



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1XW8 / pdb_00001xw8
Title : X-ray structure of putative lactam utilization protein YBGL. Northeast Structural Genomics Consortium target ET90.
Authors : Kuzin, A.P.; Chen, Y.; Vorobiev, S.M.; Acton, T.B.; Ma, L.-C.; Xiao, R.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2004-10-29
Resolution : 2.00 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
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

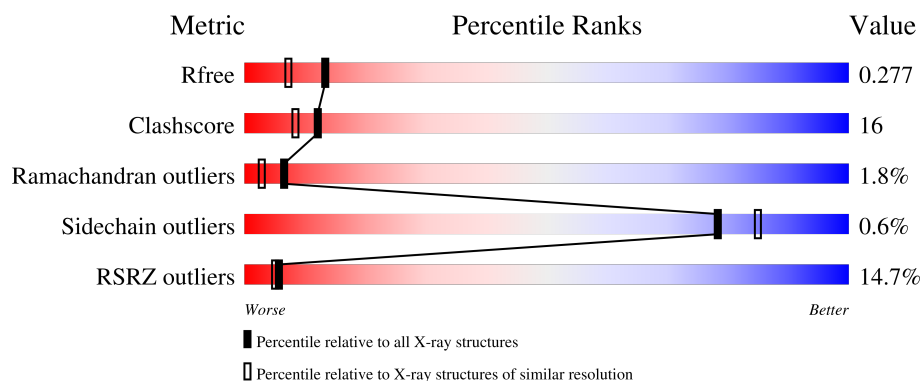
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	252	13% 63% 27% • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1758 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 UPF0271 protein ybgL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	Se	0	0	0
			1699	1060	308	320	5	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P75746
A	40	MSE	MET	modified residue	UNP P75746
A	71	MSE	MET	modified residue	UNP P75746
A	100	MSE	MET	modified residue	UNP P75746
A	108	MSE	MET	modified residue	UNP P75746
A	194	MSE	MET	modified residue	UNP P75746
A	245	LEU	-	expression tag	UNP P75746
A	246	GLU	-	expression tag	UNP P75746
A	247	HIS	-	expression tag	UNP P75746
A	248	HIS	-	expression tag	UNP P75746
A	249	HIS	-	expression tag	UNP P75746
A	250	HIS	-	expression tag	UNP P75746
A	251	HIS	-	expression tag	UNP P75746
A	252	HIS	-	expression tag	UNP P75746

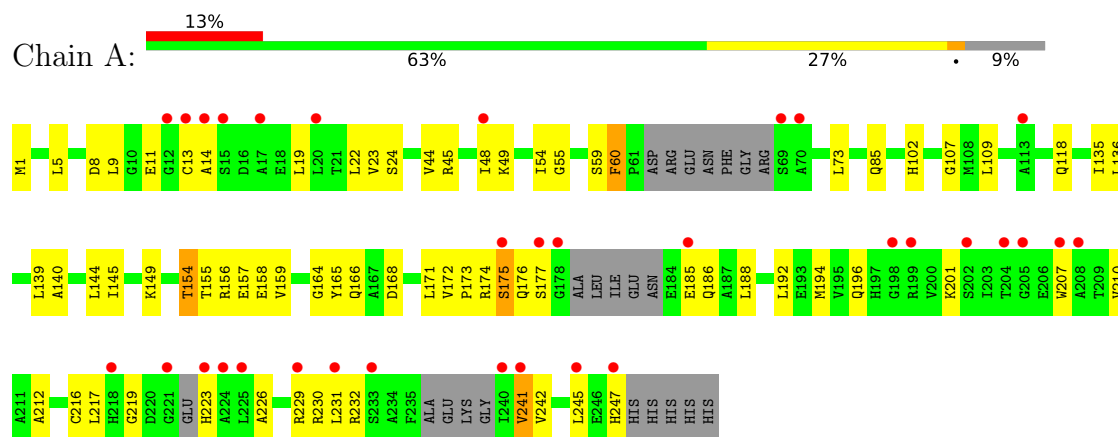
- Molecule 2 is water.

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

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: UPF0271 protein ybgL



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	72.67Å 37.21Å 79.80Å 90.00° 93.97° 90.00°	Depositor
Resolution (Å)	25.86 – 2.00 25.86 – 2.00	Depositor EDS
% Data completeness (in resolution range)	82.5 (25.86-2.00) 89.7 (25.86-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.75 (at 1.99Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.241 , 0.265 0.254 , 0.277	Depositor DCC
R_{free} test set	1153 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.8	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	1758	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.37% 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

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	0.38	0/1717	0.90	4/2312 (0.2%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	GLN	N-CA-C	-11.05	99.79	113.28
1	A	73	LEU	N-CA-C	-5.41	100.82	109.04
1	A	60	PHE	N-CA-C	-5.08	102.78	110.39
1	A	154	THR	N-CA-C	-5.05	102.38	109.96

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	1699	0	1694	53	0
2	A	59	0	0	0	0
All	All	1758	0	1694	53	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 16.

All (53) 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:136:LEU:HD11	1:A:144:LEU:HG	1.47	0.96
1:A:194:MSE:HE2	1:A:210:VAL:HG21	1.63	0.81
1:A:5:LEU:HD13	1:A:217:LEU:HD11	1.68	0.75
1:A:156:ARG:HG2	1:A:245:LEU:HD22	1.74	0.68
1:A:59:SER:H	1:A:85:GLN:HE22	1.43	0.66
1:A:156:ARG:HH12	1:A:247:HIS:HD2	1.46	0.64
1:A:155:THR:O	1:A:156:ARG:HD2	1.98	0.64
1:A:158:GLU:OE1	1:A:216:CYS:HB2	1.98	0.63
1:A:139:LEU:HD11	1:A:171:LEU:HD21	1.79	0.63
1:A:139:LEU:HD11	1:A:171:LEU:CD2	2.31	0.61
1:A:173:PRO:HB2	1:A:177:SER:HA	1.83	0.60
1:A:201:LYS:NZ	1:A:207:TRP:HE1	2.00	0.60
1:A:19:LEU:HD12	1:A:22:LEU:HD11	1.84	0.59
1:A:145:ILE:O	1:A:149:LYS:HG2	2.02	0.59
1:A:226:ALA:HA	1:A:229:ARG:HH11	1.67	0.59
1:A:156:ARG:HH12	1:A:247:HIS:CD2	2.22	0.58
1:A:174:ARG:O	1:A:175:SER:HB3	2.02	0.58
1:A:5:LEU:O	1:A:23:VAL:HG22	2.03	0.57
1:A:154:THR:HG21	1:A:247:HIS:HB3	1.86	0.56
1:A:1:MSE:HE1	1:A:196:GLN:HG2	1.91	0.53
1:A:156:ARG:NH1	1:A:247:HIS:HB2	2.25	0.52
1:A:55:GLY:HA3	1:A:102:HIS:CE1	2.46	0.51
1:A:156:ARG:HG2	1:A:245:LEU:HD13	1.91	0.51
1:A:135:ILE:HD13	1:A:245:LEU:HB2	1.93	0.49
1:A:22:LEU:O	1:A:232:ARG:HD2	2.12	0.49
1:A:8:ASP:O	1:A:9:LEU:HD23	2.13	0.49
1:A:173:PRO:HD2	1:A:177:SER:HB2	1.94	0.49
1:A:19:LEU:HD22	1:A:219:GLY:HA3	1.95	0.49
1:A:145:ILE:HA	1:A:155:THR:HG21	1.96	0.46
1:A:24:SER:HB2	1:A:242:VAL:HG12	1.95	0.46
1:A:44:VAL:HG13	1:A:54:ILE:HD13	1.97	0.45
1:A:171:LEU:HD22	1:A:171:LEU:N	2.32	0.45
1:A:194:MSE:CE	1:A:210:VAL:HG21	2.41	0.45
1:A:11:GLU:C	1:A:13:CYS:H	2.26	0.43
1:A:48:ILE:HG13	1:A:49:LYS:N	2.33	0.43
1:A:155:THR:C	1:A:156:ARG:HD2	2.43	0.43
1:A:60:PHE:CE2	1:A:109:LEU:HD13	2.53	0.43
1:A:159:VAL:HG11	1:A:212:ALA:HB2	2.01	0.43
1:A:173:PRO:HB2	1:A:177:SER:CA	2.49	0.43
1:A:201:LYS:HZ1	1:A:207:TRP:HE1	1.67	0.43
1:A:188:LEU:O	1:A:192:LEU:HD23	2.18	0.42
1:A:174:ARG:O	1:A:175:SER:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LEU:HD23	1:A:231:LEU:O	2.20	0.42
1:A:156:ARG:HG2	1:A:245:LEU:CD2	2.47	0.42
1:A:45:ARG:O	1:A:48:ILE:HG12	2.19	0.42
1:A:13:CYS:SG	1:A:14:ALA:N	2.92	0.42
1:A:223:HIS:CD2	1:A:226:ALA:HB2	2.54	0.42
1:A:140:ALA:HA	1:A:157:GLU:HB3	2.01	0.41
1:A:164:GLY:O	1:A:172:VAL:HG12	2.19	0.41
1:A:166:GLN:HB2	1:A:168:ASP:OD1	2.19	0.41
1:A:185:GLU:OE1	1:A:230:ARG:HD3	2.20	0.41
1:A:165:TYR:CE2	1:A:194:MSE:HE1	2.56	0.41
1:A:241:VAL:O	1:A:241:VAL:HG13	2.21	0.41

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	220/252 (87%)	207 (94%)	9 (4%)	4 (2%)	6 3

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	VAL
1	A	175	SER
1	A	176	GLN
1	A	107	GLY

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	168/180 (93%)	167 (99%)	1 (1%)	78	85

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	85	GLN
1	A	102	HIS
1	A	111	ASN
1	A	112	GLN
1	A	190	GLN
1	A	196	GLN
1	A	247	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

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	224/252 (88%)	0.91	33 (14%) 6 5	15, 34, 64, 82	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	177	SER	4.9
1	A	178	GLY	4.8
1	A	175	SER	4.8
1	A	247	HIS	4.4
1	A	224	ALA	4.0
1	A	225	LEU	3.8
1	A	221	GLY	3.6
1	A	240	ILE	3.6
1	A	207	TRP	3.3
1	A	223	HIS	3.0
1	A	13	CYS	3.0
1	A	14	ALA	3.0
1	A	15	SER	2.9
1	A	17	ALA	2.9
1	A	69	SER	2.7
1	A	185	GLU	2.7
1	A	113	ALA	2.6
1	A	208	ALA	2.6
1	A	202	SER	2.5
1	A	20	LEU	2.5
1	A	231	LEU	2.5
1	A	233	SER	2.4
1	A	204	THR	2.4
1	A	48	ILE	2.3
1	A	229	ARG	2.3
1	A	218	HIS	2.2
1	A	241	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	205	GLY	2.2
1	A	12	GLY	2.2
1	A	198	GLY	2.2
1	A	245	LEU	2.1
1	A	70	ALA	2.1
1	A	199	ARG	2.0

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.