



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:33 PM GMT

PDB ID : 1G1L  
Title : THE STRUCTURAL BASIS OF THE CATALYTIC MECHANISM AND  
REGULATION OF GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE (RMLA). TDP-GLUCOSE COMPLEX.  
Authors : Blankenfeldt, W.; Asuncion, M.; Lam, J.S.; Naimsmith, J.H.  
Deposited on : 2000-10-12  
Resolution : 1.77 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

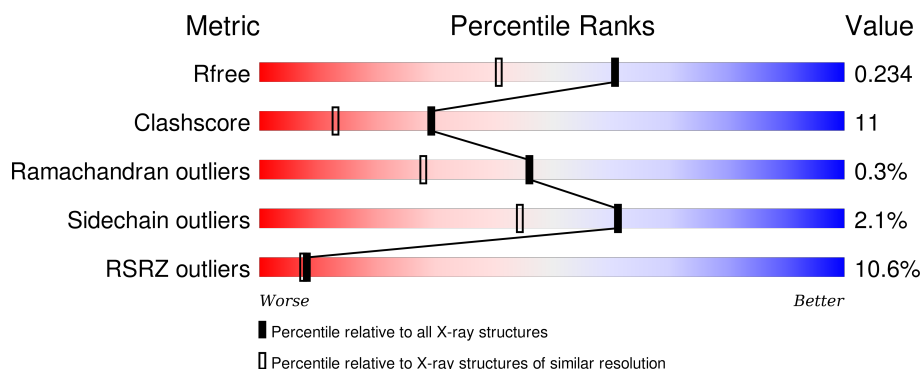
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.77 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))
$R_{free}$	91344	6655 (1.80-1.76)
Clashscore	102246	7658 (1.80-1.76)
Ramachandran outliers	100387	7570 (1.80-1.76)
Sidechain outliers	100360	7569 (1.80-1.76)
RSRZ outliers	91569	6671 (1.80-1.76)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	293	<div> <div>8%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
1	B	293	<div> <div>6%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
1	C	293	<div> <div>12%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
1	D	293	<div> <div>15%</div> <div>76%</div> <div>21%</div> <div>.</div> </div>
1	E	293	<div> <div>14%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	293	
1	G	293	
1	H	293	

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	3802	-	-	X	-
2	SO4	A	3817	-	-	-	X
2	SO4	A	3818	-	-	X	-
2	SO4	B	3701	-	-	X	-
2	SO4	B	3804	-	-	-	X
2	SO4	E	3810	-	-	X	-
2	SO4	G	3702	-	-	X	-
2	SO4	G	3813	-	-	-	X
2	SO4	H	3703	-	-	X	-
2	SO4	H	3814	-	-	-	X
2	SO4	H	3816	-	-	-	X
4	CIT	A	3800	-	-	-	X
4	CIT	A	3801	-	-	X	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22376 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 GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	9	0
			2361	1508	398	449	6			
1	B	293	Total	C	N	O	S	0	5	0
			2333	1489	395	442	7			
1	C	292	Total	C	N	O	S	0	6	0
			2335	1492	392	445	6			
1	D	292	Total	C	N	O	S	0	5	0
			2330	1487	397	440	6			
1	E	292	Total	C	N	O	S	0	5	0
			2320	1481	391	442	6			
1	F	293	Total	C	N	O	S	0	9	0
			2362	1508	395	452	7			
1	G	292	Total	C	N	O	S	0	6	0
			2334	1491	393	444	6			
1	H	292	Total	C	N	O	S	0	4	0
			2313	1477	390	440	6			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



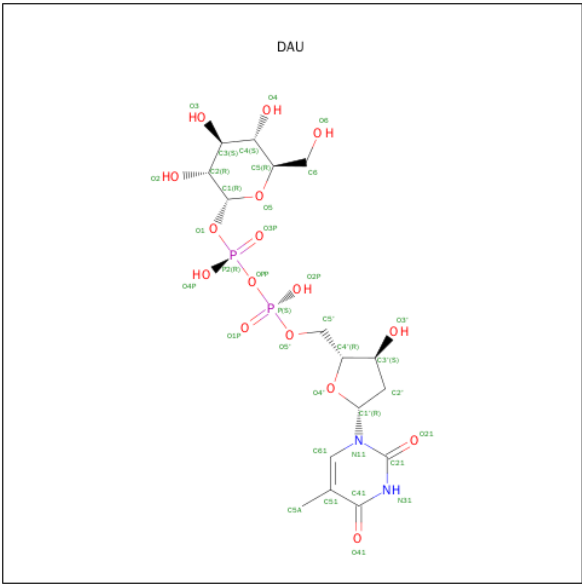
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total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

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

- Molecule 3 is 2'DEOXY-THYMIDINE-5'-DIPHOSPHO-ALPHA-D-GLUCOSE (three-letter code: DAU) (formula: C<sub>16</sub>H<sub>26</sub>N<sub>2</sub>O<sub>16</sub>P<sub>2</sub>).



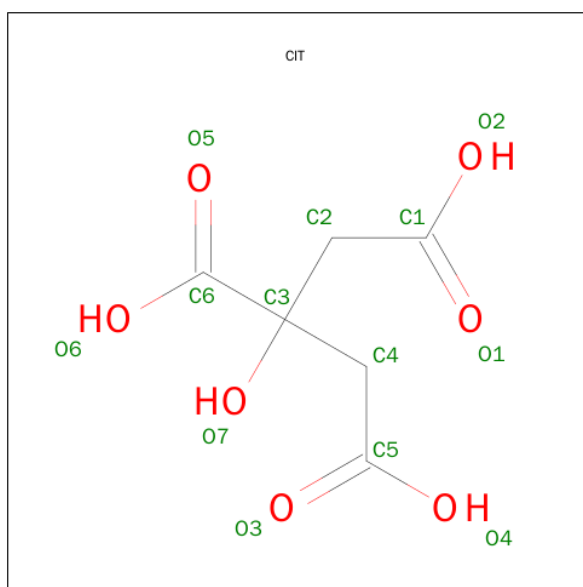
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O P	0	0
			36	16	2	16 2		
3	A	1	Total	C	N	O P	0	0
			36	16	2	16 2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	B	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	C	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	C	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	D	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	D	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	E	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	E	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	F	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	F	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	H	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	H	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	G	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	G	1	Total	C	N	O	P	0	0
			36	16	2	16	2		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		
4	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is water.

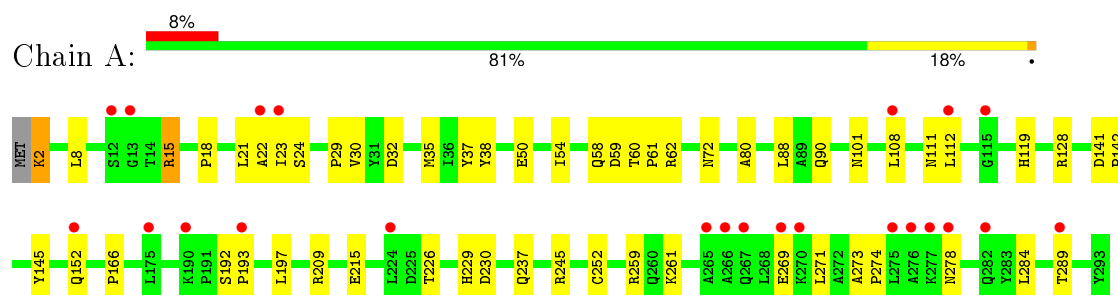
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	406	Total	O	0	0
			406	406		
5	B	414	Total	O	1	0
			414	414		
5	C	358	Total	O	0	0
			358	358		
5	D	309	Total	O	0	0
			309	309		
5	E	324	Total	O	0	0
			324	324		
5	F	325	Total	O	0	0
			325	325		
5	G	420	Total	O	0	0
			420	420		
5	H	415	Total	O	1	0
			415	415		



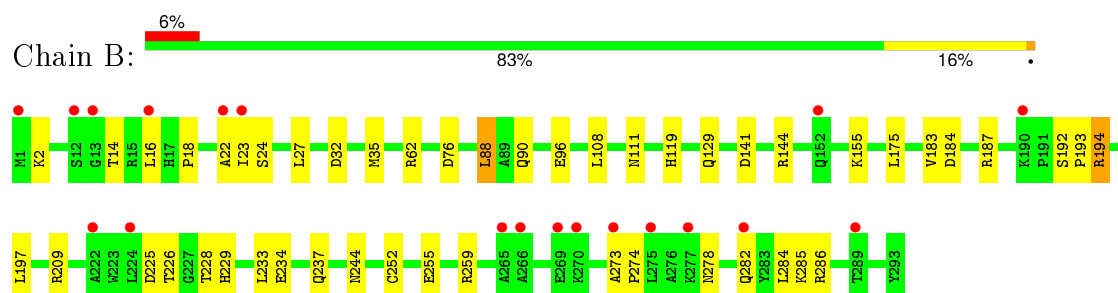
### 3 Residue-property plots [i](#)

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.

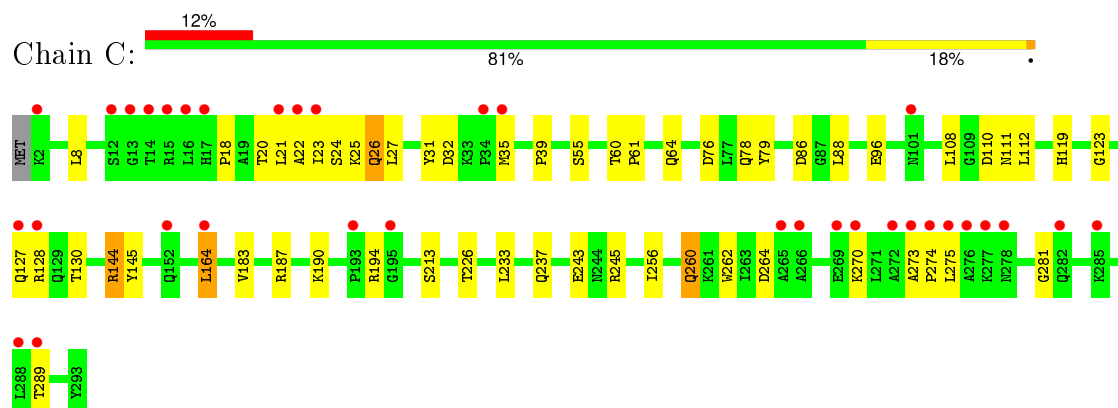
#### • Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE



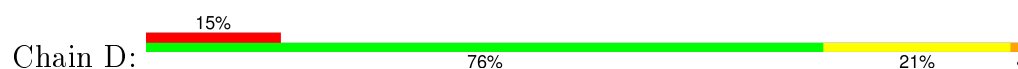
#### • Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE

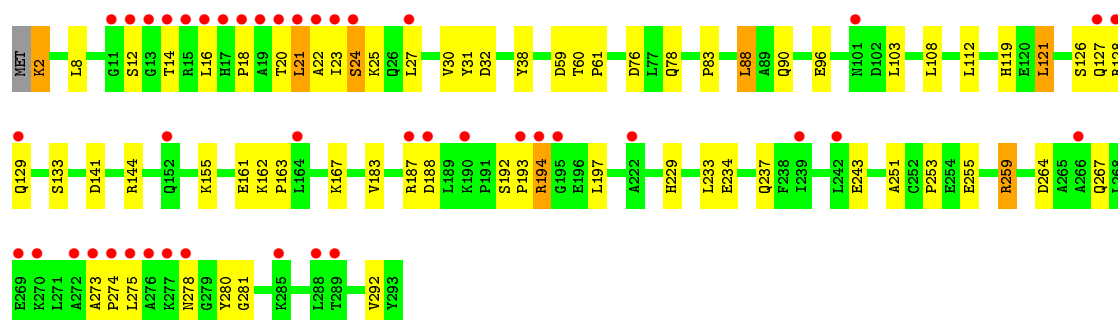


#### • Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE

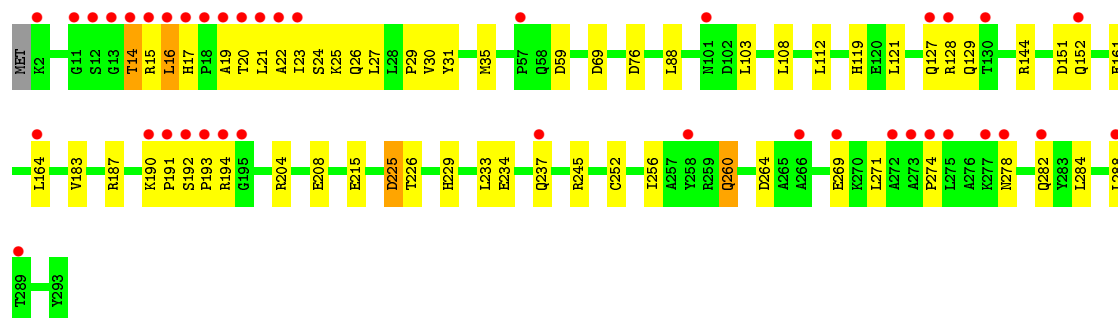
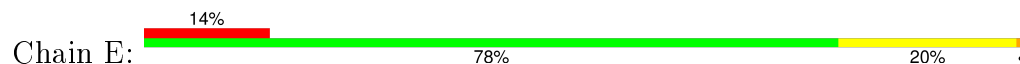


#### • Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE

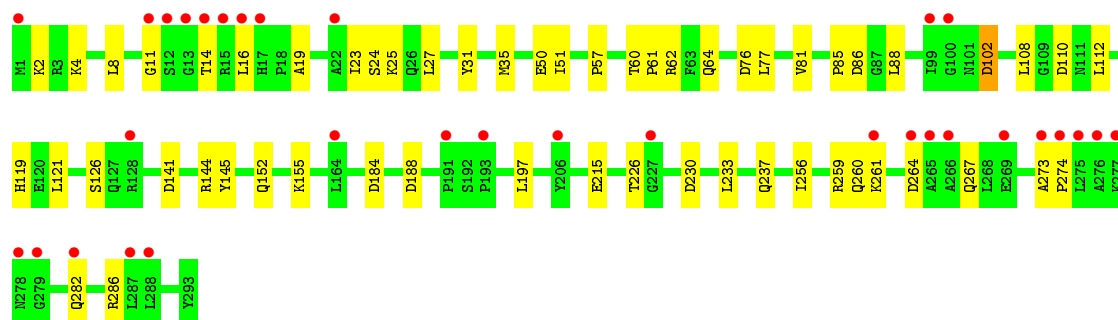
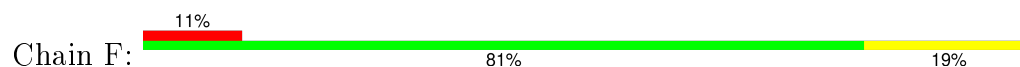




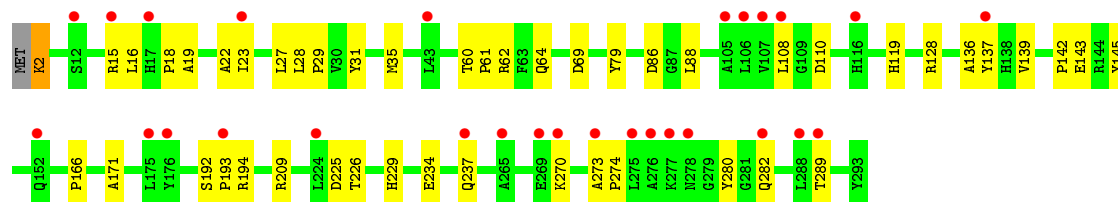
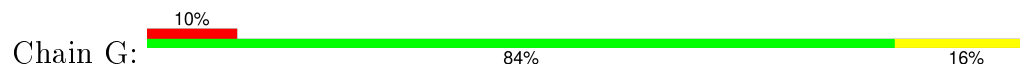
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE



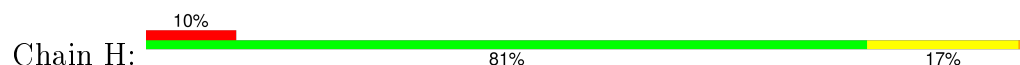
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

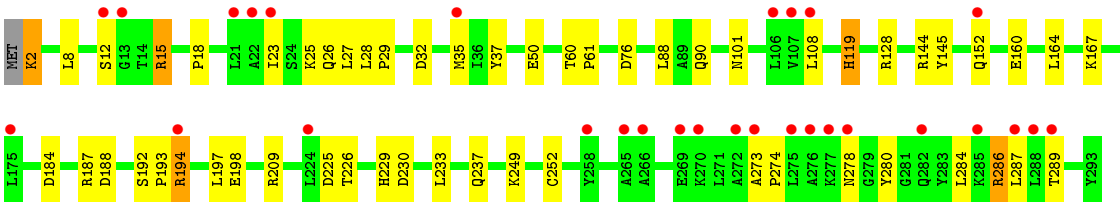


• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE



• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.58 Å   73.41 Å   134.29 Å 89.94°   80.61°   80.93°	Depositor
Resolution (Å)	40.64 – 1.77 40.64 – 1.77	Depositor EDS
% Data completeness (in resolution range)	93.3 (40.64-1.77) 93.9 (40.64-1.77)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 1.77 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.156   ,   0.215 0.181   ,   0.234	Depositor DCC
$R_{free}$ test set	12192 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.4	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 67.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 242338 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	22376	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: DAU, SO4, CIT

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	1.08	3/2413 (0.1%)	1.05	5/3274 (0.2%)
1	B	1.07	0/2383	1.06	9/3231 (0.3%)
1	C	1.02	1/2386 (0.0%)	1.00	3/3237 (0.1%)
1	D	1.03	1/2380 (0.0%)	1.11	13/3227 (0.4%)
1	E	0.96	0/2370	0.98	5/3215 (0.2%)
1	F	1.05	0/2413	1.05	9/3273 (0.3%)
1	G	1.10	3/2385 (0.1%)	1.05	7/3236 (0.2%)
1	H	1.07	2/2363 (0.1%)	1.05	8/3206 (0.2%)
All	All	1.05	10/19093 (0.1%)	1.04	59/25899 (0.2%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	37	TYR	CD1-CE1	6.24	1.48	1.39
1	C	55	SER	CB-OG	5.62	1.49	1.42
1	A	37	TYR	CD1-CE1	5.60	1.47	1.39
1	A	215	GLU	CD-OE1	5.36	1.31	1.25
1	A	128	ARG	CB-CG	-5.34	1.38	1.52

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	194	ARG	NE-CZ-NH2	-12.19	114.20	120.30
1	D	259[A]	ARG	NE-CZ-NH1	11.50	126.05	120.30
1	D	259[B]	ARG	NE-CZ-NH1	11.50	126.05	120.30
1	G	209	ARG	NE-CZ-NH2	-10.86	114.87	120.30
1	D	259[A]	ARG	NE-CZ-NH2	-10.77	114.92	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2361	0	2330	65	0
1	B	2333	0	2320	46	0
1	C	2335	0	2309	61	0
1	D	2330	0	2316	72	0
1	E	2320	0	2300	77	0
1	F	2362	0	2335	45	1
1	G	2334	0	2309	42	0
1	H	2313	0	2294	53	0
2	A	25	0	0	4	0
2	B	10	0	0	2	0
2	C	10	0	0	1	0
2	D	10	0	0	0	0
2	E	20	0	0	3	0
2	F	5	0	0	0	0
2	G	15	0	0	4	0
2	H	20	0	0	3	0
3	A	72	0	48	3	0
3	B	72	0	48	2	0
3	C	72	0	48	3	0
3	D	72	0	48	1	0
3	E	72	0	48	3	0
3	F	72	0	48	4	0
3	G	72	0	48	0	0
3	H	72	0	48	2	0
4	A	26	0	10	12	0
5	A	406	0	0	22	1
5	B	414	0	0	18	1
5	C	358	0	0	20	0
5	D	309	0	0	16	2
5	E	324	0	0	26	1
5	F	325	0	0	11	0
5	G	420	0	0	13	1
5	H	415	0	0	9	1
All	All	22376	0	18907	431	4

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 431 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)
4:A:3801:CIT:H22	5:A:4214:HOH:O	1.33	1.26
1:A:119[B]:HIS:ND1	5:A:4023:HOH:O	1.65	1.24
1:C:237[B]:GLN:NE2	1:D:237[B]:GLN:OE1	1.70	1.23
1:C:27:LEU:HD12	5:C:4073:HOH:O	1.51	1.10
1:A:101[B]:ASN:OD1	5:A:4055:HOH:O	1.69	1.09

All (4) 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)
5:D:3941:HOH:O	5:H:4205:HOH:O[1_565]	2.12	0.08
5:D:4087:HOH:O	5:E:4106:HOH:O[1_655]	2.14	0.06
5:A:4001:HOH:O	5:B:4113:HOH:O[1_565]	2.19	0.01
1:F:64:GLN:OE1	5:G:4216:HOH:O[1_455]	2.19	0.01

## 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	299/293 (102%)	295 (99%)	4 (1%)	0	100	100
1	B	296/293 (101%)	292 (99%)	4 (1%)	0	100	100
1	C	296/293 (101%)	293 (99%)	2 (1%)	1 (0%)	46	28
1	D	295/293 (101%)	289 (98%)	5 (2%)	1 (0%)	46	28
1	E	295/293 (101%)	290 (98%)	3 (1%)	2 (1%)	26	11
1	F	300/293 (102%)	296 (99%)	3 (1%)	1 (0%)	46	28
1	G	296/293 (101%)	293 (99%)	2 (1%)	1 (0%)	46	28
1	H	294/293 (100%)	291 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2371/2344 (101%)	2339 (99%)	26 (1%)	6 (0%)	46	28

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	31	TYR
1	D	31	TYR
1	E	14	THR
1	E	31	TYR
1	F	31	TYR

### 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	248/240 (103%)	244 (98%)	4 (2%)	70	57
1	B	245/240 (102%)	240 (98%)	5 (2%)	63	47
1	C	245/240 (102%)	240 (98%)	5 (2%)	63	47
1	D	244/240 (102%)	238 (98%)	6 (2%)	55	37
1	E	244/240 (102%)	238 (98%)	6 (2%)	55	37
1	F	249/240 (104%)	243 (98%)	6 (2%)	57	38
1	G	245/240 (102%)	242 (99%)	3 (1%)	78	69
1	H	243/240 (101%)	237 (98%)	6 (2%)	55	37
All	All	1963/1920 (102%)	1922 (98%)	41 (2%)	61	44

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	24	SER
1	E	16	LEU
1	H	119	HIS
1	D	119	HIS
1	E	14	THR



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	282	GLN
1	F	65	GLN
1	H	229	HIS
1	F	17	HIS
1	F	152	GLN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

41 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	DAU	A	3500	-	30,38,38	1.09	3 (10%)	44,58,58	2.15	14 (31%)
3	DAU	A	3501	-	30,38,38	0.93	1 (3%)	44,58,58	1.30	4 (9%)
2	SO4	A	3700	-	4,4,4	0.23	0	6,6,6	0.29	0
4	CIT	A	3800	-	3,12,12	0.79	0	3,17,17	1.33	0
4	CIT	A	3801	-	3,12,12	1.14	0	3,17,17	0.95	0
2	SO4	A	3802	-	4,4,4	0.37	0	6,6,6	0.33	0
2	SO4	A	3803	-	4,4,4	0.61	0	6,6,6	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	3817	-	4,4,4	0.40	0	6,6,6	0.24	0
2	SO4	A	3818	-	4,4,4	0.41	0	6,6,6	0.34	0
3	DAU	B	3502	-	30,38,38	1.02	3 (10%)	44,58,58	1.80	8 (18%)
3	DAU	B	3503	-	30,38,38	0.78	0	44,58,58	1.64	5 (11%)
2	SO4	B	3701	-	4,4,4	0.27	0	6,6,6	0.28	0
2	SO4	B	3804	-	4,4,4	0.18	0	6,6,6	0.42	0
3	DAU	C	3504	-	30,38,38	1.12	2 (6%)	44,58,58	2.27	15 (34%)
3	DAU	C	3505	-	30,38,38	1.18	1 (3%)	44,58,58	2.09	5 (11%)
2	SO4	C	3805	-	4,4,4	0.70	0	6,6,6	0.87	1 (16%)
2	SO4	C	3806	-	4,4,4	0.38	0	6,6,6	0.30	0
3	DAU	D	3506	-	30,38,38	1.13	3 (10%)	44,58,58	2.52	13 (29%)
3	DAU	D	3507	-	30,38,38	0.93	1 (3%)	44,58,58	1.62	4 (9%)
2	SO4	D	3807	-	4,4,4	0.32	0	6,6,6	0.29	0
2	SO4	D	3819	-	4,4,4	0.66	0	6,6,6	0.54	0
3	DAU	E	3508	-	30,38,38	1.02	3 (10%)	44,58,58	2.09	13 (29%)
3	DAU	E	3509	-	30,38,38	1.00	1 (3%)	44,58,58	1.71	5 (11%)
2	SO4	E	3808	-	4,4,4	0.68	0	6,6,6	0.30	0
2	SO4	E	3809	-	4,4,4	0.23	0	6,6,6	0.22	0
2	SO4	E	3810	-	4,4,4	0.66	0	6,6,6	0.69	0
2	SO4	E	3820	-	4,4,4	0.36	0	6,6,6	0.72	0
3	DAU	F	3510	-	30,38,38	1.19	2 (6%)	44,58,58	2.38	13 (29%)
3	DAU	F	3511	-	30,38,38	0.82	1 (3%)	44,58,58	1.69	7 (15%)
2	SO4	F	3811	-	4,4,4	0.23	0	6,6,6	0.56	0
3	DAU	G	3514	-	30,38,38	1.08	3 (10%)	44,58,58	1.78	8 (18%)
3	DAU	G	3515	-	30,38,38	0.92	2 (6%)	44,58,58	1.31	4 (9%)
2	SO4	G	3702	-	4,4,4	0.28	0	6,6,6	0.50	0
2	SO4	G	3812	-	4,4,4	0.62	0	6,6,6	0.57	0
2	SO4	G	3813	-	4,4,4	0.24	0	6,6,6	0.59	0
3	DAU	H	3512	-	30,38,38	1.01	3 (10%)	44,58,58	2.01	12 (27%)
3	DAU	H	3513	-	30,38,38	0.99	2 (6%)	44,58,58	1.60	4 (9%)
2	SO4	H	3703	-	4,4,4	0.22	0	6,6,6	0.27	0
2	SO4	H	3814	1	4,4,4	0.41	0	6,6,6	0.41	0
2	SO4	H	3815	-	4,4,4	0.68	0	6,6,6	0.21	0
2	SO4	H	3816	-	4,4,4	0.22	0	6,6,6	0.46	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	DAU	A	3500	-	-	0/19/55/55	0/3/3/3
3	DAU	A	3501	-	-	0/19/55/55	0/3/3/3
2	SO4	A	3700	-	-	0/0/0/0	0/0/0/0
4	CIT	A	3800	-	-	0/6/16/16	0/0/0/0
4	CIT	A	3801	-	-	0/6/16/16	0/0/0/0
2	SO4	A	3802	-	-	0/0/0/0	0/0/0/0
2	SO4	A	3803	-	-	0/0/0/0	0/0/0/0
2	SO4	A	3817	-	-	0/0/0/0	0/0/0/0
2	SO4	A	3818	-	-	0/0/0/0	0/0/0/0
3	DAU	B	3502	-	-	0/19/55/55	0/3/3/3
3	DAU	B	3503	-	-	0/19/55/55	0/3/3/3
2	SO4	B	3701	-	-	0/0/0/0	0/0/0/0
2	SO4	B	3804	-	-	0/0/0/0	0/0/0/0
3	DAU	C	3504	-	-	0/19/55/55	0/3/3/3
3	DAU	C	3505	-	-	0/19/55/55	0/3/3/3
2	SO4	C	3805	-	-	0/0/0/0	0/0/0/0
2	SO4	C	3806	-	-	0/0/0/0	0/0/0/0
3	DAU	D	3506	-	-	0/19/55/55	0/3/3/3
3	DAU	D	3507	-	-	0/19/55/55	0/3/3/3
2	SO4	D	3807	-	-	0/0/0/0	0/0/0/0
2	SO4	D	3819	-	-	0/0/0/0	0/0/0/0
3	DAU	E	3508	-	-	0/19/55/55	0/3/3/3
3	DAU	E	3509	-	-	0/19/55/55	0/3/3/3
2	SO4	E	3808	-	-	0/0/0/0	0/0/0/0
2	SO4	E	3809	-	-	0/0/0/0	0/0/0/0
2	SO4	E	3810	-	-	0/0/0/0	0/0/0/0
2	SO4	E	3820	-	-	0/0/0/0	0/0/0/0
3	DAU	F	3510	-	-	0/19/55/55	0/3/3/3
3	DAU	F	3511	-	-	0/19/55/55	0/3/3/3
2	SO4	F	3811	-	-	0/0/0/0	0/0/0/0
3	DAU	G	3514	-	-	0/19/55/55	0/3/3/3
3	DAU	G	3515	-	-	0/19/55/55	0/3/3/3
2	SO4	G	3702	-	-	0/0/0/0	0/0/0/0
2	SO4	G	3812	-	-	0/0/0/0	0/0/0/0
2	SO4	G	3813	-	-	0/0/0/0	0/0/0/0
3	DAU	H	3512	-	-	0/19/55/55	0/3/3/3
3	DAU	H	3513	-	-	0/19/55/55	0/3/3/3
2	SO4	H	3703	-	-	0/0/0/0	0/0/0/0
2	SO4	H	3814	1	-	0/0/0/0	0/0/0/0
2	SO4	H	3815	-	-	0/0/0/0	0/0/0/0
2	SO4	H	3816	-	-	0/0/0/0	0/0/0/0

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3510	DAU	C61-N11	-2.35	1.31	1.35
3	G	3514	DAU	O4'-C1'	2.02	1.47	1.42
3	G	3514	DAU	P-O1P	2.07	1.58	1.51
3	G	3515	DAU	C41-N31	2.07	1.36	1.33
3	F	3511	DAU	P2-O3P	2.08	1.58	1.51

The worst 5 of 135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	3510	DAU	O5-C1-O1	-8.37	100.33	111.36
3	C	3504	DAU	P-OPP-P2	-6.49	114.51	132.73
3	C	3505	DAU	C51-C41-N31	-6.26	118.17	125.14
3	A	3500	DAU	P-OPP-P2	-6.23	115.23	132.73
3	E	3508	DAU	P-OPP-P2	-6.22	115.27	132.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3500	DAU	1	0
3	A	3501	DAU	2	0
4	A	3800	CIT	3	0
4	A	3801	CIT	9	0
2	A	3802	SO4	2	0
2	A	3818	SO4	2	0
3	B	3502	DAU	2	0
2	B	3701	SO4	2	0
3	C	3504	DAU	3	0
2	C	3806	SO4	1	0
3	D	3506	DAU	1	0
3	E	3508	DAU	3	0
2	E	3810	SO4	2	0
2	E	3820	SO4	1	0
3	F	3510	DAU	4	0
2	G	3702	SO4	4	0
3	H	3512	DAU	1	0
3	H	3513	DAU	1	0
2	H	3703	SO4	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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	292/293 (99%)	0.49	23 (7%) 15 14	4, 10, 20, 30	0
1	B	293/293 (100%)	0.43	19 (6%) 22 21	4, 9, 21, 34	0
1	C	292/293 (99%)	0.63	34 (11%) 6 6	6, 10, 32, 47	0
1	D	292/293 (99%)	0.82	43 (14%) 3 3	5, 11, 36, 49	0
1	E	292/293 (99%)	0.83	40 (13%) 4 4	6, 12, 36, 56	0
1	F	293/293 (100%)	0.61	32 (10%) 7 7	4, 10, 29, 48	0
1	G	292/293 (99%)	0.56	28 (9%) 10 9	4, 9, 20, 66	0
1	H	292/293 (99%)	0.61	29 (9%) 9 8	5, 10, 21, 28	0
All	All	2338/2344 (99%)	0.62	248 (10%) 8 7	4, 10, 26, 66	0

The worst 5 of 248 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	23	ILE	11.7
1	D	23	ILE	10.8
1	D	22	ALA	10.0
1	E	15	ARG	7.8
1	F	14	THR	7.4

### 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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	H	3816	5/5	0.92	0.19	6.26	39,43,45,46	0
2	SO4	A	3817	5/5	0.89	0.34	6.00	38,44,46,47	0
2	SO4	G	3813	5/5	0.94	0.27	5.26	38,38,43,45	0
4	CIT	A	3801	13/13	0.63	0.28	3.70	55,57,60,61	0
2	SO4	H	3814	5/5	0.88	0.24	3.00	57,58,58,58	0
2	SO4	B	3804	5/5	0.90	0.23	2.84	45,45,50,52	0
4	CIT	A	3800	13/13	0.63	0.23	2.29	47,51,55,57	0
2	SO4	G	3702	5/5	0.96	0.28	1.93	39,40,41,44	0
2	SO4	A	3700	5/5	0.89	0.22	1.04	55,55,56,59	0
2	SO4	E	3810	5/5	0.95	0.15	0.52	35,38,41,44	0
2	SO4	H	3703	5/5	0.96	0.21	0.42	49,49,50,52	0
3	DAU	C	3505	36/36	0.96	0.12	0.24	10,14,20,22	0
3	DAU	A	3501	36/36	0.97	0.12	0.18	8,11,15,16	0
3	DAU	B	3503	36/36	0.96	0.12	0.13	10,12,17,18	0
3	DAU	B	3502	36/36	0.94	0.12	0.08	8,16,28,30	0
3	DAU	E	3509	36/36	0.96	0.12	0.06	11,15,21,22	0
3	DAU	F	3510	36/36	0.92	0.12	0.06	12,18,28,34	0
2	SO4	B	3701	5/5	0.89	0.18	0.03	53,54,55,57	0
3	DAU	A	3500	36/36	0.92	0.12	0.03	10,17,29,30	0
3	DAU	G	3514	36/36	0.93	0.12	-0.01	9,15,27,30	0
3	DAU	H	3512	36/36	0.93	0.12	-0.08	10,18,28,31	0
3	DAU	G	3515	36/36	0.97	0.11	-0.08	8,12,16,16	0
3	DAU	F	3511	36/36	0.97	0.11	-0.12	10,15,22,23	0
3	DAU	D	3507	36/36	0.96	0.12	-0.13	9,15,18,19	0
3	DAU	H	3513	36/36	0.96	0.11	-0.14	10,13,17,17	0
3	DAU	E	3508	36/36	0.92	0.11	-0.40	11,24,34,36	0
3	DAU	C	3504	36/36	0.93	0.10	-0.43	11,17,30,31	0
3	DAU	D	3506	36/36	0.92	0.10	-0.49	12,19,31,32	0
2	SO4	E	3808	5/5	0.96	0.16	-	47,50,54,54	0
2	SO4	E	3809	5/5	0.90	0.21	-	46,50,51,53	0
2	SO4	F	3811	5/5	0.94	0.20	-	43,44,47,49	0
2	SO4	D	3807	5/5	0.94	0.21	-	45,47,47,47	0
2	SO4	D	3819	5/5	0.87	0.17	-	44,44,45,49	0
2	SO4	A	3818	5/5	0.82	0.36	-	46,49,50,52	0
2	SO4	A	3802	5/5	0.94	0.31	-	62,63,64,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	H	3815	5/5	0.97	0.10	-	38,38,40,43	0
2	SO4	C	3806	5/5	0.92	0.25	-	42,46,49,49	0
2	SO4	C	3805	5/5	0.98	0.10	-	38,41,45,46	0
2	SO4	G	3812	5/5	0.96	0.12	-	41,42,43,48	0
2	SO4	A	3803	5/5	0.96	0.11	-	37,38,39,44	0
2	SO4	E	3820	5/5	0.87	0.20	-	48,48,49,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.