



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 11:58 AM EDT

PDB ID : 3GRH
Title : Crystal structure of escherichia coli ybhc
Authors : Eklof, J.M.; Tan, T.C.; Divne, C.; Brumer, H.
Deposited on : 2009-03-25
Resolution : 1.70 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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

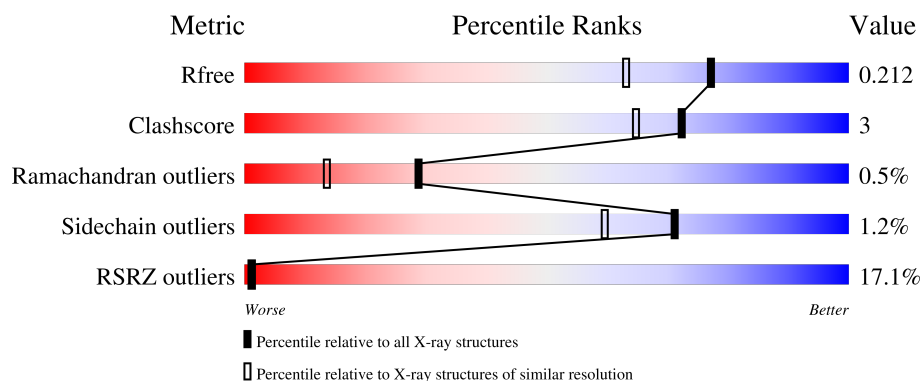
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	422	<div> <div>16%</div> <div>86%</div> <div>7% • 6%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3287 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 Acyl-CoA thioester hydrolase ybgC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3044	1891	546	599	8			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP P46130
A	-21	HIS	-	expression tag	UNP P46130
A	-20	HIS	-	expression tag	UNP P46130
A	-19	HIS	-	expression tag	UNP P46130
A	-18	HIS	-	expression tag	UNP P46130
A	-17	HIS	-	expression tag	UNP P46130
A	-16	HIS	-	expression tag	UNP P46130
A	-15	SER	-	expression tag	UNP P46130
A	-14	SER	-	expression tag	UNP P46130
A	-13	GLY	-	expression tag	UNP P46130
A	-12	VAL	-	expression tag	UNP P46130
A	-11	ASP	-	expression tag	UNP P46130
A	-10	LEU	-	expression tag	UNP P46130
A	-9	GLY	-	expression tag	UNP P46130
A	-8	THR	-	expression tag	UNP P46130
A	-7	GLU	-	expression tag	UNP P46130
A	-6	ASN	-	expression tag	UNP P46130
A	-5	LEU	-	expression tag	UNP P46130
A	-4	TYR	-	expression tag	UNP P46130
A	-3	PHE	-	expression tag	UNP P46130
A	-2	GLN	-	expression tag	UNP P46130
A	-1	SER	-	expression tag	UNP P46130
A	0	MET	-	initiating methionine	UNP P46130

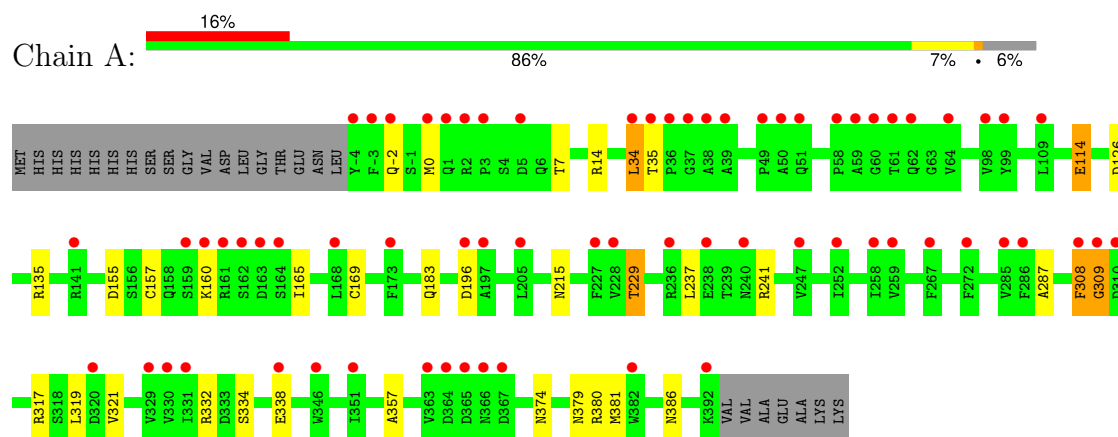
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	243	Total 243	O 243	0	0

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: Acyl-CoA thioester hydrolase ybgC



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	79.20Å 79.20Å 159.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.70 28.95 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-1.70) 99.9 (28.95-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.79 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.193 , 0.208 0.198 , 0.212	Depositor DCC
R_{free} test set	1308 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 59.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.039 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3287	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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	1.10	3/3111 (0.1%)	1.01	10/4242 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	GLU	CB-CG	11.85	1.74	1.52
1	A	114	GLU	CG-CD	7.71	1.63	1.51
1	A	114	GLU	CD-OE2	6.89	1.33	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	A	126	ASP	CB-CG-OD1	7.39	124.95	118.30
1	A	196	ASP	CB-CG-OD1	7.08	124.67	118.30
1	A	381	MET	CG-SD-CE	-7.06	88.91	100.20
1	A	241	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	114	GLU	OE1-CD-OE2	-5.20	117.06	123.30
1	A	14	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	155	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	A	135	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	332	ARG	NE-CZ-NH1	5.02	122.81	120.30

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	3044	0	2915	19	0
2	A	243	0	0	0	0
All	All	3287	0	2915	19	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 3.

All (19) 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:114:GLU:CG	1:A:114:GLU:CB	1.74	1.59
1:A:160:LYS:NZ	1:A:169:CYS:SG	2.40	0.94
1:A:334:SER:H	1:A:386:ASN:HD22	1.35	0.72
1:A:157:CYS:HG	1:A:169:CYS:HG	1.36	0.71
1:A:34:LEU:HD12	1:A:34:LEU:O	1.92	0.70
1:A:374:ASN:HD22	1:A:380:ARG:HH11	1.40	0.69
1:A:357:ALA:H	1:A:379:ASN:HD22	1.41	0.68
1:A:-2:GLN:HG3	1:A:0:MET:HE1	1.92	0.51
1:A:334:SER:H	1:A:386:ASN:ND2	2.09	0.48
1:A:-2:GLN:HG3	1:A:0:MET:CE	2.44	0.47
1:A:0:MET:CE	1:A:0:MET:HA	2.45	0.47
1:A:319:LEU:HG	1:A:321:VAL:HG13	1.99	0.45
1:A:357:ALA:H	1:A:379:ASN:ND2	2.11	0.45
1:A:308:PHE:O	1:A:309:GLY:O	2.35	0.45
1:A:183:GLN:HA	1:A:215:ASN:O	2.18	0.44
1:A:160:LYS:NZ	1:A:165:ILE:O	2.45	0.42
1:A:229:THR:HB	1:A:237:LEU:CD2	2.51	0.41
1:A:287:ALA:HA	1:A:317:ARG:O	2.20	0.41
1:A:338:GLU:OE1	1:A:338:GLU:HA	2.21	0.40

There are no symmetry-related clashes.

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	395/422 (94%)	379 (96%)	14 (4%)	2 (0%)	29	13

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	GLY
1	A	308	PHE

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	325/346 (94%)	321 (99%)	4 (1%)	71	59

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	34	LEU
1	A	35	THR
1	A	229	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	183	GLN
1	A	215	ASN
1	A	249	ASN
1	A	269	ASN
1	A	280	GLN
1	A	302	ASN
1	A	374	ASN
1	A	379	ASN
1	A	386	ASN

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 ⓘ

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	397/422 (94%)	0.93	68 (17%) ⓘ ⓘ	6, 15, 30, 48	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	PRO	10.9
1	A	37	GLY	10.6
1	A	308	PHE	9.8
1	A	35	THR	8.5
1	A	60	GLY	8.1
1	A	38	ALA	7.7
1	A	364	ASP	7.3
1	A	59	ALA	7.2
1	A	366	ASN	6.9
1	A	365	ASP	6.7
1	A	367	ASP	6.2
1	A	-2	GLN	5.5
1	A	61	THR	5.4
1	A	34	LEU	5.2
1	A	310	ASP	5.2
1	A	-3	PHE	5.1
1	A	163	ASP	5.1
1	A	338	GLU	4.5
1	A	5	ASP	4.3
1	A	-4	TYR	3.9
1	A	329	VAL	3.9
1	A	50	ALA	3.8
1	A	161	ARG	3.6
1	A	39	ALA	3.5
1	A	363	VAL	3.5
1	A	0	MET	3.5
1	A	62	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	162	SER	3.4
1	A	392	LYS	3.4
1	A	197	ALA	3.3
1	A	247	VAL	3.2
1	A	267	PHE	3.2
1	A	64	VAL	3.1
1	A	141	ARG	3.1
1	A	58	PRO	3.1
1	A	285	VAL	3.0
1	A	236	ARG	2.9
1	A	351	ILE	2.7
1	A	173	PHE	2.7
1	A	51	GLN	2.7
1	A	346	TRP	2.6
1	A	331	ILE	2.5
1	A	3	PRO	2.5
1	A	330	VAL	2.5
1	A	168	LEU	2.5
1	A	240	ASN	2.5
1	A	286	PHE	2.5
1	A	98	VAL	2.5
1	A	109	LEU	2.5
1	A	1	GLN	2.4
1	A	196	ASP	2.4
1	A	2	ARG	2.4
1	A	259	VAL	2.4
1	A	164	SER	2.3
1	A	99	TYR	2.3
1	A	309	GLY	2.3
1	A	159	SER	2.3
1	A	205	LEU	2.2
1	A	252	ILE	2.2
1	A	272	PHE	2.2
1	A	258	ILE	2.2
1	A	160	LYS	2.2
1	A	49	PRO	2.1
1	A	227	PHE	2.1
1	A	228	VAL	2.1
1	A	320	ASP	2.1
1	A	238	GLU	2.0
1	A	382	TRP	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 monosaccharides 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.