



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2022 – 02:11 PM EDT

PDB ID : 7N6H
Title : The crystal structure of the GH30 subfamily 10 enzyme, AcXbh30A from *Acetivibrio clariflavus*
Authors : Tan, K.; St John, F.J.
Deposited on : 2021-06-08
Resolution : 1.28 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
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)	:	2.29

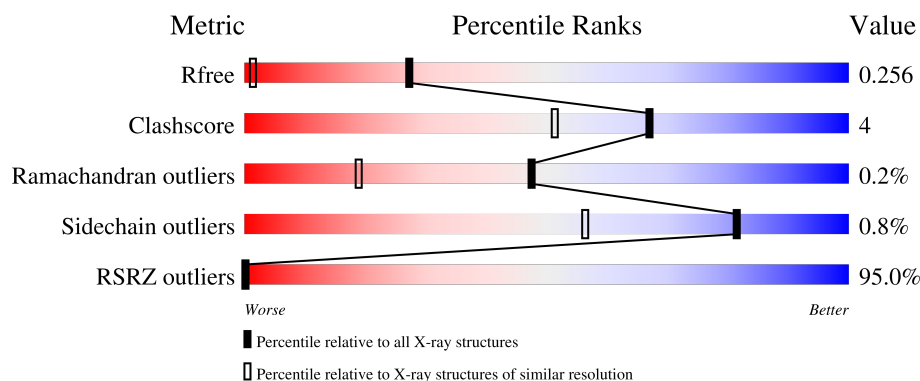
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.28 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	1850 (1.30-1.26)
Clashscore	141614	1926 (1.30-1.26)
Ramachandran outliers	138981	1860 (1.30-1.26)
Sidechain outliers	138945	1859 (1.30-1.26)
RSRZ outliers	127900	1807 (1.30-1.26)

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	444	<div> <div>92%</div> <div>89% 9%</div> </div>
1	B	444	<div> <div>93%</div> <div>88% 9%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	A	504	-	-	-	X
2	CL	A	506	-	-	-	X
2	CL	A	508	-	-	X	-
2	CL	A	511	-	-	-	X
2	CL	A	515	-	-	X	-
2	CL	B	503	-	-	X	-
2	CL	B	507	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7649 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 AcXbh30A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	3	0
			3454	2194	570	679	11			
1	B	433	Total	C	N	O	S	0	1	0
			3443	2187	569	676	11			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	MET	-	initiating methionine	UNP G8LU16
A	464	LEU	-	expression tag	UNP G8LU16
A	465	GLU	-	expression tag	UNP G8LU16
A	466	HIS	-	expression tag	UNP G8LU16
A	467	HIS	-	expression tag	UNP G8LU16
A	468	HIS	-	expression tag	UNP G8LU16
A	469	HIS	-	expression tag	UNP G8LU16
A	470	HIS	-	expression tag	UNP G8LU16
A	471	HIS	-	expression tag	UNP G8LU16
B	28	MET	-	initiating methionine	UNP G8LU16
B	464	LEU	-	expression tag	UNP G8LU16
B	465	GLU	-	expression tag	UNP G8LU16
B	466	HIS	-	expression tag	UNP G8LU16
B	467	HIS	-	expression tag	UNP G8LU16
B	468	HIS	-	expression tag	UNP G8LU16
B	469	HIS	-	expression tag	UNP G8LU16
B	470	HIS	-	expression tag	UNP G8LU16
B	471	HIS	-	expression tag	UNP G8LU16

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	15	Total	Cl	0	0
			15	15		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	8	Total	Cl	0	0
			8	8		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	388	Total	O	0	0
			388	388		
4	B	329	Total	O	0	0
			329	329		

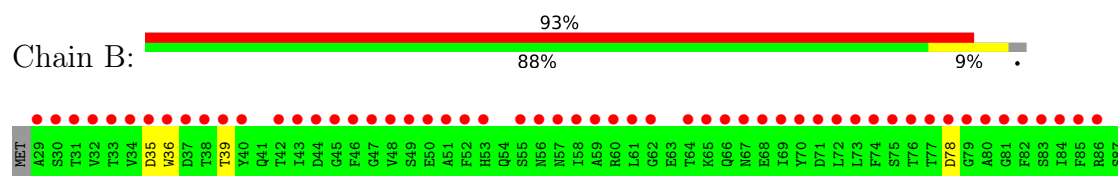
3 Residue-property plots

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 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: AcXbh30A



• Molecule 1: AcXbh30A



L448	P388	C328	G268	S208	M148	I88
F449	K389	F329	S269	P209	M149	L89
M450	T390	T331	S270	E210	T150	G90
S451	G391	T331	Y271	E211	T151	D91
L452	K392	N332	I272	L212	N152	G92
T453	F393	N333	P273	R213	G153	G93
T454	A394	G334	F274	I214	S154	T94
F455	I395	E335	T275	F215	V155	H95
V396	V396	G336	T276	M216	V156	G96
O457	A397	L337	T277	R217	G157	H97
I398	I398	I338	K278	D218	G158	A98
N399	N399	K339	S279	Y219	S159	D99
M400	M400	K340	K280	L220	L160	D100
G401	G401	D341	G281	V221	R161	G101
M402	M402	L342	K282	T222	L162	P102
S403	S403	N343	G283	T223	D163	M103
K404	K404	S344	I284	F224	K164	M104
Q405	Q405	K345	W285	D225	Y165	T105
S406	S406	T346	M286	K226	Q166	M106
HIS	HIS	Y347	T287	E227	A167	Q107
HIS	HIS	K348	E288	N228	Y168	P108
Y409	Y409	V349	V289	I229	A169	A109
T410	T410	A350	S290	T230	T170	E110
L411	L411	K351	D291	A231	Y171	D111
K412	K412	R352	M292	K232	L172	V112
G413	G413	L353	N293	V233	A173	W113
F414	F414	T354	G294	F234	E174	D114
S415	S415	T355	N295	F235	H175	W115
P416	P416	I356	D296	A236	L176	M116
A417	A417	G357	T297	E237	K177	E117
S418	S418	Q358	T298	N238	M178	S118
V419	V419	F359	I299	M239	Y179	N119
T420	T420	S360	N300	S240	K180	D120
P421	P421	R361	D301	F241	S181	D121
Y422	Y422	F362	G302	N242	K182	Q122
T423	T423	I363	L303	E243	F183	Q122
T424	T424	R364	R304	Q244	G184	I123
S425	S425	P365	W305	Y245	T185	P124
S426	S426	G366	A306	A246	E186	M125
T427	T427	W367	K307	I247	I187	I126
Q428	Q428	Q368	E308	N248	T188	M127
N429	N429	R369	I309	S249	H189	A128
L430	L430	I370	H310	L250	I190	I129
E431	E431	E371	D311	N251	G191	Q130
K432	K432	A372	F312	D252	I192	S131
G433	G433	T373	M313	P253	Q193	K132
S434	S434	K374	T314	L254	N194	Y133
D435	D435	N375	I315	A255	E195	G134
I436	I436	P376	T316	V256	P196	V135
T437	T437	W377	F317	K257	N197	D136
V438	V438	S378	G318	R258	L198	Q137
N439	N439	N379	N319	R259	E199	I138
M440	M440	V380	A320	D260	T200	L139
S441	S441	Y381	W321	I261	Y140	Y140
S442	S442	V382	F322	V262	S201	T141
F443	F443	T383	Y323	Q263	Y202	W142
S444	S444	A384	W324	A264	S203	W143
F445	F445	Y385	W325	H265	S204	S144
E446	E446	K386	G326	N266	C205	P145
L447	L447	D387	A327	Y267	W207	P146
						A147

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.87Å 108.02Å 66.84Å 90.00° 90.14° 90.00°	Depositor
Resolution (Å)	41.18 – 1.28 41.18 – 1.28	Depositor EDS
% Data completeness (in resolution range)	96.3 (41.18-1.28) 96.2 (41.18-1.28)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	13.51 (at 1.28Å)	Xtriage
Refinement program	PHENIX (1.19_4092: ???)	Depositor
R, R_{free}	0.202 , 0.254 0.203 , 0.256	Depositor DCC
R_{free} test set	10529 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	13.1	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 26.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.387 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7649	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CL, ACT

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	0.24	0/3544	0.47	0/4821
1	B	0.24	0/3533	0.46	0/4806
All	All	0.24	0/7077	0.47	0/9627

There are no bond length outliers.

There are no bond angle outliers.

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	3454	0	3292	24	0
1	B	3443	0	3281	24	0
2	A	15	0	0	8	0
2	B	8	0	0	5	0
3	A	8	0	6	0	0
3	B	4	0	3	0	0
4	A	388	0	0	4	0
4	B	329	0	0	3	0
All	All	7649	0	6582	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 4.

The worst 5 of 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)
2:A:510:CL:CL	4:A:896:HOH:O	2.38	0.78
1:A:213:ARG:NE	2:A:503:CL:CL	2.50	0.73
2:A:515:CL:CL	4:A:860:HOH:O	2.43	0.73
2:A:514:CL:CL	4:A:952:HOH:O	2.53	0.61
1:A:404:LYS:HG3	1:A:449:PRO:HD3	1.85	0.59

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	433/444 (98%)	418 (96%)	14 (3%)	1 (0%)	47	19
1	B	432/444 (97%)	418 (97%)	13 (3%)	1 (0%)	47	19
All	All	865/888 (97%)	836 (97%)	27 (3%)	2 (0%)	47	19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	TRP
1	B	324	TRP

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	376/384 (98%)	373 (99%)	3 (1%)	81	56
1	B	374/384 (97%)	371 (99%)	3 (1%)	81	56
All	All	750/768 (98%)	744 (99%)	6 (1%)	81	56

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	324	TRP
1	B	329	PHE
1	B	378	SER
1	A	324	TRP
1	A	206	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 23 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ACT	A	517	-	3,3,3	1.25	0	3,3,3	1.32	0
3	ACT	B	509	-	3,3,3	1.28	0	3,3,3	1.27	0
3	ACT	A	516	-	3,3,3	1.27	0	3,3,3	1.41	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	433/444 (97%)	4.62	410 (94%) 0 0	10, 15, 21, 38	0
1	B	433/444 (97%)	4.76	413 (95%) 0 0	9, 14, 21, 34	0
All	All	866/888 (97%)	4.69	823 (95%) 0 0	9, 15, 21, 38	0

The worst 5 of 823 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	29	ALA	36.8
1	B	306	ALA	14.5
1	B	146	PRO	12.5
1	B	246	ALA	11.7
1	B	329	PHE	11.5

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ACT	A	517	4/4	0.30	0.31	21,21,22,22	0
3	ACT	A	516	4/4	0.33	0.29	17,18,20,21	0
2	CL	A	511	1/1	0.37	0.49	33,33,33,33	0
2	CL	A	506	1/1	0.39	0.45	45,45,45,45	0
2	CL	A	501	1/1	0.46	0.29	39,39,39,39	0
2	CL	A	509	1/1	0.48	0.38	68,68,68,68	0
2	CL	A	502	1/1	0.49	0.15	31,31,31,31	0
2	CL	A	513	1/1	0.49	0.22	49,49,49,49	0
2	CL	A	503	1/1	0.51	0.20	52,52,52,52	0
3	ACT	B	509	4/4	0.61	0.31	24,24,26,27	0
2	CL	A	510	1/1	0.64	0.20	50,50,50,50	0
2	CL	B	507	1/1	0.66	0.54	79,79,79,79	0
2	CL	B	506	1/1	0.66	0.20	27,27,27,27	0
2	CL	A	507	1/1	0.67	0.33	23,23,23,23	0
2	CL	B	501	1/1	0.72	0.25	33,33,33,33	0
2	CL	B	505	1/1	0.73	0.25	38,38,38,38	0
2	CL	A	505	1/1	0.73	0.11	29,29,29,29	0
2	CL	A	514	1/1	0.74	0.21	45,45,45,45	0
2	CL	B	502	1/1	0.74	0.10	23,23,23,23	0
2	CL	A	512	1/1	0.75	0.22	40,40,40,40	0
2	CL	A	504	1/1	0.76	0.46	48,48,48,48	0
2	CL	A	515	1/1	0.78	0.21	26,26,26,26	0
2	CL	A	508	1/1	0.81	0.17	22,22,22,22	0
2	CL	B	504	1/1	0.82	0.24	39,39,39,39	0
2	CL	B	508	1/1	0.88	0.16	45,45,45,45	0
2	CL	B	503	1/1	0.91	0.06	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.