



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:17 AM GMT

PDB ID : 3E31
Title : H. influenzae beta-carbonic anhydrase, variant V47A
Authors : Rowlett, R.S.; Lee, J.
Deposited on : 2008-08-05
Resolution : 2.95 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

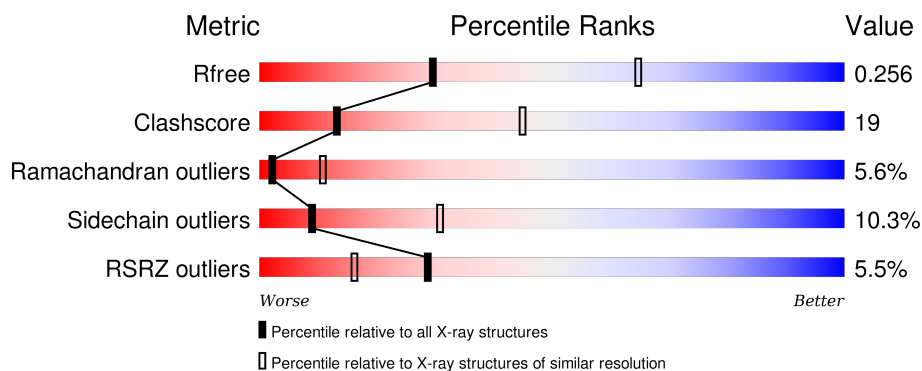
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	91344	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	229	<div> <div>3%</div> <div>46%</div> <div>26%</div> <div>7%</div> <div>•</div> <div>20%</div> </div>
1	B	229	<div> <div>5%</div> <div>50%</div> <div>24%</div> <div>•</div> <div>•</div> <div>21%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2905 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 Carbonic anhydrase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1452	923	261	261	7			
1	B	181	Total	C	N	O	S	0	0	0
			1435	912	258	258	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ALA	VAL	ENGINEERED	UNP P45148
B	47	ALA	VAL	ENGINEERED	UNP P45148

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	6	Total	O	0	0
			6	6		

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

[illegible]

Chain B:

5% 50% 24% 21%

MET ASP LYS ILE LYS GLN LEU PHE ALA ASN ASN THR SER TRP ALA GLN ARG MET LYS LYS GLU GLU ALA ASP HIS GLN T34 P35 H36 Y37 L38 W39 I40 G41 C42 S43 D44 S45 R46 A47 P48 A49 E50 K51 L52 T53 R54 L55 E56 P57 G58 E59 I60 R64 Q62 Y63 W67 L68 R69 T93 H98 T99 N100 C101 H105 L113 G114 L115 T116 L120 F128 K129 L133 L134 G135 K136 L137 R142 A143 D144 T147 Y156 M157 L158 L159 R160 T161 S162 I163 L176 Y181 D182 Y183 M184 D185 G186 R187

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	82.28 Å 82.28 Å 188.78 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.72 – 2.95 37.71 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (37.72-2.95) 99.9 (37.71-2.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.69 (at 2.95 Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.197 , 0.247 0.203 , 0.256	Depositor DCC
R_{free} test set	718 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	80.9	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 65.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 14323 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2905	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.76	0/1484	0.80	0/2014
1	B	0.79	1/1467 (0.1%)	0.82	0/1991
All	All	0.77	1/2951 (0.0%)	0.81	0/4005

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	42	CYS	CB-SG	-6.05	1.72	1.82

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190	ASP	Peptide
1	A	49	ALA	Peptide
1	B	192	GLY	Peptide
1	B	213	SER	Peptide

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	1452	0	1447	57	0
1	B	1435	0	1428	54	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	0	1	0
3	B	6	0	0	3	0
All	All	2905	0	2875	109	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 19.

The worst 5 of 109 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:B:214:ILE:O	1:B:214:ILE:HG22	1.67	0.94
1:B:213:SER:O	3:B:235:HOH:O	1.85	0.94
1:B:52:LEU:HD21	1:B:181:TYR:CE2	2.12	0.83
1:A:116:ILE:HD11	1:A:120:LEU:HD11	1.62	0.79
1:A:116:ILE:HD11	1:A:120:LEU:CD1	2.15	0.76

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	181/229 (79%)	153 (84%)	15 (8%)	13 (7%)	1 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	179/229 (78%)	151 (84%)	21 (12%)	7 (4%)	4	19
All	All	360/458 (79%)	304 (84%)	36 (10%)	20 (6%)	2	11

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	54	ASN
1	B	136	LYS
1	B	143	ALA
1	A	44	ASP
1	A	45	SER

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	157/200 (78%)	138 (88%)	19 (12%)	6	23
1	B	155/200 (78%)	142 (92%)	13 (8%)	14	42
All	All	312/400 (78%)	280 (90%)	32 (10%)	9	31

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	VAL
1	A	211	ARG
1	B	196	THR
1	A	198	ARG
1	A	215	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	B	54	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

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 [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	183/229 (79%)	0.30	8 (4%)	38 22	25, 41, 63, 67	0
1	B	181/229 (79%)	0.42	12 (6%)	22 11	24, 39, 71, 78	0
All	All	364/458 (79%)	0.36	20 (5%)	29 16	24, 40, 64, 78	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	49	ALA	4.8
1	A	34	THR	4.3
1	A	215	LEU	4.2
1	B	59	GLU	4.2
1	A	191	GLN	3.8

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	B	230	1/1	0.99	0.09	-1.24	51,51,51,51	0
2	ZN	A	230	1/1	0.99	0.08	-2.13	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.