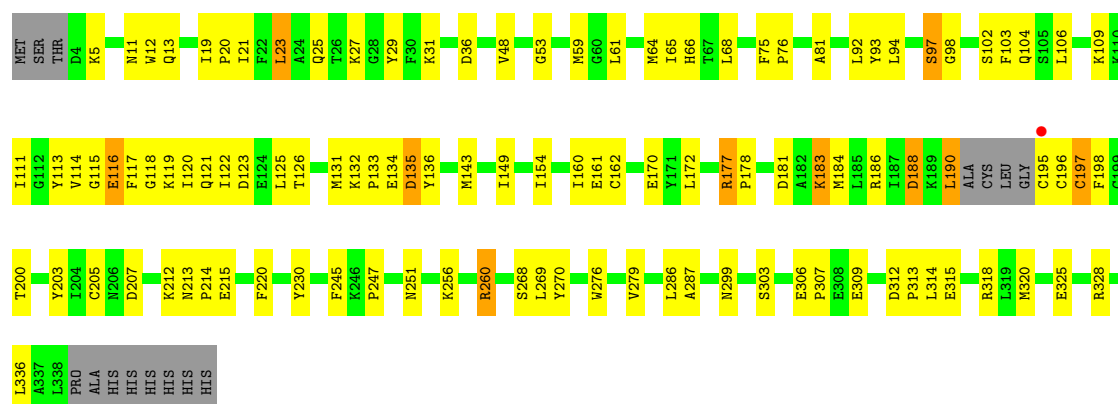
• Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5





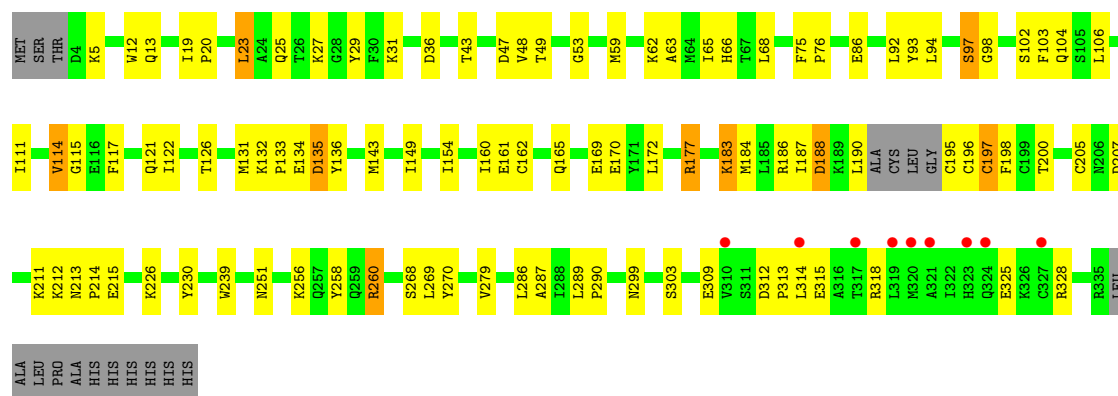
• Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5

Chain G: 64% 29%



• Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5

Chain H: 3% 66% 27% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.48Å 191.84Å 101.89Å 90.00° 112.72° 90.00°	Depositor
Resolution (Å)	19.92 – 2.90 19.92 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.92-2.90) 99.0 (19.92-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_353)	Depositor
R, R_{free}	0.221 , 0.263 0.220 , 0.261	Depositor DCC
R_{free} test set	3091 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.496	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.049 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20876	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.87% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PLP

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	0.70	2/2563 (0.1%)	0.90	5/3458 (0.1%)
1	B	0.64	0/2695	0.88	8/3637 (0.2%)
1	C	0.59	0/2736	0.88	4/3693 (0.1%)
1	D	0.58	0/2723	0.87	8/3674 (0.2%)
1	E	0.65	1/2475 (0.0%)	0.87	8/3340 (0.2%)
1	F	0.62	0/2704	0.87	7/3648 (0.2%)
1	G	0.62	1/2712 (0.0%)	0.89	7/3659 (0.2%)
1	H	0.56	0/2691	0.86	6/3630 (0.2%)
All	All	0.62	4/21299 (0.0%)	0.88	53/28739 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	120	ILE	CA-CB	-5.57	1.47	1.54
1	E	114	VAL	CA-CB	-5.51	1.47	1.54
1	A	114	VAL	CA-CB	-5.50	1.47	1.54
1	A	114	VAL	C-O	-5.39	1.18	1.24

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	VAL	N-CA-C	11.13	120.99	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	114	VAL	N-CA-C	9.62	119.58	110.53
1	G	115	GLY	N-CA-C	9.12	134.79	113.18
1	B	114	VAL	N-CA-C	8.52	118.43	110.42
1	C	114	VAL	N-CA-C	8.48	118.50	110.53

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	133	PRO	Mainchain,Peptide

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	2505	0	2525	72	0
1	B	2634	0	2652	61	0
1	C	2674	0	2703	72	0
1	D	2662	0	2688	71	1
1	E	2417	0	2422	68	1
1	F	2643	0	2667	68	2
1	G	2651	0	2678	74	0
1	H	2630	0	2649	72	0
2	A	15	0	6	13	0
2	B	15	0	6	4	0
2	E	15	0	6	6	0
2	H	15	0	6	3	0
All	All	20876	0	21008	545	2

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 13.

The worst 5 of 545 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:C:125:LEU:HD13	1:C:190:LEU:HD11	1.37	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:177:ARG:HH11	1:H:177:ARG:HG2	1.25	1.02
1:A:177:ARG:HH11	1:A:177:ARG:HG2	1.22	1.00
1:E:177:ARG:HG2	1:E:177:ARG:HH11	1.25	0.99
1:F:177:ARG:HG2	1:F:177:ARG:HH11	1.28	0.98

All (2) 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:F:218:ARG:NH1	1:E:292:ASP:OD2[1_455]	2.05	0.15
1:F:96:GLY:O	1:D:108:GLY:CA[2_656]	2.17	0.03

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	306/346 (88%)	298 (97%)	7 (2%)	1 (0%)	36	65
1	B	325/346 (94%)	314 (97%)	11 (3%)	0	100	100
1	C	333/346 (96%)	325 (98%)	8 (2%)	0	100	100
1	D	329/346 (95%)	317 (96%)	12 (4%)	0	100	100
1	E	296/346 (86%)	288 (97%)	7 (2%)	1 (0%)	36	65
1	F	326/346 (94%)	318 (98%)	8 (2%)	0	100	100
1	G	327/346 (94%)	317 (97%)	10 (3%)	0	100	100
1	H	324/346 (94%)	313 (97%)	9 (3%)	2 (1%)	21	51
All	All	2566/2768 (93%)	2490 (97%)	72 (3%)	4 (0%)	43	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	GLY
1	H	115	GLY
1	H	103	PHE
1	E	115	GLY

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	270/299 (90%)	255 (94%)	15 (6%)	19	50
1	B	285/299 (95%)	267 (94%)	18 (6%)	16	45
1	C	289/299 (97%)	269 (93%)	20 (7%)	14	41
1	D	288/299 (96%)	267 (93%)	21 (7%)	13	38
1	E	261/299 (87%)	248 (95%)	13 (5%)	22	53
1	F	286/299 (96%)	268 (94%)	18 (6%)	16	45
1	G	287/299 (96%)	267 (93%)	20 (7%)	14	40
1	H	285/299 (95%)	267 (94%)	18 (6%)	16	45
All	All	2251/2392 (94%)	2108 (94%)	143 (6%)	16	44

5 of 143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	190	LEU
1	G	251	ASN
1	H	170	GLU
1	B	309	GLU
1	B	303	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	66	HIS
1	G	66	HIS

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Mol	Chain	Res	Type
1	G	248	GLN
1	C	248	GLN
1	A	11	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](#)

4 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	PLP	E	400	1	15,15,16	1.73	2 (13%)	21,22,23	2.08	7 (33%)
2	PLP	A	400	1	15,15,16	1.87	1 (6%)	21,22,23	3.50	5 (23%)
2	PLP	B	400	1	15,15,16	1.98	3 (20%)	21,22,23	1.88	4 (19%)
2	PLP	H	400	1	15,15,16	1.83	3 (20%)	21,22,23	1.96	5 (23%)

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	PLP	E	400	1	-	3/6/6/8	0/1/1/1
2	PLP	A	400	1	-	4/6/6/8	0/1/1/1
2	PLP	B	400	1	-	5/6/6/8	0/1/1/1
2	PLP	H	400	1	-	3/6/6/8	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	PLP	O3-C3	-6.12	1.22	1.36
2	B	400	PLP	O3-C3	-5.81	1.23	1.36
2	H	400	PLP	O3-C3	-5.60	1.24	1.36
2	E	400	PLP	O3-C3	-5.15	1.25	1.36
2	B	400	PLP	C2-N1	2.77	1.38	1.33

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	PLP	O4P-C5A-C5	13.40	134.47	109.36
2	H	400	PLP	O4P-C5A-C5	6.97	122.42	109.36
2	B	400	PLP	O4P-C5A-C5	6.08	120.75	109.36
2	E	400	PLP	O4P-C5A-C5	5.63	119.90	109.36
2	A	400	PLP	C5A-C5-C6	-5.20	110.89	119.36

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	PLP	C4-C5-C5A-O4P
2	A	400	PLP	C6-C5-C5A-O4P
2	B	400	PLP	C4-C5-C5A-O4P
2	B	400	PLP	C5A-O4P-P-O1P
2	B	400	PLP	C5A-O4P-P-O2P

There are no ring outliers.

4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	400	PLP	6	0
2	A	400	PLP	13	0
2	B	400	PLP	4	0
2	H	400	PLP	3	0

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 [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	314/346 (90%)	-0.04	9 (2%) 53 45	25, 52, 96, 128	0
1	B	329/346 (95%)	-0.05	0 100 100	33, 54, 97, 125	0
1	C	335/346 (96%)	-0.11	5 (1%) 72 64	33, 55, 101, 143	0
1	D	333/346 (96%)	0.02	7 (2%) 63 54	30, 55, 100, 128	0
1	E	302/346 (87%)	-0.07	7 (2%) 61 52	30, 52, 94, 130	0
1	F	330/346 (95%)	-0.09	4 (1%) 76 69	29, 53, 99, 127	0
1	G	331/346 (95%)	-0.16	1 (0%) 90 87	33, 56, 100, 130	0
1	H	328/346 (94%)	0.08	9 (2%) 56 47	34, 57, 102, 130	0
All	All	2602/2768 (94%)	-0.05	42 (1%) 70 62	25, 54, 100, 143	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	320	MET	5.3
1	H	324	GLN	4.8
1	A	320	MET	4.6
1	A	314	LEU	4.5
1	H	310	VAL	3.4

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
2	PLP	H	400	15/16	0.91	0.07	41,54,63,77	0
2	PLP	B	400	15/16	0.95	0.07	26,47,58,68	0
2	PLP	E	400	15/16	0.96	0.06	28,35,53,54	0
2	PLP	A	400	15/16	0.96	0.05	22,32,54,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.