WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Sep 10, 2023 – 08:13 AM EDT

PDB ID	:	4H67
Title	:	Crystal structure of HMP synthase Thi5 from S. cerevisiae
Authors	:	Coquille, S.C.; Roux, C.; Fitzpatrick, T.; Thore, S.
Deposited on	:	2012-09-19
Resolution	:	2.70 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

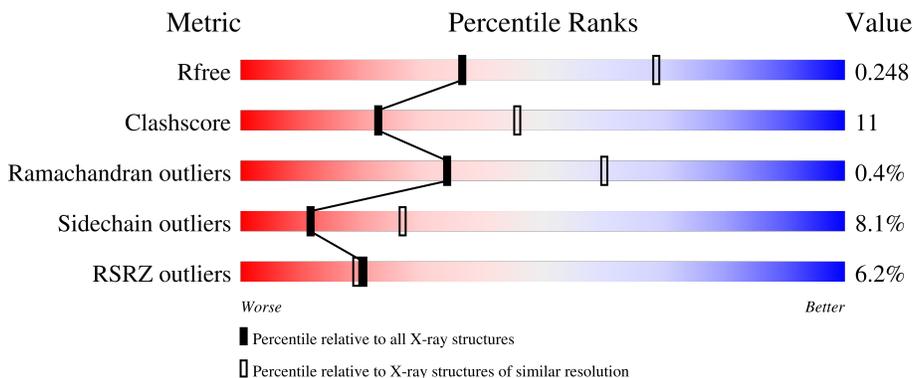|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.70 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	Percentile Ranks	Value
Rfree		0.248
Clashscore		11
Ramachandran outliers		0.4%
Sidechain outliers		8.1%
RSRZ outliers		6.2%

Worse ... *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	3% ... 73% ... 21% .. .
1	B	346	5% ... 69% ... 16% .. . 11%
1	C	346	8% ... 71% ... 23% ...
1	D	346	4% ... 74% ... 19% ...
1	E	346	5% ... 68% ... 17% .. 12%

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Mol	Chain	Length	Quality of chain
1	F	346	6% · · · · · · · 73% · · · · · · 20% · ·
1	G	346	6% · · · · · · · 71% · · · · · · 19% · · 6%
1	H	346	9% · · · · · · · 68% · · · · · · 16% · · 12%

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	SO4	A	403	-	-	X	-
2	SO4	C	406	-	-	X	-
2	SO4	D	403	-	-	X	-
2	SO4	G	402	-	-	X	-
2	SO4	H	401	-	-	X	-

2   Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 20928 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	A	337	Total	C	N	O	S	0	0	0
			2701	1741	450	494	16			
1	B	307	Total	C	N	O	S	0	0	0
			2457	1592	399	452	14			
1	C	338	Total	C	N	O	S	0	0	0
			2696	1736	449	494	17			
1	D	335	Total	C	N	O	S	0	0	0
			2668	1720	438	492	18			
1	E	305	Total	C	N	O	S	0	0	0
			2440	1580	396	449	15			
1	F	335	Total	C	N	O	S	0	0	0
			2668	1720	438	492	18			
1	G	326	Total	C	N	O	S	0	0	0
			2609	1682	428	483	16			
1	H	305	Total	C	N	O	S	0	0	0
			2440	1580	396	450	14			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	240	SER	LYS	engineered mutation	UNP P43534
A	241	GLY	GLU	engineered mutation	UNP P43534
A	317	THR	GLN	engineered mutation	UNP P43534
A	341	HIS	-	expression tag	UNP P43534
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	240	SER	LYS	engineered mutation	UNP P43534
B	241	GLY	GLU	engineered mutation	UNP P43534
B	317	THR	GLN	engineered mutation	UNP P43534
B	341	HIS	-	expression tag	UNP P43534

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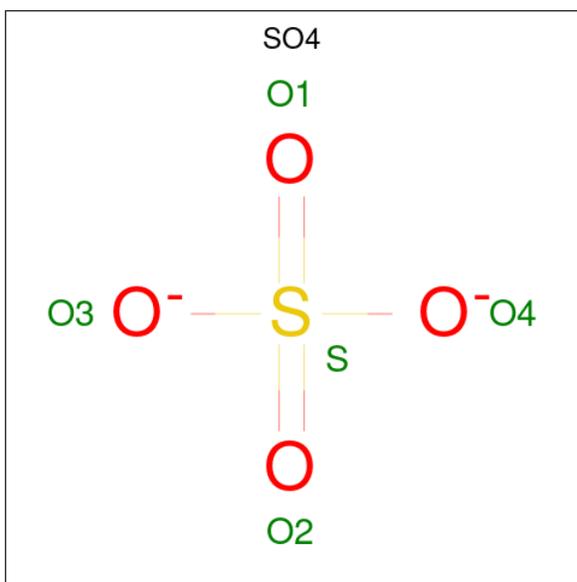
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Chain	Residue	Modelled	Actual	Comment	Reference
B	342	HIS	-	expression tag	UNP P43534
B	343	HIS	-	expression tag	UNP P43534
B	344	HIS	-	expression tag	UNP P43534
B	345	HIS	-	expression tag	UNP P43534
B	346	HIS	-	expression tag	UNP P43534
C	240	SER	LYS	engineered mutation	UNP P43534
C	241	GLY	GLU	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	240	SER	LYS	engineered mutation	UNP P43534
D	241	GLY	GLU	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	240	SER	LYS	engineered mutation	UNP P43534
E	241	GLY	GLU	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
F	240	SER	LYS	engineered mutation	UNP P43534
F	241	GLY	GLU	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
G	240	SER	LYS	engineered mutation	UNP P43534

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Chain	Residue	Modelled	Actual	Comment	Reference
G	241	GLY	GLU	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	240	SER	LYS	engineered mutation	UNP P43534
H	241	GLY	GLU	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 SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	D	1	Total 5	O 4	S 1	0	0
2	D	1	Total 5	O 4	S 1	0	0
2	D	1	Total 5	O 4	S 1	0	0
2	E	1	Total 5	O 4	S 1	0	0
2	F	1	Total 5	O 4	S 1	0	0
2	G	1	Total 5	O 4	S 1	0	0
2	G	1	Total 5	O 4	S 1	0	0
2	H	1	Total 5	O 4	S 1	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).

PLP
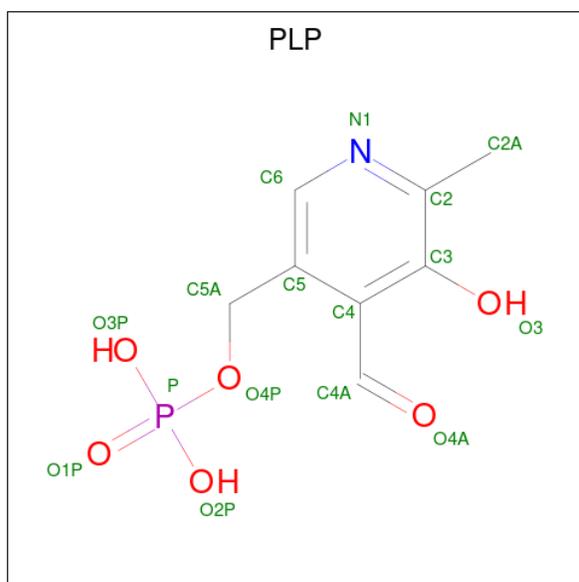
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 15	C 8	N 1	O 5	P 1	0	0

- Molecule 4 is water.

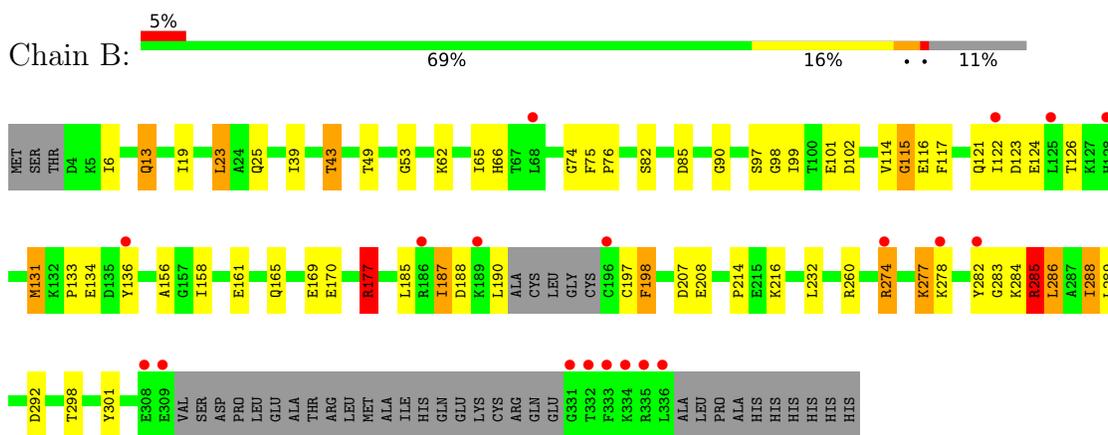| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total 31	O 31	0	0
4	B	20	Total 20	O 20	0	0
4	C	25	Total 25	O 25	0	0
4	D	15	Total 15	O 15	0	0
4	E	14	Total 14	O 14	0	0
4	F	14	Total 14	O 14	0	0
4	G	13	Total 13	O 13	0	0
4	H	17	Total 17	O 17	0	0

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.
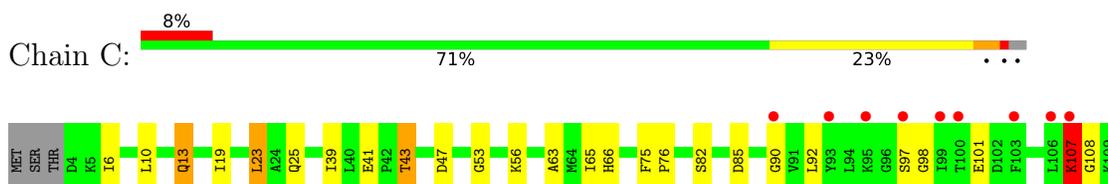
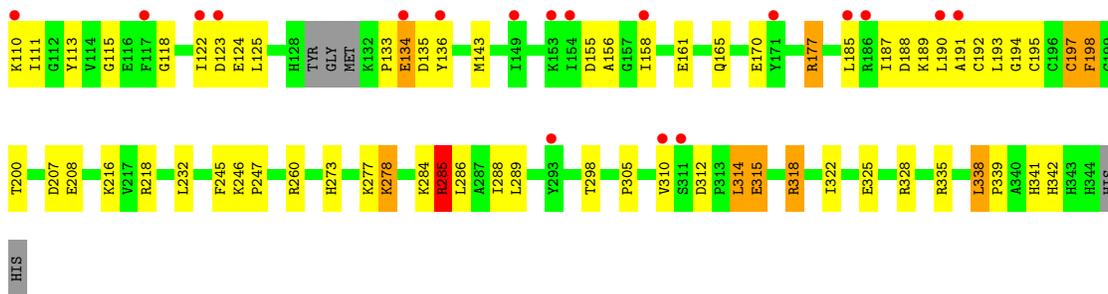• Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5

Chain A:

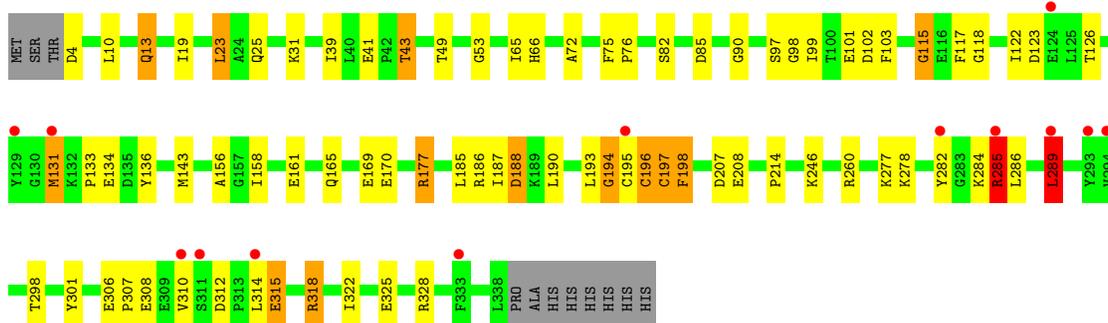• Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5

Chain B:

• Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5

Chain C:

K110 I111 G112 Y113 V114 G115 E116 F117 G118 I122 D123 E124 L125 H128 TYR GLY MET K132 P133 E134 D135 Y136 M143 I149 K153 I154 D155 A156 G157 I158 E161 Q165 E170 Y171 R177 L185 R186 I187 D188 K189 L190 A191 C192 L193 G194 C195 C196 C197 F198 C199

T200 D207 E208 K216 V217 R218 L232 F245 K246 P247 R260 H273 K277 K278 K284 R285 L286 A287 I288 L289 Y293 T298 P305 V310 S311 D312 P313 L314 E315 R318 I322 E325 R328 R335 L338 P339 A340 H341 H342 H343 H344 HIS

HIS

• Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5

Chain D:

4%

74% 19% • • •

MET SER THR D4 L10 Q13 I19 L23 A24 Q25 K31 I39 L40 E41 P42 T43 T49 G53 I65 H66 A72 F75 P76 S82 D85 G90 S97 G98 I99 T100 E101 D102 F103 G115 E116 F117 G118 I122 D123 E124 L125 T126

Y129 G130 M131 K132 P133 E134 D135 Y136 M143 A156 G157 I158 E161 Q165 E169 E170 R177 L185 R186 I187 D188 K189 L190 L193 G194 C195 C196 C197 F198 D207 E208 P214 K246 R260 K277 K278 Y282 G283 K284 R285 L286 L289 Y293 V294

T298 Y301 E306 P307 E308 E309 V310 S311 D312 P313 L314 E315 R318 I322 E325 R328 F333 L338 PRO ALA HIS HIS HIS HIS HIS HIS

• Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5

Chain E:

5%

68% 17% • • 12%

MET SER T3 D4 K5 I6 L10 Q13 I19 L23 A24 Q25 I39 L40 E41 P42 T43 G53 I65 F75 P76 S82 D85 G90 S97 G98 I99 T100 E101 D102 G115 E116 F117 G118 K119 I120 Q121 I122 D123 E124 L125 T126 Y129 G130 M131 K132

P133 E134 D135 Y136 A156 G157 I158 E161 Q165 E170 R177 L185 R186 I187 D188 LYS ALA CYS LEU GLY C195 C196 C197 F198 D207 E208 P214 E215 K216 K225 L232 K246 R260 Y270 K277 K284 R285 L286 A287 I288 L289 D292

T298 Y301 W304 P305 E306 P307 E308 GLU VAL SER ASP PRO LEU GLU ALA THR ARG LEU MET ALA ILE HIS GLN GLU LYS CYS ARG GLN GLU GLY T332 F333 K334 R335 L336 ALA LEU PRO ALA HIS HIS HIS HIS HIS HIS

• Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5

Chain F:

6%

73% 20% • •

MET SER THR D4 K5 I6 Q13 I19 L23 A24 Q25 I39 T43 G53 I65 H66 F75 P76 S82 D85 G90 S97 G98 I99 T100 E101 D102 F103 Q104 V114 G115 E116 F117 G118 K119 I120 Q121 I122 D123 E124 L125 T126 K127 H128 M131 K132

P133 E134 D135 Y136 M143 K153 A156 G157 I158 E161 Q165 E170 R177 L185 R186 I187 D188 K189 L190 A191 C192 L193 G194 C195 C196 C197 F198 D207 E208 P214 E215 K216 L232 K246 Y270 K277 K278 Y282 G283 K284 R285 L286 A287 I288 L289
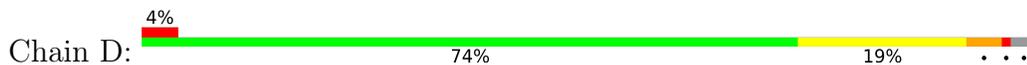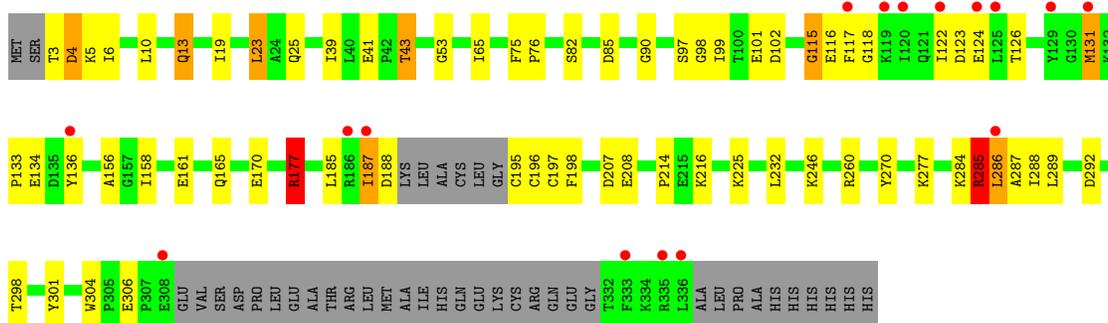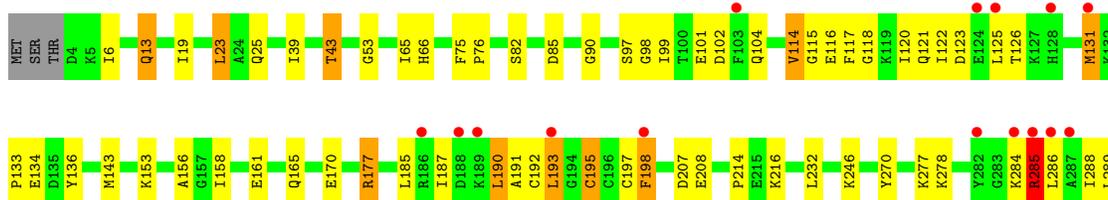
• Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5

Chain G:

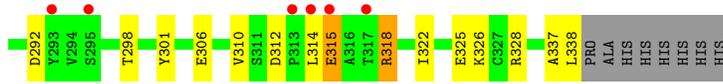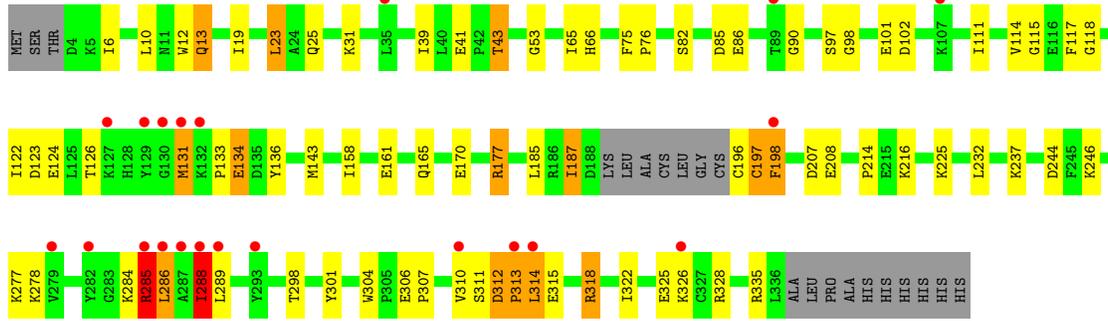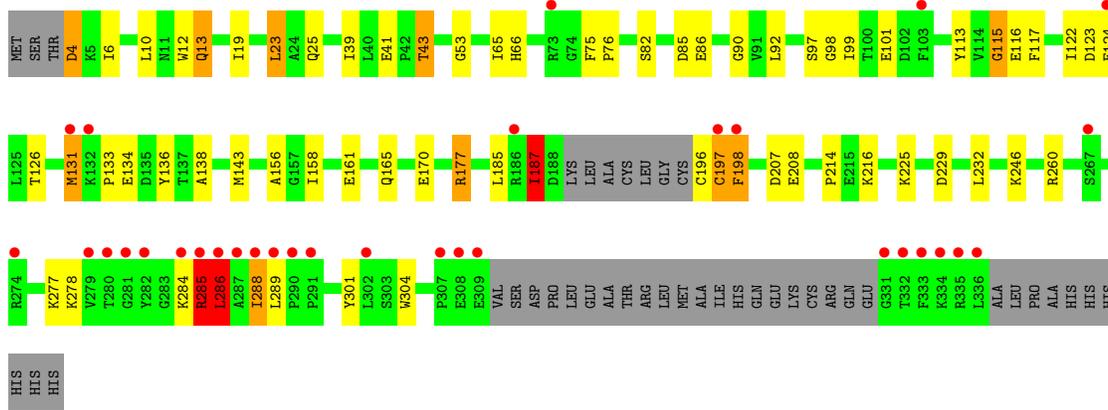• Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5

Chain H:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.79Å 188.46Å 101.67Å 90.00° 112.51° 90.00°	Depositor
Resolution (Å)	49.14 – 2.70 49.14 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.3 (49.14-2.70) 95.3 (49.14-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.207 , 0.247 0.207 , 0.248	Depositor DCC
R_{free} test set	2010 reflections (2.81%)	wwPDB-VP
Wilson B-factor (Å^2)	62.4	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 59.0	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.064 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20928	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, 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	0.65	1/2768 (0.0%)	0.69	1/3739 (0.0%)
1	B	0.61	0/2515	0.89	6/3394 (0.2%)
1	C	0.60	0/2761	0.71	2/3730 (0.1%)
1	D	0.58	0/2730	0.70	3/3687 (0.1%)
1	E	0.58	0/2498	0.70	2/3373 (0.1%)
1	F	0.55	0/2730	0.70	4/3687 (0.1%)
1	G	0.57	0/2670	0.69	2/3605 (0.1%)
1	H	0.58	0/2498	0.67	2/3372 (0.1%)
All	All	0.59	1/21170 (0.0%)	0.72	22/28587 (0.1%)

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	G	0	1
1	H	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	CYS	CB-SG	-6.62	1.71	1.82

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	274	ARG	NE-CZ-NH1	-23.03	108.79	120.30
1	B	274	ARG	NE-CZ-NH2	21.24	130.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	274	ARG	CD-NE-CZ	11.09	139.12	123.60
1	F	115	GLY	N-CA-C	9.30	136.36	113.10
1	B	285	ARG	NE-CZ-NH1	7.39	124.00	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	288	ILE	Peptide
1	H	187	ILE	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	2701	0	2699	75	3
1	B	2457	0	2466	51	0
1	C	2696	0	2702	85	1
1	D	2668	0	2684	71	1
1	E	2440	0	2446	49	1
1	F	2668	0	2684	59	0
1	G	2609	0	2614	65	0
1	H	2440	0	2444	45	0
2	A	15	0	0	3	0
2	C	30	0	0	6	0
2	D	15	0	0	3	0
2	E	5	0	0	1	0
2	F	5	0	0	1	0
2	G	10	0	0	3	0
2	H	5	0	0	2	0
3	B	15	0	6	5	0
4	A	31	0	0	1	0
4	B	20	0	0	2	0
4	C	25	0	0	5	0
4	D	15	0	0	1	0
4	E	14	0	0	0	0
4	F	14	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	13	0	0	1	0
4	H	17	0	0	3	0
All	All	20928	0	20745	477	3

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 11.

The worst 5 of 477 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:312:ASP:HB3	1:A:315:GLU:CB	1.64	1.27
1:A:274:ARG:NH2	1:A:310:VAL:HG11	1.58	1.16
1:D:118:GLY:N	2:D:403:SO4:O4	1.77	1.15
1:C:193:LEU:CG	1:C:194:GLY:H	1.55	1.13
1:C:115:GLY:N	2:C:406:SO4:O2	1.82	1.10

All (3) 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:285:ARG:NH1	1:D:314:LEU:CD2[1_455]	1.41	0.79
1:A:218:ARG:NH1	1:E:292:ASP:OD2[1_455]	1.94	0.26
1:A:96:GLY:O	1:C:107:LYS:O[2_656]	2.11	0.09

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	333/346 (96%)	324 (97%)	8 (2%)	1 (0%)	41	66
1	B	301/346 (87%)	290 (96%)	9 (3%)	2 (1%)	22	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	334/346 (96%)	320 (96%)	14 (4%)	0	100	100
1	D	333/346 (96%)	323 (97%)	9 (3%)	1 (0%)	41	66
1	E	299/346 (86%)	290 (97%)	7 (2%)	2 (1%)	22	46
1	F	333/346 (96%)	322 (97%)	11 (3%)	0	100	100
1	G	322/346 (93%)	312 (97%)	7 (2%)	3 (1%)	17	40
1	H	299/346 (86%)	286 (96%)	11 (4%)	2 (1%)	22	46
All	All	2554/2768 (92%)	2467 (97%)	76 (3%)	11 (0%)	34	60

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	GLY
1	B	115	GLY
1	E	115	GLY
1	B	187	ILE
1	G	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	291/298 (98%)	265 (91%)	26 (9%)	9	22
1	B	265/298 (89%)	246 (93%)	19 (7%)	14	34
1	C	291/298 (98%)	266 (91%)	25 (9%)	10	24
1	D	288/298 (97%)	264 (92%)	24 (8%)	11	25
1	E	264/298 (89%)	246 (93%)	18 (7%)	16	36
1	F	288/298 (97%)	265 (92%)	23 (8%)	12	27
1	G	282/298 (95%)	256 (91%)	26 (9%)	9	21
1	H	263/298 (88%)	244 (93%)	19 (7%)	14	34
All	All	2232/2384 (94%)	2052 (92%)	180 (8%)	11	27

5 of 180 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	43	THR
1	G	134	GLU
1	F	131	MET
1	F	286	LEU
1	G	277	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	66	HIS
1	D	66	HIS
1	H	66	HIS

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

18 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	SO4	C	402	-	4,4,4	0.12	0	6,6,6	0.28	0
2	SO4	H	401	-	4,4,4	1.90	1 (25%)	6,6,6	0.93	0
3	PLP	B	400	1	15,15,16	1.88	4 (26%)	20,22,23	2.21	6 (30%)
2	SO4	F	401	-	4,4,4	0.64	0	6,6,6	0.61	0
2	SO4	D	401	-	4,4,4	0.14	0	6,6,6	0.29	0
2	SO4	A	402	-	4,4,4	0.21	0	6,6,6	0.37	0
2	SO4	A	403	-	4,4,4	0.61	0	6,6,6	0.55	0
2	SO4	A	401	-	4,4,4	0.10	0	6,6,6	0.64	0
2	SO4	C	401	-	4,4,4	0.23	0	6,6,6	0.61	0
2	SO4	C	404	-	4,4,4	0.21	0	6,6,6	0.30	0
2	SO4	C	405	-	4,4,4	0.17	0	6,6,6	0.28	0
2	SO4	C	406	-	4,4,4	0.58	0	6,6,6	0.90	0
2	SO4	D	402	-	4,4,4	0.20	0	6,6,6	0.46	0
2	SO4	C	403	-	4,4,4	0.29	0	6,6,6	0.38	0
2	SO4	D	403	-	4,4,4	0.64	0	6,6,6	0.63	0
2	SO4	G	401	-	4,4,4	0.13	0	6,6,6	0.28	0
2	SO4	G	402	-	4,4,4	0.64	0	6,6,6	0.38	0
2	SO4	E	401	-	4,4,4	0.55	0	6,6,6	0.67	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	PLP	B	400	1	-	3/6/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	400	PLP	O3-C3	-5.17	1.25	1.37
3	B	400	PLP	C2-N1	2.56	1.38	1.33
2	H	401	SO4	O2-S	2.30	1.58	1.46
3	B	400	PLP	P-O3P	-2.14	1.46	1.54
3	B	400	PLP	C3-C4	2.08	1.44	1.40

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	400	PLP	C4A-C4-C5	-6.79	113.94	120.94
3	B	400	PLP	C4A-C4-C3	3.64	126.66	120.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	400	PLP	O3-C3-C4	2.44	124.54	118.10
3	B	400	PLP	C2A-C2-C3	2.31	123.75	120.89
3	B	400	PLP	O2P-P-O1P	2.27	119.56	110.68

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	400	PLP	C5A-O4P-P-O1P
3	B	400	PLP	C5A-O4P-P-O2P
3	B	400	PLP	C5A-O4P-P-O3P

There are no ring outliers.

11 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	402	SO4	1	0
2	H	401	SO4	2	0
3	B	400	PLP	5	0
2	F	401	SO4	1	0
2	A	403	SO4	3	0
2	C	404	SO4	1	0
2	C	406	SO4	4	0
2	D	403	SO4	3	0
2	G	401	SO4	1	0
2	G	402	SO4	2	0
2	E	401	SO4	1	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 ⓘ

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(Å²)	Q<0.9
1	A	337/346 (97%)	0.38	12 (3%)	42	42	41, 65, 118, 135	0
1	B	307/346 (88%)	0.43	19 (6%)	20	19	40, 64, 113, 138	0
1	C	338/346 (97%)	0.58	27 (7%)	12	10	43, 66, 123, 142	0
1	D	335/346 (96%)	0.24	13 (3%)	39	38	42, 65, 124, 135	0
1	E	305/346 (88%)	0.39	16 (5%)	27	25	41, 66, 113, 134	0
1	F	335/346 (96%)	0.38	21 (6%)	20	19	44, 67, 126, 144	0
1	G	326/346 (94%)	0.29	21 (6%)	19	18	40, 68, 126, 143	0
1	H	305/346 (88%)	0.53	32 (10%)	6	4	45, 68, 115, 136	0
All	All	2588/2768 (93%)	0.40	161 (6%)	20	19	40, 66, 122, 144	0

The worst 5 of 161 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	336	LEU	8.6
1	F	314	LEU	7.6
1	B	333	PHE	7.6
1	G	286	LEU	6.9
1	H	285	ARG	6.4

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 ⓘ

There are no monosaccharides in this entry.

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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	SO4	C	403	5/5	0.69	0.20	91,95,140,159	0
3	PLP	B	400	15/16	0.82	0.25	56,81,103,112	0
2	SO4	C	405	5/5	0.84	0.22	102,106,139,147	0
2	SO4	E	401	5/5	0.87	0.16	54,96,118,118	0
2	SO4	C	406	5/5	0.87	0.17	85,95,107,115	0
2	SO4	A	402	5/5	0.89	0.17	65,109,111,125	0
2	SO4	G	402	5/5	0.90	0.16	68,88,95,111	0
2	SO4	F	401	5/5	0.90	0.15	66,75,111,112	0
2	SO4	C	404	5/5	0.92	0.12	60,87,142,158	0
2	SO4	D	403	5/5	0.92	0.22	61,73,105,132	0
2	SO4	C	401	5/5	0.92	0.17	59,92,104,110	0
2	SO4	D	402	5/5	0.93	0.12	68,70,85,92	0
2	SO4	D	401	5/5	0.93	0.17	74,86,112,122	0
2	SO4	A	403	5/5	0.94	0.11	77,80,93,100	0
2	SO4	H	401	5/5	0.95	0.12	85,87,96,99	0
2	SO4	G	401	5/5	0.95	0.13	51,95,108,113	0
2	SO4	A	401	5/5	0.96	0.15	55,66,77,103	0
2	SO4	C	402	5/5	0.97	0.16	54,55,80,94	0

6.5 Other polymers (i)

There are no such residues in this entry.