



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 01:32 AM UTC

PDB ID : 3K85 / pdb_00003k85
Title : Crystal structure of a D-glycero-D-manno-heptose 1-phosphate kinase from *Bacteriodes thetaiotaomicron*
Authors : Palani, K.; Kumaran, D.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2009-10-13
Resolution : 2.28 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

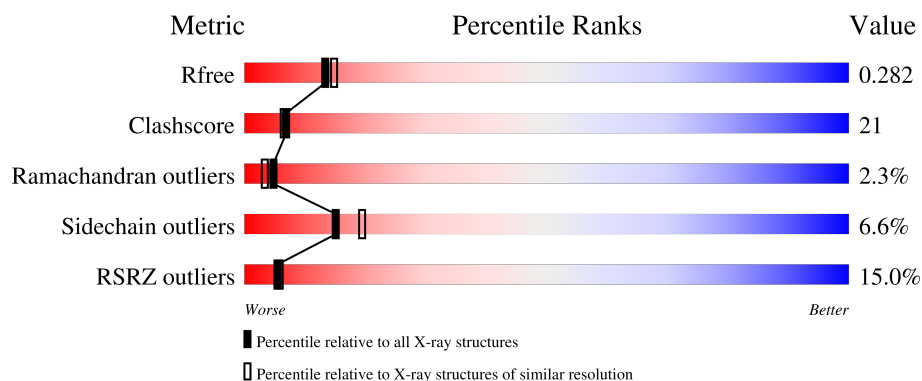
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	357	
1	B	357	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 4879 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 D-glycero-D-manno-heptose 1-phosphate kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	Se	0	0	0
			2371	1517	391	450	4	9			
1	B	306	Total	C	N	O	S	Se	0	0	0
			2371	1517	391	450	4	9			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MSE	-	expression tag	UNP Q8AAJ0
A	1	SER	-	expression tag	UNP Q8AAJ0
A	2	LEU	-	expression tag	UNP Q8AAJ0
A	349	GLU	-	expression tag	UNP Q8AAJ0
A	350	GLY	-	expression tag	UNP Q8AAJ0
A	351	HIS	-	expression tag	UNP Q8AAJ0
A	352	HIS	-	expression tag	UNP Q8AAJ0
A	353	HIS	-	expression tag	UNP Q8AAJ0
A	354	HIS	-	expression tag	UNP Q8AAJ0
A	355	HIS	-	expression tag	UNP Q8AAJ0
A	356	HIS	-	expression tag	UNP Q8AAJ0
B	0	MSE	-	expression tag	UNP Q8AAJ0
B	1	SER	-	expression tag	UNP Q8AAJ0
B	2	LEU	-	expression tag	UNP Q8AAJ0
B	349	GLU	-	expression tag	UNP Q8AAJ0
B	350	GLY	-	expression tag	UNP Q8AAJ0
B	351	HIS	-	expression tag	UNP Q8AAJ0
B	352	HIS	-	expression tag	UNP Q8AAJ0
B	353	HIS	-	expression tag	UNP Q8AAJ0
B	354	HIS	-	expression tag	UNP Q8AAJ0
B	355	HIS	-	expression tag	UNP Q8AAJ0
B	356	HIS	-	expression tag	UNP Q8AAJ0

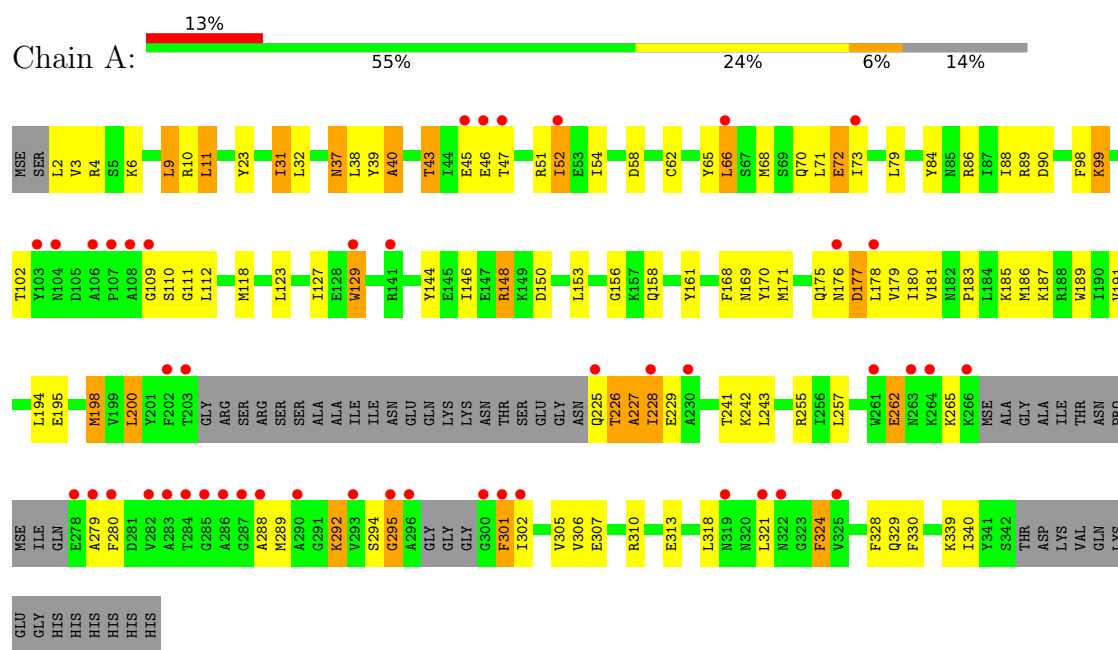
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	75	Total 75	O 75	0	0
2	B	62	Total 62	O 62	0	0

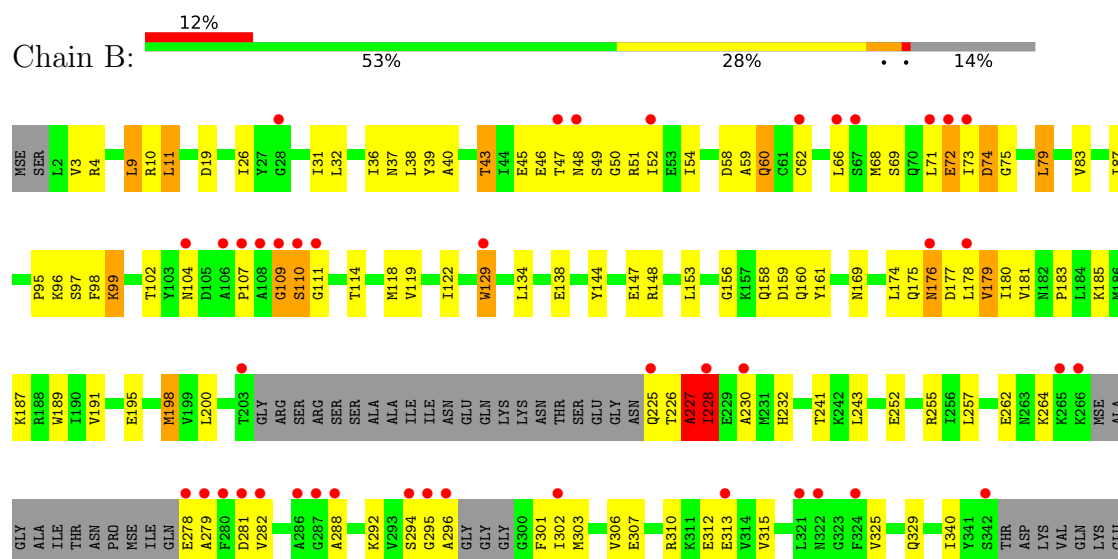
3 Residue-property plots [i](#)

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: D-glycero-D-manno-heptose 1-phosphate kinase



- Molecule 1: D-glycero-D-manno-heptose 1-phosphate kinase



GLY
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	71.89Å 149.47Å 141.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.95 – 2.28 40.95 – 2.28	Depositor EDS
% Data completeness (in resolution range)	94.1 (40.95-2.28) 94.2 (40.95-2.28)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.05Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.254 , 0.282 0.254 , 0.282	Depositor DCC
R_{free} test set	1677 reflections (3.61%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.682	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4879	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% 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](#)

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	0.44	0/2404	0.95	10/3224 (0.3%)
1	B	0.43	0/2404	0.96	10/3224 (0.3%)
All	All	0.43	0/4808	0.96	20/6448 (0.3%)

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	GLU	N-CA-C	-7.86	102.80	111.36
1	A	39	TYR	N-CA-C	7.80	120.92	109.69
1	B	281	ASP	N-CA-C	-7.50	104.17	112.72
1	B	39	TYR	N-CA-C	7.40	121.13	109.81
1	B	75	GLY	N-CA-C	-6.82	105.48	115.63

There are no chirality outliers.

There are no planarity outliers.

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	2371	0	2364	96	0
1	B	2371	0	2364	111	0
2	A	75	0	0	1	0
2	B	62	0	0	4	0
All	All	4879	0	4728	201	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 21.

The worst 5 of 201 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:B:257:LEU:HD22	1:B:292:LYS:HB2	1.51	0.91
1:A:180:ILE:HD12	1:B:243:LEU:HD13	1.53	0.90
1:A:58:ASP:OD1	1:A:102:THR:HG22	1.71	0.89
1:A:185:LYS:HG2	1:B:185:LYS:HG2	1.60	0.83
1:A:2:LEU:HD11	1:A:4:ARG:NH1	1.93	0.83

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	298/357 (84%)	277 (93%)	14 (5%)	7 (2%)	5	3
1	B	298/357 (84%)	270 (91%)	21 (7%)	7 (2%)	5	3
All	All	596/714 (84%)	547 (92%)	35 (6%)	14 (2%)	5	3

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	SER
1	A	279	ALA
1	A	295	GLY
1	B	177	ASP
1	B	228	ILE

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	249/277 (90%)	233 (94%)	16 (6%)	16	20
1	B	249/277 (90%)	232 (93%)	17 (7%)	14	18
All	All	498/554 (90%)	465 (93%)	33 (7%)	15	19

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	228	ILE
1	B	262	GLU
1	B	329	GLN
1	A	280	PHE
1	A	262	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	329	GLN
1	B	319	ASN
1	B	70	GLN
1	B	60	GLN
1	B	169	ASN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	297/357 (83%)	0.90	46 (15%) 5 5	18, 38, 77, 91	0
1	B	297/357 (83%)	0.84	43 (14%) 6 6	17, 40, 67, 82	0
All	All	594/714 (83%)	0.87	89 (14%) 5 6	17, 39, 73, 91	0

The worst 5 of 89 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	295	GLY	6.9
1	A	287	GLY	6.8
1	A	286	ALA	6.0
1	B	108	ALA	5.8
1	B	280	PHE	5.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.