



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 05:02 AM EST

PDB ID : 1CVD  
Title : STRUCTURAL CONSEQUENCES OF REDESIGNING A PROTEIN-ZINC  
BINDING SITE  
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Deposited on : unknown  
Resolution : 2.20 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](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

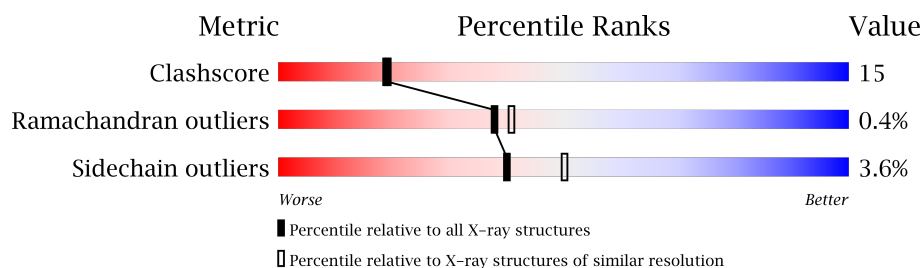
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	255	 64% 32% ..

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2139 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 II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2025	1300	345	377	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	CYS	HIS	CONFLICT	UNP P00918

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

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

- Molecule 3 is water.

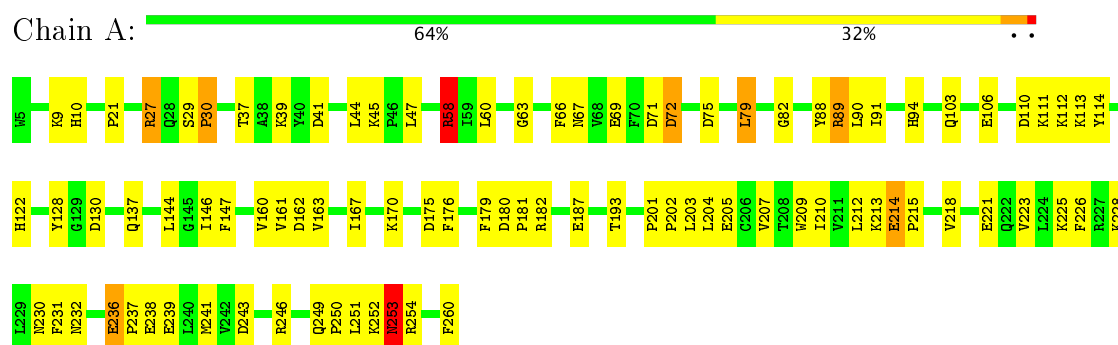
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	113	Total	O	0	0
			113	113		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

Note EDS was not executed.

#### • Molecule 1: CARBONIC ANHYDRASE II



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.70 Å   41.70 Å   73.00 Å 90.00°   104.60°   90.00°	Depositor
Resolution (Å)	7.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.184 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2139	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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	1.41	4/2084 (0.2%)	1.71	30/2829 (1.1%)

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	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	GLU	CD-OE1	6.25	1.32	1.25
1	A	238	GLU	CD-OE2	-6.17	1.18	1.25
1	A	214	GLU	CD-OE2	-5.49	1.19	1.25
1	A	228	LYS	C-O	5.16	1.33	1.23

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	ARG	NE-CZ-NH1	13.94	127.27	120.30
1	A	88	TYR	CB-CG-CD1	8.79	126.27	121.00
1	A	88	TYR	CB-CG-CD2	-8.53	115.89	121.00
1	A	162	ASP	CB-CG-OD2	-8.41	110.73	118.30
1	A	89	ARG	NE-CZ-NH2	-7.73	116.43	120.30
1	A	58	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	A	130	ASP	CB-CG-OD2	-7.44	111.60	118.30
1	A	130	ASP	CB-CG-OD1	7.22	124.79	118.30
1	A	214	GLU	OE1-CD-OE2	-7.21	114.64	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	PHE	CB-CG-CD1	-7.07	115.85	120.80
1	A	162	ASP	CB-CG-OD1	6.69	124.32	118.30
1	A	106	GLU	CG-CD-OE1	6.31	130.93	118.30
1	A	187	GLU	OE1-CD-OE2	6.30	130.86	123.30
1	A	94	HIS	N-CA-CB	6.15	121.68	110.60
1	A	72	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	246	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	236	GLU	CG-CD-OE1	6.01	130.31	118.30
1	A	79	LEU	CA-CB-CG	6.00	129.09	115.30
1	A	175	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	10	HIS	CA-CB-CG	-5.92	103.54	113.60
1	A	214	GLU	CG-CD-OE2	5.83	129.97	118.30
1	A	238	GLU	CG-CD-OE2	5.56	129.43	118.30
1	A	37	THR	CA-CB-CG2	5.51	120.11	112.40
1	A	106	GLU	CG-CD-OE2	-5.50	107.31	118.30
1	A	58	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	147	PHE	CB-CG-CD1	-5.40	117.02	120.80
1	A	27	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	A	207	VAL	CA-CB-CG2	5.22	118.73	110.90
1	A	89	ARG	CB-CA-C	-5.06	100.28	110.40
1	A	71	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	58	ARG	Sidechain

## 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	2025	0	1980	59	0
2	A	1	0	0	0	0
3	A	113	0	0	2	0
All	All	2139	0	1980	59	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 15.

All (59) 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:253:ASN:HD22	1:A:254:ARG:N	1.74	0.85
1:A:58:ARG:HD2	1:A:69:GLU:OE1	1.75	0.85
1:A:161:VAL:HG13	1:A:225:LYS:HD3	1.70	0.73
1:A:253:ASN:HD22	1:A:253:ASN:C	1.93	0.69
1:A:253:ASN:ND2	1:A:254:ARG:N	2.41	0.69
1:A:60:LEU:HD23	1:A:67:ASN:O	1.94	0.67
1:A:236:GLU:HB3	1:A:237:PRO:HD2	1.77	0.66
1:A:110:ASP:O	1:A:111:LYS:HB2	1.97	0.64
1:A:161:VAL:CG1	1:A:225:LYS:HD3	2.28	0.63
1:A:63:GLY:HA3	1:A:170:LYS:NZ	2.14	0.62
1:A:60:LEU:HD21	1:A:67:ASN:HB2	1.83	0.61
1:A:252:LYS:O	1:A:253:ASN:CG	2.41	0.58
1:A:47:LEU:HD11	1:A:210:ILE:HG21	1.85	0.57
1:A:72:ASP:OD2	1:A:91:ILE:HD12	2.05	0.57
1:A:63:GLY:HA3	1:A:170:LYS:HZ3	1.70	0.57
1:A:45:LYS:O	1:A:82:GLY:HA2	2.05	0.56
1:A:213:LYS:HD3	1:A:260:PHE:CZ	2.42	0.55
1:A:213:LYS:HD3	1:A:260:PHE:CE2	2.43	0.54
1:A:167:ILE:HG13	1:A:167:ILE:O	2.07	0.54
1:A:128:TYR:CE1	1:A:137:GLN:HG3	2.44	0.52
1:A:58:ARG:CD	1:A:69:GLU:OE1	2.54	0.52
1:A:112:LYS:HE3	1:A:114:TYR:CZ	2.44	0.52
1:A:103:GLN:NE2	1:A:243:ASP:OD1	2.43	0.52
1:A:112:LYS:HE3	1:A:114:TYR:CE2	2.46	0.51
1:A:58:ARG:HD2	1:A:69:GLU:CD	2.31	0.50
1:A:160:VAL:O	1:A:163:VAL:HG12	2.12	0.50
1:A:218:VAL:CG2	1:A:223:VAL:HG23	2.42	0.50
1:A:180:ASP:OD2	1:A:182:ARG:NH2	2.30	0.49
1:A:29:SER:HB3	1:A:30:PRO:HA	1.94	0.49
1:A:128:TYR:CZ	1:A:137:GLN:HG3	2.50	0.47
1:A:249:GLN:HB3	1:A:250:PRO:HD2	1.97	0.47
1:A:60:LEU:N	1:A:60:LEU:HD23	2.31	0.46
1:A:231:PHE:HD2	1:A:239:GLU:HG2	1.80	0.46
1:A:27:ARG:HG3	1:A:205:GLU:HB3	1.97	0.46
1:A:201:PRO:HA	1:A:203:LEU:HG	1.99	0.45
1:A:163:VAL:HG11	1:A:176:PHE:CE1	2.52	0.45
1:A:60:LEU:O	1:A:66:PHE:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:THR:HA	1:A:209:TRP:O	2.18	0.44
1:A:41:ASP:CG	1:A:44:LEU:HD13	2.37	0.44
1:A:202:PRO:HG2	1:A:204:LEU:HG	2.00	0.44
1:A:250:PRO:HB2	1:A:252:LYS:HG3	2.00	0.44
1:A:146:ILE:HG12	1:A:212:LEU:HD12	1.99	0.44
1:A:214:GLU:HA	1:A:215:PRO:HD3	1.80	0.44
1:A:60:LEU:HD22	1:A:69:GLU:OE2	2.18	0.43
1:A:253:ASN:ND2	1:A:253:ASN:C	2.60	0.43
1:A:21:PRO:HD2	3:A:270:HOH:O	2.18	0.43
1:A:180:ASP:HA	1:A:181:PRO:HD2	1.93	0.43
1:A:218:VAL:HG23	1:A:223:VAL:HG23	2.01	0.42
1:A:251:LEU:O	1:A:252:LYS:HB2	2.19	0.42
1:A:9:LYS:HG3	1:A:9:LYS:O	2.20	0.42
1:A:41:ASP:OD1	1:A:41:ASP:C	2.58	0.41
1:A:113:LYS:NZ	3:A:342:HOH:O	2.49	0.41
1:A:230:ASN:HB3	1:A:232:ASN:OD1	2.21	0.41
1:A:89:ARG:O	1:A:122:HIS:HA	2.20	0.41
1:A:223:VAL:O	1:A:226:PHE:HB2	2.21	0.41
1:A:41:ASP:HB3	1:A:44:LEU:HD13	2.01	0.41
1:A:231:PHE:CE1	1:A:241:MET:HG3	2.56	0.41
1:A:218:VAL:HG21	1:A:223:VAL:HG23	2.04	0.40
1:A:75:ASP:OD1	1:A:89:ARG:NE	2.54	0.40

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	253/255 (99%)	239 (94%)	13 (5%)	1 (0%)	38 41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	ASN

### 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	220/220 (100%)	212 (96%)	8 (4%)	40 50

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	A	39	LYS
1	A	58	ARG
1	A	79	LEU
1	A	90	LEU
1	A	144	LEU
1	A	221	GLU
1	A	253	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	136	GLN
1	A	158	GLN
1	A	253	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

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.