



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:40 PM UTC

PDB ID : 1GQQ / pdb_00001gqq
Title : MURC - Crystal structure of the apo-enzyme from Haemophilus influenzae
Authors : Skarzynski, T.; Cleasby, A.; Domenici, E.; Gevi, M.; Shaw, J.
Deposited on : 2001-12-03
Resolution : 3.10 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

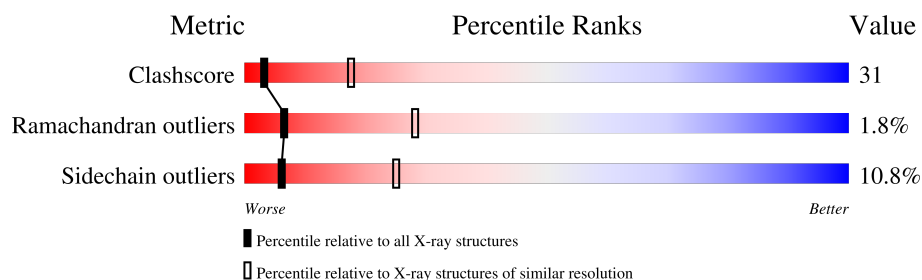
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	475	
1	B	475	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6578 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 UDP-N-ACETYLMURAMATE-L-ALANINE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3292	2081	573	623	15			
1	B	427	Total	C	N	O	S	0	0	0
			3286	2078	572	621	15			

GLY	ASP	F206	E207	K208	M209	K210	A211	T212	L217	H218	N219	L220	P221	F222	Y223	G224	L225	A226	V227	M228	C229	A230	D231	D232	P233	V234	L235	M236	E237	L238	V239	P240	K241	V242	G243	R244	Q245	V246	I247	T248	Y249	S252	E253	Q254	A255	D256	Y257	R258	I259	E260	D261	Y262	F263	Q264	T265	G266	F267																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.51Å 99.48Å 180.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.88 – 3.10	Depositor
% Data completeness (in resolution range)	100.0 (19.88-3.10)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.239 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6578	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

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	1.74	53/3346 (1.6%)	1.77	70/4525 (1.5%)
1	B	1.34	27/3341 (0.8%)	1.50	39/4519 (0.9%)
All	All	1.55	80/6687 (1.2%)	1.64	109/9044 (1.2%)

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	ILE	CA-CB	-13.82	1.36	1.53
1	A	357	ILE	CA-CB	-11.23	1.41	1.54
1	A	400	MET	SD-CE	-10.57	1.53	1.79
1	A	473	TRP	C-O	-10.35	1.11	1.24
1	B	411	ILE	CA-CB	-8.54	1.44	1.54

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	SER	N-CA-C	-11.65	98.38	112.59
1	B	252	SER	N-CA-C	9.39	123.39	109.59
1	A	336	PRO	CA-C-N	-8.67	109.08	122.60
1	A	336	PRO	C-N-CA	-8.67	109.08	122.60
1	B	349	HIS	N-CA-C	-8.08	100.84	110.13

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	3292	0	3295	180	0
1	B	3286	0	3288	230	0
All	All	6578	0	6583	404	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 31.

The worst 5 of 404 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:105:ILE:HD11	1:A:110:MET:HG2	1.23	1.16
1:A:417:LYS:HD3	1:A:417:LYS:N	1.66	1.08
1:B:39:LEU:HD13	1:B:45:ILE:HG12	1.42	1.02
1:B:287:VAL:HG12	1:B:288:PRO:HD2	1.39	0.99
1:B:80:VAL:HG21	1:B:105:ILE:HD12	1.44	0.98

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	420/475 (88%)	384 (91%)	30 (7%)	6 (1%)	9	34
1	B	419/475 (88%)	376 (90%)	34 (8%)	9 (2%)	5	25
All	All	839/950 (88%)	760 (91%)	64 (8%)	15 (2%)	6	28

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	ASP
1	B	55	VAL
1	B	72	GLU

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Mol	Chain	Res	Type
1	B	253	GLU
1	B	219	ASN

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	349/387 (90%)	313 (90%)	36 (10%)	7	27
1	B	348/387 (90%)	309 (89%)	39 (11%)	6	24
All	All	697/774 (90%)	622 (89%)	75 (11%)	6	25

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	270	HIS
1	B	453	LEU
1	B	280	ARG
1	B	348	HIS
1	A	350	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	19	GLN
1	B	74	HIS
1	B	337	ASN
1	B	61	GLN
1	B	99	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.