



wwPDB X-ray Structure Validation Summary Report i

Mar 1, 2014 – 12:04 AM GMT

PDB ID : 1H5T
Title : THYMIDYLYLTRANSFERASECOMPLEXED WITH THYMIDYLYLDIPHOSPHATE-GLUCOSE
Authors : Rosano, C.; Zuccotti, S.; Bolognesi, M.
Deposited on : 2001-05-25
Resolution : 1.90 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

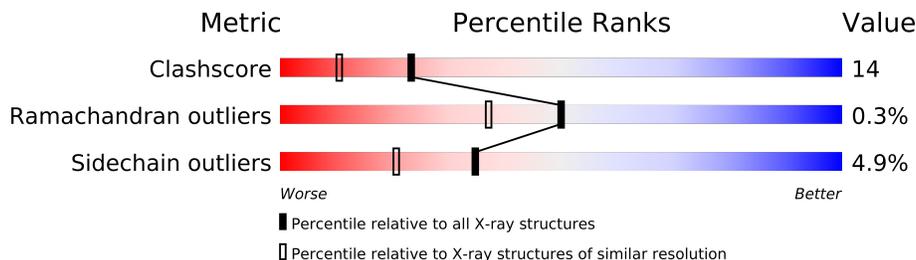
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.90 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))
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	293	
1	C	293	
1	D	293	
2	B	293	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9839 atoms, of which 0 are hydrogen and 0 are deuterium.

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 GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERAS E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	290	2277	1459	378	429	11	25	0	0
1	C	290	2269	1455	378	425	11	16	0	0
1	D	290	2273	1457	378	427	11	10	0	0

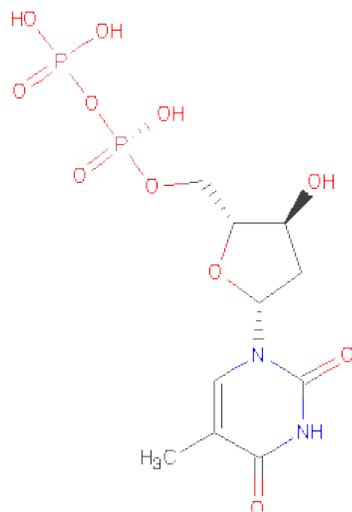
- Molecule 2 is a protein called GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERAS E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	290	2270	1455	378	428	9	18	0	0

There are 2 discrepancies between the modelled and reference sequences:

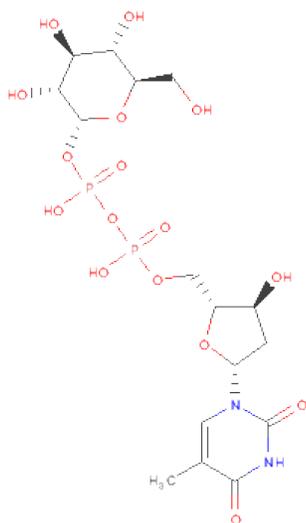
Chain	Residue	Modelled	Actual	Comment	Reference
B	217	LEU	MET	CONFLICT	UNP P37744
B	288	GLN	MET	CONFLICT	UNP P37744

- Molecule 3 is THYMIDINE-5'-DIPHOSPHATE (three-letter code: TYD) (formula: $C_{10}H_{16}N_2O_{11}P_2$).



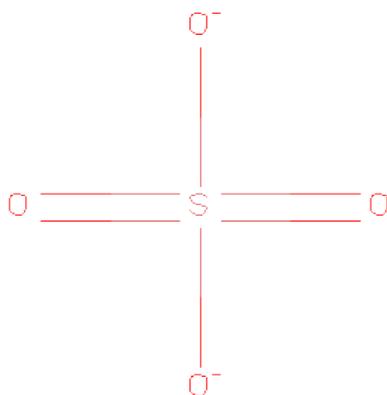
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			
3	A	1	Total	25	10	2	11	2	0	0
3	B	1	Total	25	10	2	11	2	0	0
3	C	1	Total	25	10	2	11	2	0	0
3	D	1	Total	25	10	2	11	2	0	0

- Molecule 4 is 2'-DEOXY-THYMIDINE-5'-DIPHOSPHO-ALPHA-D-GLUCOSE (three-letter code: DAU) (formula: C₁₆H₂₆N₂O₁₆P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	Total 36	C 16	N 2	O 16	P 2	0	0
4	B	1	Total 36	C 16	N 2	O 16	P 2	0	0
4	C	1	Total 36	C 16	N 2	O 16	P 2	0	0
4	D	1	Total 36	C 16	N 2	O 16	P 2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	146	Total 146	O 146	0	0
6	B	99	Total 99	O 99	0	0
6	C	119	Total 119	O 119	0	0
6	D	137	Total 137	O 137	0	0

3 Residue-property plots i

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

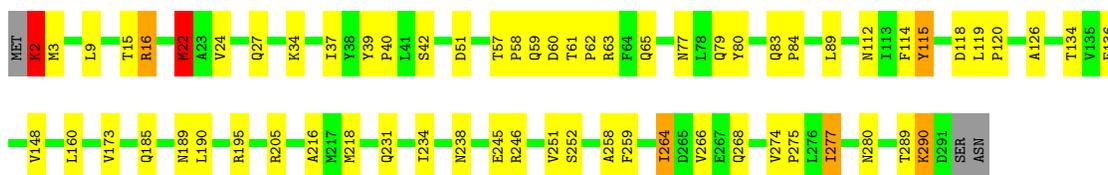
- Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain A:



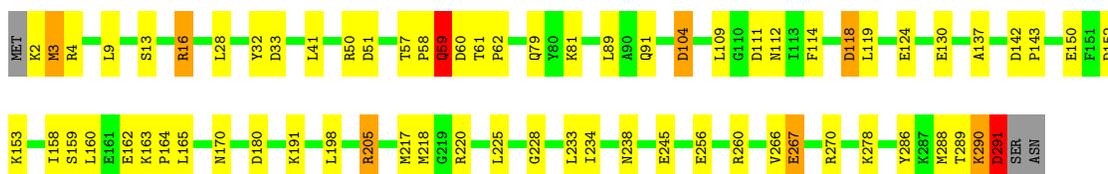
- Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain C:



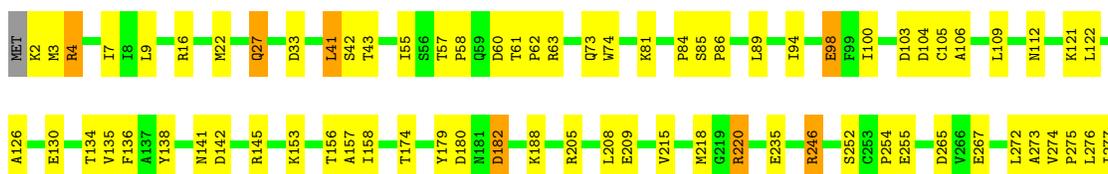
- Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain D:



- Molecule 2: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain B:



M280	L285	Q288	P293	K290	D291	SER	ASN
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4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.81Å 119.49Å 81.17Å 90.00° 112.67° 90.00°	Depositor
Resolution (Å)	12.00 – 1.90	Depositor
% Data completeness (in resolution range)	97.4 (12.00-1.90)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.174 , 0.224	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	9839	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

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: TYD, DAU, SO4

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	0.93	2/2324 (0.1%)	1.01	8/3145 (0.3%)
1	C	0.87	2/2316 (0.1%)	1.06	11/3134 (0.4%)
1	D	1.25	3/2320 (0.1%)	1.12	12/3140 (0.4%)
2	B	0.87	5/2317 (0.2%)	0.94	7/3138 (0.2%)
All	All	0.99	12/9277 (0.1%)	1.03	38/12557 (0.3%)

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	4
2	B	1	1
All	All	1	5

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	59	GLN	CG-CD	42.29	2.48	1.51
1	D	290	LYS	CA-CB	15.68	1.88	1.53
1	A	245	GLU	CG-CD	-15.36	1.28	1.51
1	C	290	LYS	CB-CG	12.06	1.85	1.52
2	B	291	ASP	N-CA	-11.12	1.24	1.46

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	59	GLN	CG-CD-NE2	-24.54	57.80	116.70
1	C	290	LYS	CB-CA-C	18.41	147.22	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	290	LYS	CA-CB-CG	-10.94	89.34	113.40
1	D	291	ASP	CB-CG-OD2	-9.01	110.19	118.30
1	C	290	LYS	CA-C-O	8.01	136.92	120.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	174	THR	CB

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	106	ALA	Mainchain
1	D	137	ALA	Mainchain
1	D	267	GLU	Mainchain
1	D	291	ASP	Sidechain
1	D	59	GLN	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2277	0	2284	65	0
1	C	2269	0	2275	70	0
1	D	2273	0	2280	67	0
2	B	2270	0	2271	71	0
3	A	25	0	13	0	0
3	B	25	0	13	0	0
3	C	25	0	13	0	0
3	D	25	0	13	0	0
4	A	36	0	16	2	0
4	B	36	0	16	1	0
4	C	36	0	16	2	0
4	D	36	0	16	1	0
5	D	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	146	0	0	12	1
6	B	99	0	0	8	1
6	C	119	0	0	5	1
6	D	137	0	0	14	1
All	All	9839	0	9226	265	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

The worst 5 of 265 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:112:ASN:ND2	1:C:114:PHE:CE1	1.74	1.55
1:D:217:MET:SD	1:D:217:MET:CE	2.01	1.46
2:B:142:ASP:OD2	2:B:145:ARG:NH1	1.67	1.27
1:A:63:ARG:CG	1:A:63:ARG:HH11	1.63	1.11
1:A:63:ARG:HH11	1:A:63:ARG:HG2	0.97	1.07

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	Distance(Å)	Clash(Å)
6:A:2056:HOH:O	6:C:2051:HOH:O[1_554]	2.12	0.08
6:B:2002:HOH:O	6:D:2133:HOH:O[2_747]	2.16	0.04

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	288/293 (98%)	284 (99%)	3 (1%)	1 (0%)	50	37
1	C	288/293 (98%)	284 (99%)	4 (1%)	0	100	100
1	D	288/293 (98%)	284 (99%)	2 (1%)	2 (1%)	30	15
2	B	288/293 (98%)	282 (98%)	6 (2%)	0	100	100
All	All	1152/1172 (98%)	1134 (98%)	15 (1%)	3 (0%)	50	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	D	32	TYR
1	D	124	GLU

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	244/247 (99%)	228 (93%)	16 (7%)	24	11
1	C	242/247 (98%)	229 (95%)	13 (5%)	31	17
1	D	243/247 (98%)	236 (97%)	7 (3%)	55	44
2	B	242/247 (98%)	230 (95%)	12 (5%)	34	20
All	All	971/988 (98%)	923 (95%)	48 (5%)	35	21

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	130	GLU
2	B	267	GLU
1	D	59	GLN
2	B	153	LYS
2	B	220	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	154	ASN
1	C	27	GLN
1	C	238	ASN
2	B	27	GLN
1	C	268	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

9 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$
3	TYD	A	1292	-	26,26,26	2.08	8 (30%)	35,40,40	2.08	5 (14%)
4	DAU	A	1293	-	26,28,38	4.18	6 (23%)	32,40,58	2.21	8 (25%)
3	TYD	B	1292	-	26,26,26	2.21	7 (26%)	35,40,40	2.06	6 (17%)
4	DAU	B	1293	-	26,28,38	4.31	6 (23%)	32,40,58	2.39	12 (37%)
3	TYD	C	1292	-	26,26,26	2.28	5 (19%)	35,40,40	1.48	3 (8%)
4	DAU	C	1293	-	26,28,38	4.43	6 (23%)	32,40,58	2.35	6 (18%)
3	TYD	D	1292	-	26,26,26	1.93	6 (23%)	35,40,40	2.23	6 (17%)
4	DAU	D	1293	1	26,28,38	4.28	6 (23%)	32,40,58	2.20	8 (25%)
5	SO4	D	1294	-	4,4,4	0.16	0	6,6,6	0.29	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	TYD	A	1292	-	-	0/13/28/28	0/2/2/2
4	DAU	A	1293	-	-	0/10/32/55	0/2/2/3
3	TYD	B	1292	-	-	0/13/28/28	0/2/2/2
4	DAU	B	1293	-	-	0/10/32/55	0/2/2/3
3	TYD	C	1292	-	-	0/13/28/28	0/2/2/2
4	DAU	C	1293	-	-	0/10/32/55	0/2/2/3
3	TYD	D	1292	-	-	0/13/28/28	0/2/2/2
4	DAU	D	1293	1	-	0/10/32/55	0/2/2/3
5	SO4	D	1294	-	-	0/0/0/0	0/0/0/0

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1293	DAU	P-O1P	20.77	1.70	1.46
4	B	1293	DAU	P-O1P	20.04	1.69	1.46
4	D	1293	DAU	P-O1P	19.96	1.69	1.46
4	A	1293	DAU	P-O1P	19.37	1.68	1.46
3	C	1292	TYD	PA-O3A	-5.99	1.49	1.59

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1292	TYD	C6-N1-C2	-8.76	119.92	122.41
4	A	1293	DAU	C51-C61-N11	-8.25	116.94	125.27
4	C	1293	DAU	C51-C61-N11	-8.24	116.96	125.27
3	D	1292	TYD	C6-N1-C2	-8.22	120.07	122.41
4	B	1293	DAU	C51-C61-N11	-8.18	117.02	125.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.