wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 08:25 AM EDT

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

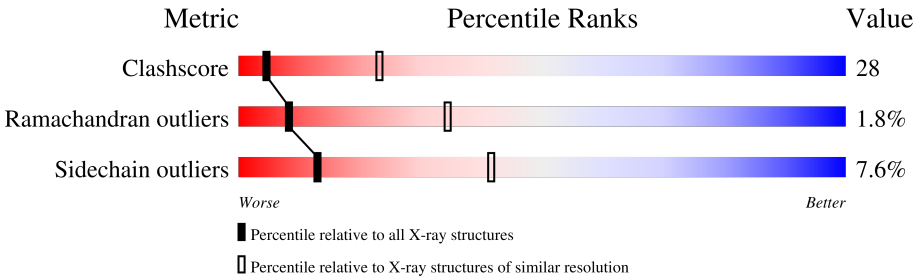
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	475	44% 36% 9% 10%
1	B	475	41% 42% 6% 10%

2 Entry composition (i)

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			

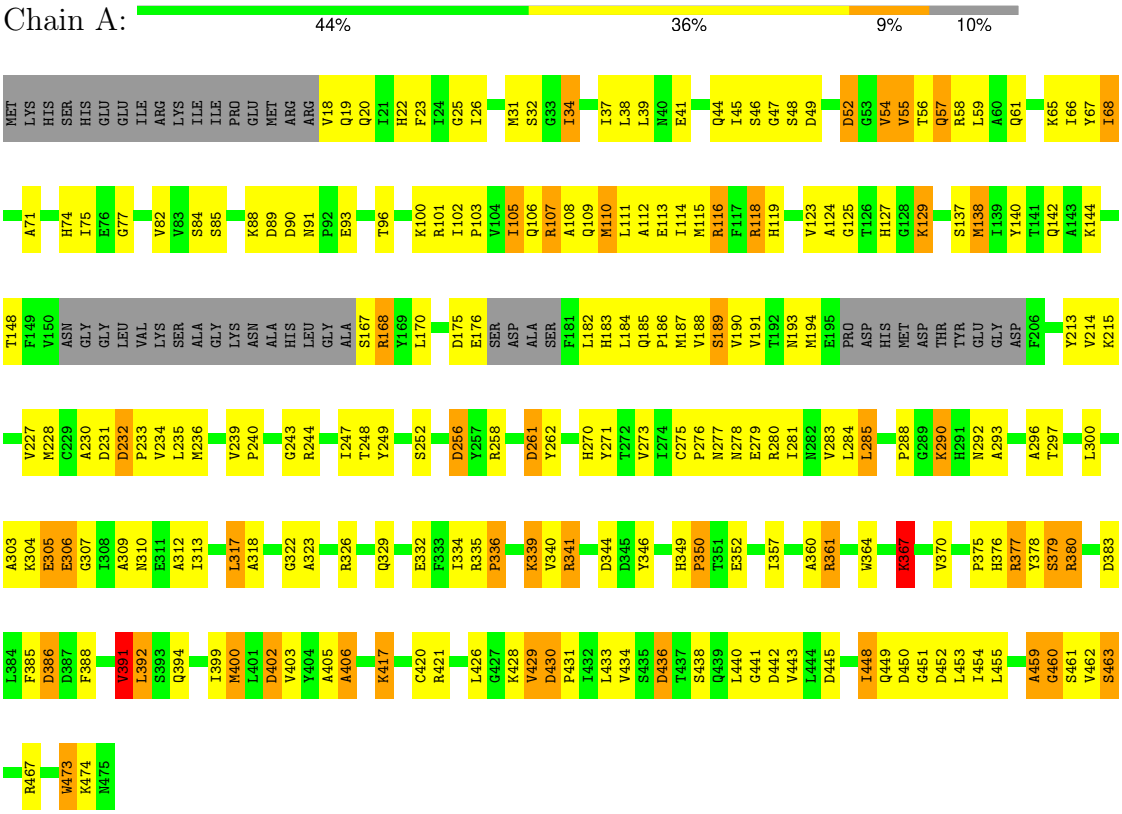
3 Residue-property plots (i)

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. 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. 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.

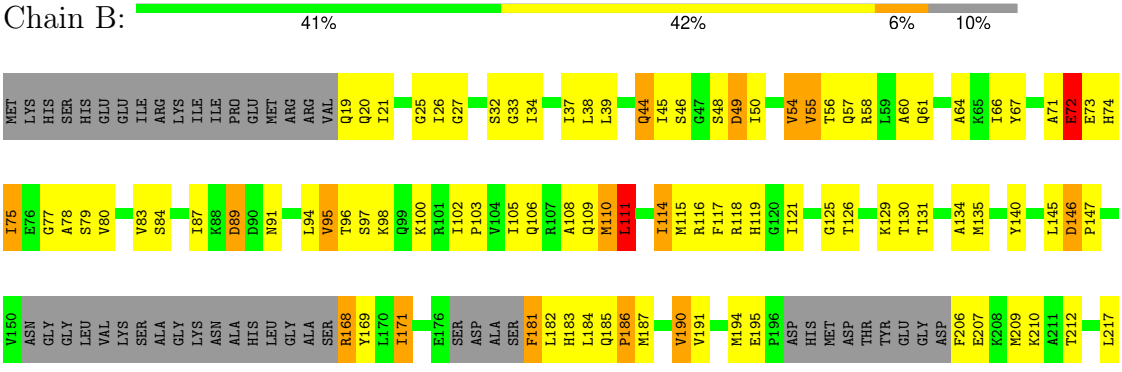
• Molecule 1: UDP-N-ACETYLMURAMATE-L-ALANINE LIGASE

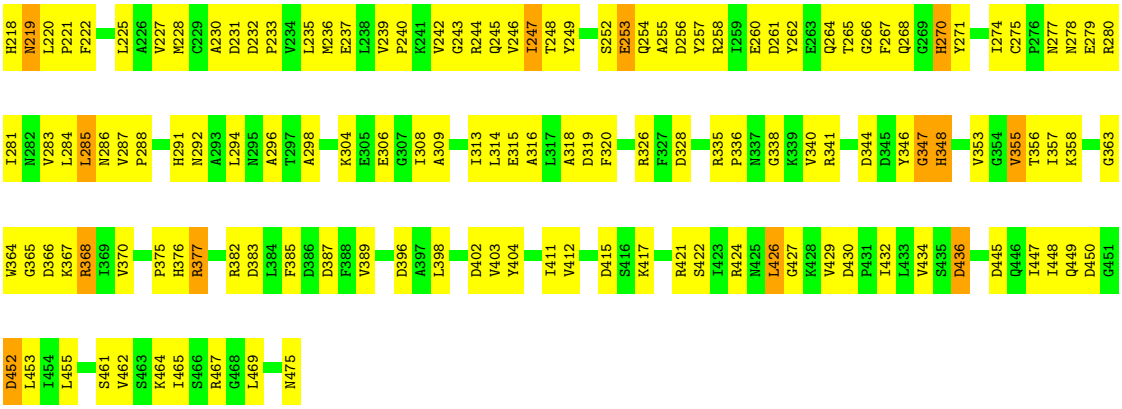
Chain A:



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

Chain B:




H218 N219 L220 P221 F222
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 E263 Q264 T265 G266 F267 Q268 G269 H270 Y271
I274 C275 P276 N277 N278 E279 R280
I281 N282 V283 L284 L285 N286 V287 P288
H291 N292 A293 L294 N295 A296 T297 A298
K304 E305 E306 G307 I308 A309
I313 L314 E315 A316 L317 A318 D319 F320
R326 F327 D328
R335 P336 N337 G338 K339 V340 R341
D344 D345 Y346 G347 H348
V353 G354 V355 T356 I357 K358
G363
W364 G365 D366 K367 R368 I369 V370
P375 H376 R377
R382 D383 L384 F385 D386 D387 F388 V389
D396 A397 L398
D402 V403 Y404
I411 V412
D415 S416 K417
R421 S422 I423 R424 M425 L426 G427 K428 V429 D430 P431 I432 L433 V434 S435 D436
D445 Q446 I447 I448 Q449 D450 G451
D452 L453 I454 L455
S461 V462 S463 K464 I465 S466 R467 G468 L469
N475

4 Data and refinement statistics (i)

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

5.1 Standard geometry

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(^{o})	Ideal(^{o})
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

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: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%)	11 40
1	B	419/475 (88%)	376 (90%)	34 (8%)	9 (2%)	7 30
All	All	839/950 (88%)	760 (91%)	64 (8%)	15 (2%)	8 34

5 of 15 Ramachandran outliers are listed below:

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

Continued on next page...

Continued from previous page...

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

5.3.2 Protein sidechains (i)

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%)	15	45
1	B	348/387 (90%)	319 (92%)	29 (8%)	11	38
All	All	697/774 (90%)	644 (92%)	53 (8%)	13	41

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

Mol	Chain	Res	Type
1	B	72	GLU
1	B	131	THR
1	B	448	ILE
1	B	75	ILE
1	B	111	LEU

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

Mol	Chain	Res	Type
1	B	74	HIS
1	B	268	GLN
1	B	264	GLN
1	B	295	ASN
1	A	254	GLN

5.3.3 RNA (i)

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 monosaccharides 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.