



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 18, 2018 – 09:38 PM EST

PDB ID : 1GQQ
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

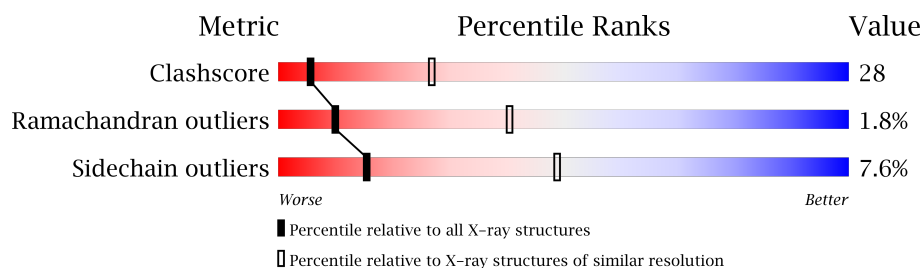
1 Overall quality at a glance

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	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)

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. 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.

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.

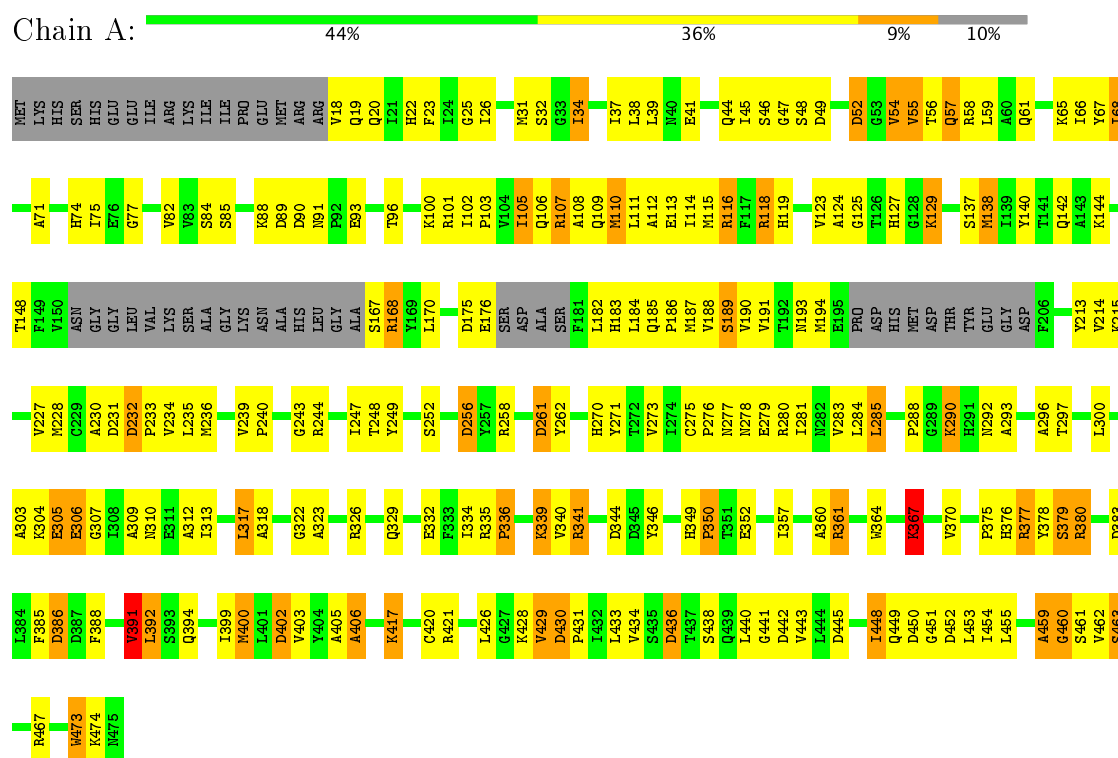
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3292	2081	573	623	15			
1	B	427	Total	C	N	O	S	0	0	0
			3286	2078	572	621	15			

3 Residue-property plots

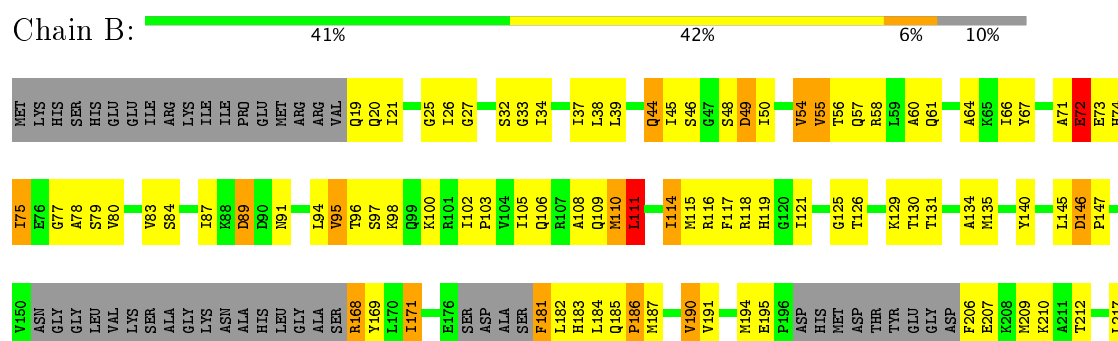
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

• Molecule 1: UDP-N-ACETYLMURAMATE-L-ALANINE LIGASE



• Molecule 1: UDP-N-ACETYLMURAMATE-L-ALANINE LIGASE



D452	H218	I281	R364	S461	S252	T248	U249	V252	X253	Y254	Z255	A256	B257	C258	D259	E260	F261	G262	H263	I264	J265	K266	L267	M268	N269	O270	P271	Q272	R273	S274	T275	U276	V277	W278	X279	Y280	Z281
L453	H219	I282	G365	V462	E253	T249			E254	Q254	A255	D256	Y257	R258	I259	E260	D261	G262	H263	I264	J265	K266	L267	M268	N269	O270	P271	Q272	R273	S274	T275	U276	V277	W278	X279	Y280	Z281
I454	H220	I283	G366	K464	F254	T250			Q254	A255	D256	Y257	R258	I259	E260	D261	G262	H263	I264	J265	K266	L267	M268	N269	O270	P271	Q272	R273	S274	T275	U276	V277	W278	X279	Y280	Z281	
L455	H221	I284	K367	I465	G255	T251			A255	D256	Y257	R258	I259	E260	D261	G262	H263	I264	J265	K266	L267	M268	N269	O270	P271	Q272	R273	S274	T275	U276	V277	W278	X279	Y280	Z281		
	H222	I285	R368	S466	F256	T252			D256	Y257	R258	I259	E260	D261	G262	H263	I264	J265	K266	L267	M268	N269	O270	P271	Q272	R273	S274	T275	U276	V277	W278	X279	Y280	Z281			
S461	H223	I286	T369	S467	G257	T253			I259	E260	D261	G262	H263	I264	J265	K266	L267	M268	N269	O270	P271	Q272	R273	S274	T275	U276	V277	W278	X279	Y280	Z281						
V462	H224	I287	V370	S468	F258	T254			E260	D261	G262	H263	I264	J265	K266	L267	M268	N269	O270	P271	Q272	R273	S274	T275	U276	V277	W278	X279	Y280	Z281							
S463	H225	I288		S469	G259	T255			D261	G262	H263	I264	J265	K266	L267	M268	N269	O270	P271	Q272	R273	S274	T275	U276	V277	W278	X279	Y280	Z281								
K464	H226	I289	P375	K465	F260	T256			I264	J265	K266	L267	M268	N269	O270	P271	Q272	R273	S274	T275	U276	V277	W278	X279	Y280	Z281											
I465	H227	I290	R376	I466	G261	T257			E261	D262	H263	I264	J265	K266	L267	M268	N269	O270	P271	Q272	R273	S274	T275	U276	V277	W278	X279	Y280	Z281								
S466	H228	I291	R377	S466	F262	T258			D262	H263	I264	J265	K266	L267	M268	N269	O270	P271	Q272	R273	S274	T275	U276	V277	W278	X279	Y280	Z281									
S467	H229	I292		S467	G263	T259			I265	D263	H264	I265	J266	K267	L268	M269	N270	O271	P272	Q273	R274	S275	T276	U277	V278	W279	X280	Y281	Z282								
R468	H230	I293	R382	R468	F264	T260			E262	D263	H264	I265	J266	K267	L268	M269	N270	O271	P272	Q273	R274	S275	T276	U277	V278	W279	X280	Y281	Z282								
L469	H231	I294	R383	L469	G265	T261			D263	H264	I265	J266	K267	L268	M269	N270	O271	P272	Q273	R274	S275	T276	U277	V278	W279	X280	Y281	Z282									
	H232	I295	L384		F266	T262			I266	D264	H265	I266	J267	K268	L269	M270	N271	O272	P273	Q274	R275	S276	T277	U278	V279	W280	X281	Y282	Z283								

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	1.33	17/3346 (0.5%)	1.38	35/4525 (0.8%)
1	B	1.00	2/3341 (0.1%)	1.17	22/4519 (0.5%)
All	All	1.18	19/6687 (0.3%)	1.28	57/9044 (0.6%)

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	ILE	CA-CB	-8.14	1.36	1.54
1	A	430	ASP	CB-CG	8.01	1.68	1.51
1	A	429	VAL	CB-CG1	-7.79	1.36	1.52
1	A	367	LYS	CE-NZ	6.82	1.66	1.49
1	B	417	LYS	CD-CE	6.52	1.67	1.51

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	ASP	CB-CG-OD1	-10.40	108.94	118.30
1	A	386	ASP	CB-CG-OD2	10.04	127.34	118.30
1	A	344	ASP	CB-CG-OD2	9.77	127.10	118.30
1	B	382	ARG	NE-CZ-NH1	-9.39	115.61	120.30
1	A	474	LYS	CD-CE-NZ	-8.13	93.00	111.70

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	165	0
1	B	3286	0	3288	213	0
All	All	6578	0	6583	372	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 28.

The worst 5 of 372 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:N	1:A:417:LYS:HD3	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%)	13	47
1	B	419/475 (88%)	376 (90%)	34 (8%)	9 (2%)	8	36
All	All	839/950 (88%)	760 (91%)	64 (8%)	15 (2%)	10	40

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%)	325 (93%)	24 (7%)	18	53
1	B	348/387 (90%)	319 (92%)	29 (8%)	13	45
All	All	697/774 (90%)	644 (92%)	53 (8%)	15	49

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	467	ARG
1	B	75	ILE
1	B	426	LEU
1	B	32	SER
1	B	50	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	446	GLN
1	B	20	GLN
1	B	449	GLN
1	A	449	GLN
1	B	19	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 carbohydrates 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.