



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:30 PM UTC

PDB ID : 7QCP / pdb_00007qcp
Title : Crystal structure of Mycobacterium hassiacum glucosyl-3-phosphoglycerate synthase at pH 7.2 - apo form
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Deposited on : 2021-11-25
Resolution : 1.11 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

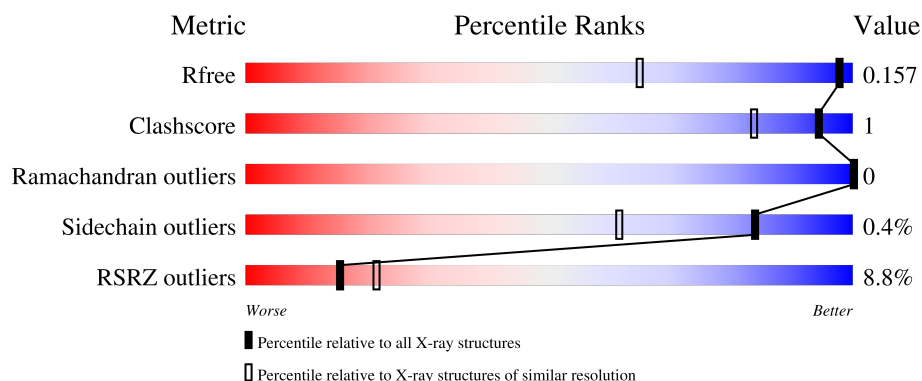
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.11 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	1985 (1.14-1.10)
Clashscore	190562	2021 (1.14-1.10)
Ramachandran outliers	187476	1978 (1.14-1.10)
Sidechain outliers	187428	1974 (1.14-1.10)
RSRZ outliers	180081	1984 (1.14-1.10)

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	327	
1	B	327	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9756 atoms, of which 4587 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 Glucosyl-3-phosphoglycerate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	287	Total	C	H	N	O	S	10	16	0
			4489	1416	2255	392	418	8			
1	B	290	Total	C	H	N	O	S	0	22	0
			4584	1436	2324	392	423	9			

There are 26 discrepancies between the modelled and reference sequences:

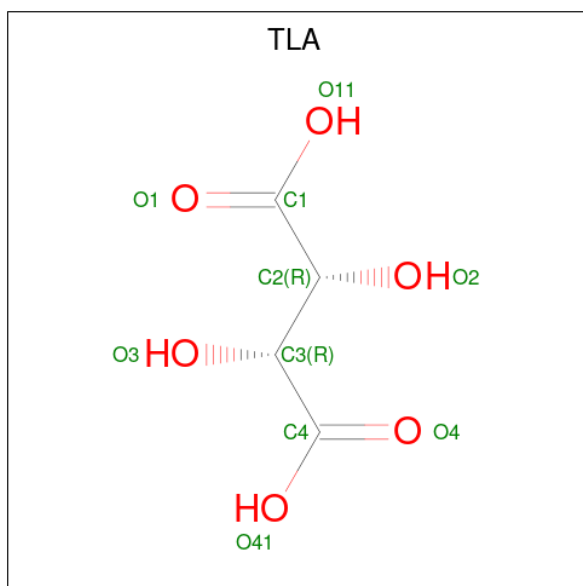
Chain	Residue	Modelled	Actual	Comment	Reference
A	315	LYS	-	linker	UNP K5B7Z4
A	316	LEU	-	linker	UNP K5B7Z4
A	317	ALA	-	linker	UNP K5B7Z4
A	318	ALA	-	linker	UNP K5B7Z4
A	319	ALA	-	linker	UNP K5B7Z4
A	320	LEU	-	linker	UNP K5B7Z4
A	321	GLU	-	linker	UNP K5B7Z4
A	322	HIS	-	expression tag	UNP K5B7Z4
A	323	HIS	-	expression tag	UNP K5B7Z4
A	324	HIS	-	expression tag	UNP K5B7Z4
A	325	HIS	-	expression tag	UNP K5B7Z4
A	326	HIS	-	expression tag	UNP K5B7Z4
A	327	HIS	-	expression tag	UNP K5B7Z4
B	315	LYS	-	linker	UNP K5B7Z4
B	316	LEU	-	linker	UNP K5B7Z4
B	317	ALA	-	linker	UNP K5B7Z4
B	318	ALA	-	linker	UNP K5B7Z4
B	319	ALA	-	linker	UNP K5B7Z4
B	320	LEU	-	linker	UNP K5B7Z4
B	321	GLU	-	linker	UNP K5B7Z4
B	322	HIS	-	expression tag	UNP K5B7Z4
B	323	HIS	-	expression tag	UNP K5B7Z4
B	324	HIS	-	expression tag	UNP K5B7Z4
B	325	HIS	-	expression tag	UNP K5B7Z4
B	326	HIS	-	expression tag	UNP K5B7Z4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	327	HIS	-	expression tag	UNP K5B7Z4

- Molecule 2 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	4	4	6		
2	B	1	Total	C	H	O	0	0
			14	4	4	6		

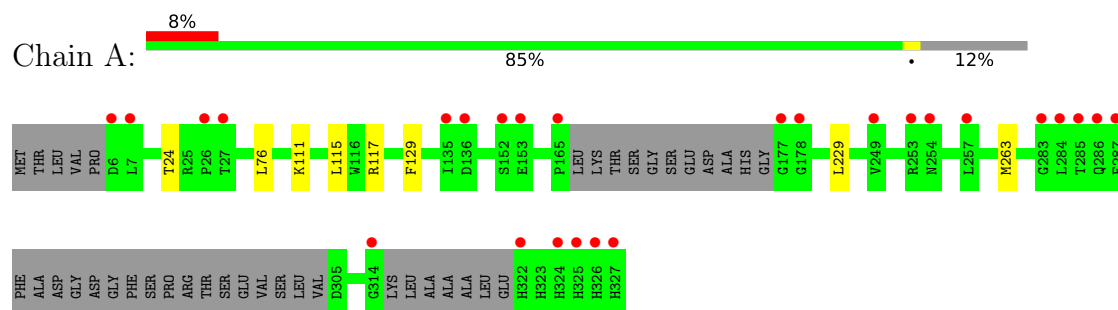
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	340	Total	O	0	5
			342	342		
3	B	310	Total	O	0	7
			313	313		

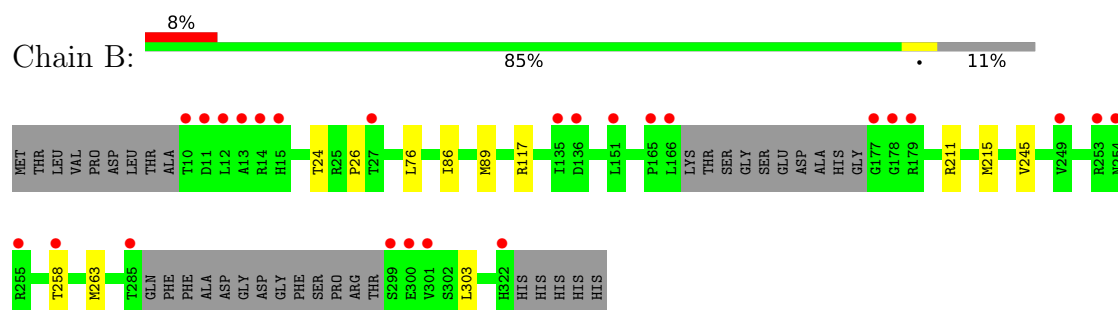
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glucosyl-3-phosphoglycerate synthase



- Molecule 1: Glucosyl-3-phosphoglycerate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.28Å 90.63Å 95.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.65 – 1.11 47.65 – 1.11	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.65-1.11) 99.9 (47.65-1.11)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 1.11Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.142 , 0.156 (Not available) , 0.157	Depositor DCC
R_{free} test set	12153 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	12.2	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	9756	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.29	0/2332	0.51	0/3181
1	B	0.27	0/2379	0.50	0/3244
All	All	0.28	0/4711	0.50	0/6425

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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ARG	Sidechain
1	B	117	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2234	2255	2218	5	0
1	B	2260	2324	2268	7	0
2	A	10	4	4	1	0
2	B	10	4	4	1	0
3	A	342	0	0	3	0
3	B	313	0	0	3	0
All	All	5169	4587	4494	12	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (12) 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:229:LEU:HD23	3:A:524:HOH:O	2.05	0.56
1:B:303:LEU:HD22	3:B:672:HOH:O	2.09	0.53
1:A:111[A]:LYS:HD3	3:A:714:HOH:O	2.09	0.52
1:B:211:ARG:HD3	1:B:215[B]:MET:HG2	1.93	0.50
1:A:24[B]:THR:HG23	3:A:543:HOH:O	2.14	0.48
1:B:26:PRO:HG3	1:B:245[B]:VAL:CG1	2.48	0.44
1:A:263[A]:MET:HE1	2:A:401:TLA:H2	1.99	0.44
1:B:263[B]:MET:SD	2:B:401:TLA:O2	2.76	0.43
1:B:24[B]:THR:HG23	3:B:538:HOH:O	2.19	0.42
1:B:86:ILE:HD12	1:B:89:MET:HE3	2.02	0.41
1:B:258:THR:HG23	3:B:709:HOH:O	2.21	0.41
1:A:115:LEU:HD22	1:A:129:PHE:CD1	2.56	0.41

There are no symmetry-related clashes.

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	295/327 (90%)	291 (99%)	4 (1%)	0	100	100
1	B	306/327 (94%)	300 (98%)	6 (2%)	0	100	100
All	All	601/654 (92%)	591 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	244/265 (92%)	243 (100%)	1 (0%)	84	61
1	B	250/265 (94%)	249 (100%)	1 (0%)	84	61
All	All	494/530 (93%)	492 (100%)	2 (0%)	84	61

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	LEU
1	B	76	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	GLN
1	B	322	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TLA	B	401	-	9,9,9	1.06	0	12,12,12	0.93	0
2	TLA	A	401	-	9,9,9	0.99	0	12,12,12	1.06	1 (8%)

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	TLA	B	401	-	-	2/12/12/12	-
2	TLA	A	401	-	-	0/12/12/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	TLA	O1-C1-C2	-2.07	116.12	121.62

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	TLA	O1-C1-C2-O2
2	B	401	TLA	O11-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	TLA	1	0
2	A	401	TLA	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(Å ²)	Q < 0.9
1	A	287/327 (87%)	0.07	26 (9%)	15 20	7, 15, 42, 71	14 (4%)
1	B	290/327 (88%)	0.12	25 (8%)	16 22	6, 16, 40, 60	15 (5%)
All	All	577/654 (88%)	0.10	51 (8%)	15 21	6, 15, 42, 71	29 (5%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	287	PHE	8.0
1	B	166	LEU	7.2
1	B	10	THR	7.1
1	A	284	LEU	6.8
1	A	285	THR	6.0
1	B	177	GLY	6.0
1	A	177	GLY	5.8
1	B	12	LEU	5.3
1	B	322	HIS	5.0
1	B	301	VAL	4.7
1	A	322	HIS	4.7
1	B	254	ASN	4.6
1	A	136	ASP	4.1
1	A	327	HIS	3.9
1	A	254	ASN	3.8
1	A	286	GLN	3.7
1	B	178	GLY	3.6
1	B	253	ARG	3.4
1	B	255	ARG	3.4
1	A	253	ARG	3.3
1	A	165	PRO	3.3
1	B	13	ALA	3.3
1	B	285	THR	3.2
1	B	249	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	299	SER	3.2
1	B	300	GLU	3.1
1	B	258	THR	3.1
1	A	314	GLY	3.1
1	A	283	GLY	3.1
1	A	325	HIS	3.0
1	A	6	ASP	2.9
1	B	135	ILE	2.9
1	A	7	LEU	2.9
1	A	135	ILE	2.9
1	A	257	LEU	2.8
1	B	27	THR	2.8
1	B	14	ARG	2.8
1	A	27	THR	2.7
1	A	249	VAL	2.6
1	B	136	ASP	2.6
1	A	326	HIS	2.6
1	B	15	HIS	2.4
1	B	11	ASP	2.4
1	A	153	GLU	2.3
1	A	324	HIS	2.3
1	A	178	GLY	2.3
1	B	179	ARG	2.3
1	B	165	PRO	2.3
1	B	151	LEU	2.3
1	A	26	PRO	2.2
1	A	152	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TLA	A	401	10/10	0.88	0.18	18,50,79,107	0
2	TLA	B	401	10/10	0.89	0.22	19,47,128,154	14

6.5 Other polymers [i](#)

There are no such residues in this entry.