



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:48 PM UTC

PDB ID : 2YNU / pdb_00002ynu
Title : Apo GIM-1 with 2Mol. Crystal structures of Pseudomonas aeruginosa GIM-1:
active site plasticity in metallo-beta-lactamases
Authors : Borra, P.S.; Samuelsen, O.; Spencer, J.; Lorentzen, M.S.; Leiros, H.-K.S.
Deposited on : 2012-10-18
Resolution : 2.06 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
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
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

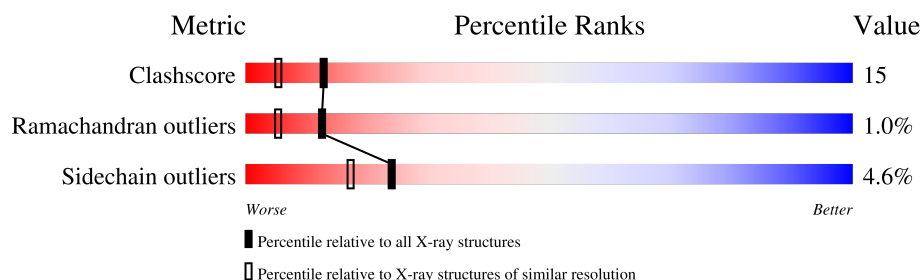
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)

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 failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	233	
1	B	233	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6971 atoms, of which 3377 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 GIM-1 PROTEIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	217	Total	C	H	N	O	S	21	11	0
			3486	1117	1731	287	348	3			
1	B	209	Total	C	H	N	O	S	90	6	0
			3307	1062	1646	271	325	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	SER	-	expression tag	UNP Q704V1
B	36	SER	-	expression tag	UNP Q704V1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	119	Total	O	0	0
			119	119		
2	B	59	Total	O	0	0
			59	59		

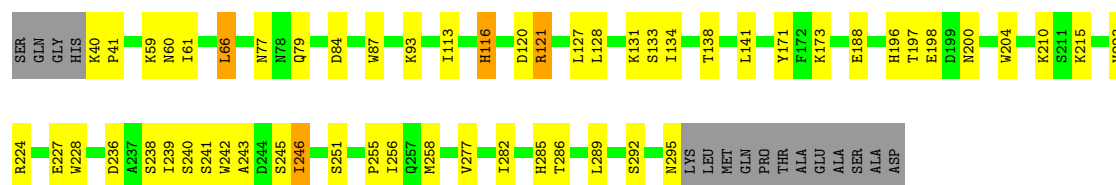
3 Residue-property plots

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 failed to run properly.

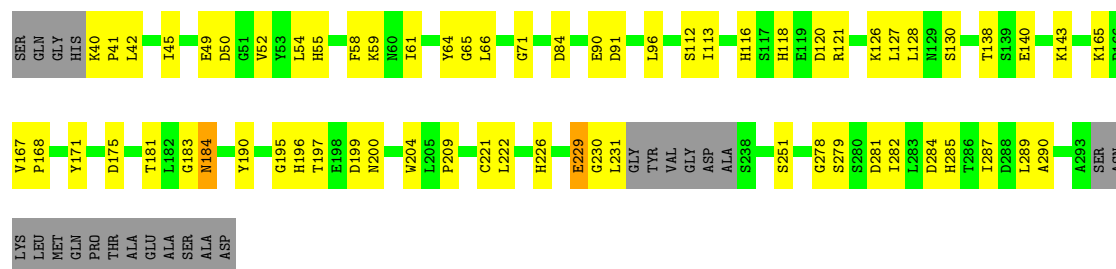
• Molecule 1: GIM-1 PROTEIN

Chain A: 



• Molecule 1: GIM-1 PROTEIN

Chain B: 



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	38.79Å 135.38Å 40.51Å 90.00° 90.23° 90.00°	Depositor
Resolution (Å)	19.71 – 2.06	Depositor
% Data completeness (in resolution range)	97.1 (19.71-2.06)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.06Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.185 , 0.235	Depositor
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.120	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for l,k,-h 0.068 for h,-k,-l 0.043 for l,-k,h	Xtriage
Total number of atoms	6971	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.42% 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	1.04	0/1822	1.01	3/2475 (0.1%)
1	B	0.76	0/1718	0.95	4/2332 (0.2%)
All	All	0.92	0/3540	0.98	7/4807 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229	GLU	N-CA-C	-7.02	105.53	112.97
1	A	256	ILE	N-CA-C	6.91	117.96	108.84
1	B	52	VAL	N-CA-C	5.69	116.31	108.12
1	A	77	ASN	CB-CA-C	-5.65	109.54	117.23
1	B	165	LYS	CA-C-N	-5.57	114.02	119.76
1	B	165	LYS	C-N-CA	-5.57	114.02	119.76
1	A	256	ILE	CB-CA-C	-5.04	104.57	111.33

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	1755	1731	1690	60	1
1	B	1661	1646	1618	45	1
2	A	119	0	0	32	2
2	B	59	0	0	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3594	3377	3308	101	3

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 15.

All (101) 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:128:LEU:O	2:A:2059:HOH:O	1.64	1.14
1:A:242:TRP:O	2:A:2105:HOH:O	1.69	1.09
1:A:134:ILE:N	2:A:2059:HOH:O	1.85	1.07
1:A:40:LYS:N	2:A:2001:HOH:O	1.87	1.07
1:A:245:SER:N	2:A:2105:HOH:O	1.99	0.93
1:A:228:TRP:O	2:A:2101:HOH:O	1.86	0.91
1:B:65:GLY:O	2:B:2008:HOH:O	1.89	0.89
1:A:120:ASP:C	2:A:2017:HOH:O	2.18	0.86
1:A:116:HIS:CD2	1:A:121:ARG:HG3	2.16	0.80
1:B:61:ILE:N	2:B:2008:HOH:O	1.90	0.78
1:A:93:LYS:NZ	2:A:2035:HOH:O	2.03	0.78
1:A:243:ALA:C	2:A:2105:HOH:O	2.29	0.75
1:B:42:LEU:O	2:B:2003:HOH:O	2.06	0.74
1:A:120:ASP:O	2:A:2017:HOH:O	2.06	0.74
1:B:251:SER:HB2	2:B:2055:HOH:O	1.88	0.73
1:A:285:HIS:NE2	2:A:2101:HOH:O	2.11	0.73
1:A:79:GLN:OE1	2:A:2026:HOH:O	2.10	0.69
1:A:173:LYS:O	2:A:2069:HOH:O	2.12	0.67
1:A:242:TRP:C	2:A:2105:HOH:O	2.30	0.65
1:B:116:HIS:CD2	1:B:121:ARG:HG3	2.32	0.64
1:A:238:SER:HB3	1:A:241[B]:SER:OG	2.00	0.61
1:B:278:GLY:HA3	1:B:282:ILE:CD1	2.31	0.61
1:B:127:LEU:O	1:B:130:SER:OG	2.13	0.58
1:A:40:LYS:HD2	1:A:66:LEU:HD21	1.86	0.58
1:A:282:ILE:O	1:A:286[B]:THR:HG23	2.03	0.58
1:A:40:LYS:HD2	1:A:66:LEU:CD2	2.35	0.57
1:A:141:LEU:HD21	2:A:2090:HOH:O	2.03	0.57
1:A:210[B]:LYS:HE3	2:A:2012:HOH:O	2.03	0.57
1:A:198:GLU:OE1	2:A:2090:HOH:O	2.18	0.56
1:A:121:ARG:CA	2:A:2017:HOH:O	2.53	0.56
1:A:224:ARG:H	1:A:286[B]:THR:CG2	2.18	0.56
1:A:141:LEU:HD11	2:A:2090:HOH:O	2.06	0.55
1:B:112:SER:HB3	1:B:128:LEU:CD1	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286[A]:THR:HA	2:A:2115:HOH:O	2.08	0.54
1:B:226:HIS:CE1	1:B:285:HIS:HB2	2.43	0.54
1:A:227:GLU:O	1:B:229:GLU:HG2	2.09	0.53
1:A:286[B]:THR:HA	2:A:2115:HOH:O	2.09	0.52
1:B:183:GLY:O	1:B:184:ASN:CB	2.58	0.52
1:A:59:LYS:HE2	1:A:87:TRP:NE1	2.25	0.51
1:A:289:LEU:HD12	2:A:2115:HOH:O	2.10	0.51
1:B:196:HIS:HB2	1:B:221:CYS:O	2.11	0.51
1:B:61:ILE:HG13	1:B:61:ILE:O	2.10	0.51
1:B:183:GLY:O	1:B:184:ASN:HB2	2.10	0.50
1:A:215:LYS:HE3	2:A:2092:HOH:O	2.12	0.50
1:A:223:VAL:HA	1:A:286[B]:THR:HG21	1.93	0.50
1:A:61:ILE:HD12	1:B:61:ILE:HD13	1.94	0.50
1:B:91:ASP:OD2	2:B:2007:HOH:O	2.20	0.49
1:A:285:HIS:CE1	2:A:2101:HOH:O	2.62	0.49
1:B:140:GLU:CD	2:B:2044:HOH:O	2.55	0.49
1:B:120:ASP:OD1	1:B:120:ASP:N	2.44	0.49
1:B:61:ILE:HA	2:B:2009:HOH:O	2.13	0.49
1:A:246:ILE:CD1	1:A:286[B]:THR:OG1	2.61	0.48
1:B:96:LEU:HD11	1:B:128:LEU:HD23	1.95	0.48
1:B:167:VAL:HB	1:B:168:PRO:HD2	1.96	0.48
1:B:40:LYS:HG3	1:B:41:PRO:HD2	1.96	0.48
1:A:127:LEU:HD11	1:A:131:LYS:HE3	1.96	0.47
1:A:258:MET:SD	1:A:277:VAL:HG11	2.54	0.47
1:A:210[A]:LYS:HE2	2:A:2047:HOH:O	2.14	0.47
1:B:45:ILE:HD11	1:B:54:LEU:HD23	1.97	0.47
1:A:246:ILE:HD12	1:A:286[B]:THR:OG1	2.14	0.47
1:A:285:HIS:O	2:A:2115:HOH:O	2.21	0.46
1:B:55:HIS:CE1	1:B:71:GLY:HA3	2.51	0.46
1:B:204:TRP:O	1:B:209:PRO:HD3	2.16	0.46
1:A:121:ARG:HA	2:A:2017:HOH:O	2.14	0.46
1:B:126:LYS:HE2	2:B:2018:HOH:O	2.15	0.46
1:B:195:GLY:HA3	1:B:222:LEU:CD1	2.45	0.46
1:A:121:ARG:NE	2:A:2017:HOH:O	2.48	0.46
1:A:224:ARG:H	1:A:286[B]:THR:HG22	1.80	0.46
1:B:96:LEU:HD21	1:B:128:LEU:HD21	1.98	0.45
1:B:58:PHE:N	2:B:2001:HOH:O	2.43	0.45
1:A:215:LYS:HD3	1:A:255:PRO:O	2.16	0.45
1:A:61:ILE:CD1	1:B:61:ILE:HD13	2.47	0.45
1:A:292:SER:O	1:A:295:ASN:OD1	2.36	0.44
1:B:199:ASP:OD1	1:B:199:ASP:N	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ARG:N	2:A:2017:HOH:O	2.43	0.44
1:B:251:SER:CB	2:B:2055:HOH:O	2.57	0.44
1:A:59:LYS:HE2	1:A:87:TRP:CD1	2.52	0.44
1:B:175:ASP:O	1:B:190:TYR:HA	2.18	0.44
1:B:61:ILE:HG13	1:B:64:TYR:HB3	2.00	0.43
1:B:279:SER:C	1:B:281:ASP:N	2.76	0.43
1:A:258:MET:CG	1:A:277:VAL:CG1	2.96	0.43
1:A:61:ILE:HD12	1:B:61:ILE:HG21	2.01	0.42
1:A:196:HIS:CD2	1:A:197:THR:HG23	2.55	0.42
1:A:41:PRO:HD2	2:A:2003:HOH:O	2.19	0.42
1:A:138:THR:O	1:A:171:TYR:HA	2.19	0.42
1:B:222:LEU:HD12	1:B:222:LEU:HA	1.86	0.42
1:B:138:THR:O	1:B:171:TYR:HA	2.19	0.42
1:B:118:HIS:CE1	1:B:197:THR:HG22	2.55	0.42
1:B:231:LEU:HD11	1:B:290:ALA:HA	2.01	0.42
1:A:242:TRP:O	1:A:242:TRP:HD1	2.03	0.41
1:A:133:SER:N	2:A:2059:HOH:O	2.53	0.41
1:B:278:GLY:HA3	1:B:282:ILE:HD11	2.01	0.41
1:A:60:ASN:HA	1:A:66:LEU:HD12	2.01	0.41
1:B:116:HIS:HD2	1:B:118:HIS:H	1.67	0.41
1:A:204:TRP:CH2	1:A:215:LYS:HA	2.56	0.41
1:A:127:LEU:O	1:A:131:LYS:HG3	2.20	0.41
1:B:278:GLY:HA3	1:B:282:ILE:HD12	2.02	0.41
1:B:284:ASP:HA	1:B:287:ILE:HD12	2.04	0.40
1:A:116:HIS:NE2	1:A:121:ARG:HG3	2.35	0.40
1:A:236:ASP:HB3	2:A:2089:HOH:O	2.21	0.40
1:B:230:GLY:O	1:B:289:LEU:HD13	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188[B]:GLU:OE2	1:B:171:TYR:OH[2_655]	1.93	0.27
2:A:2040:HOH:O	2:A:2070:HOH:O[1_655]	2.06	0.14
2:A:2024:HOH:O	2:A:2068:HOH:O[1_655]	2.08	0.12

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	226/233 (97%)	210 (93%)	15 (7%)	1 (0%)	30	23
1	B	209/233 (90%)	188 (90%)	18 (9%)	3 (1%)	9	3
All	All	435/466 (93%)	398 (92%)	33 (8%)	4 (1%)	12	7

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	84	ASP
1	A	84	ASP
1	B	184	ASN
1	B	49	GLU

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	198/199 (100%)	189 (96%)	9 (4%)	24	18
1	B	187/199 (94%)	178 (95%)	9 (5%)	23	16
All	All	385/398 (97%)	367 (95%)	18 (5%)	24	16

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LEU
1	A	113	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	116	HIS
1	A	121	ARG
1	A	200	ASN
1	A	239	ILE
1	A	240	SER
1	A	246	ILE
1	A	251	SER
1	B	50	ASP
1	B	59	LYS
1	B	66	LEU
1	B	90[A]	GLU
1	B	90[B]	GLU
1	B	113	ILE
1	B	143	LYS
1	B	181	THR
1	B	200	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	HIS
1	A	285	HIS
1	B	116	HIS
1	B	118	HIS
1	B	196	HIS
1	B	226	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.