



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 10:15 pm GMT

PDB ID : 1CNY
Title : SECONDARY INTERACTIONS SIGNIFICANTLY REMOVED FROM THE
SULFONAMIDE BINDING POCKET OF CARBONIC ANHYDRASE II IN-
FLUENCE BINDING CONSTANTS
Authors : Boriack, P.A.; Christianson, D.W.
Deposited on : 1995-07-21
Resolution : 2.30 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

<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	:	1.7.2 (RC1), CSD as538be (2017)
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)	:	recalc28949

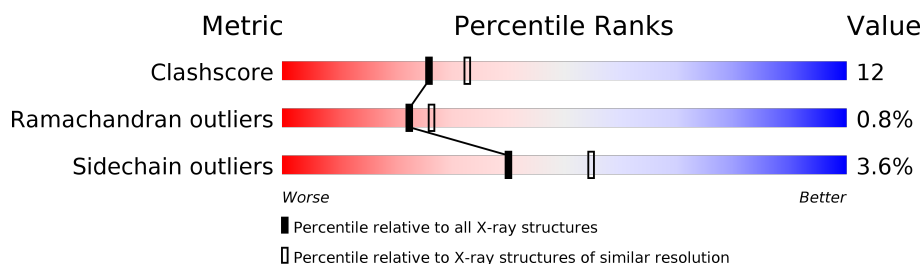
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	260	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2150 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	256	Total	C	N	O	S	0	0	0
			2039	1309	350	378	2			

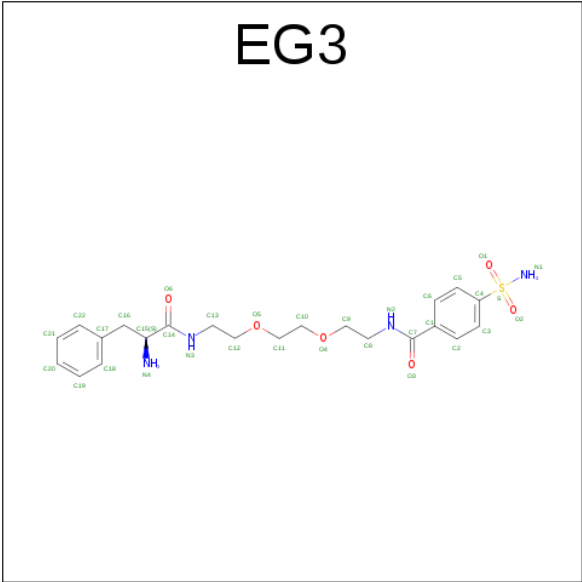
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Hg	0	0
			1	1		

- Molecule 4 is PHENYLALANYLAMINODI(ETHYLOXY)ETHYL BENZENESULFONAMIDEAMINOCARBONYLBENZENESULFONAMIDE (three-letter code: EG3) (formula: C₂₂H₃₀N₄O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	14	0
			33	22	4	6	1		

- Molecule 5 is water.

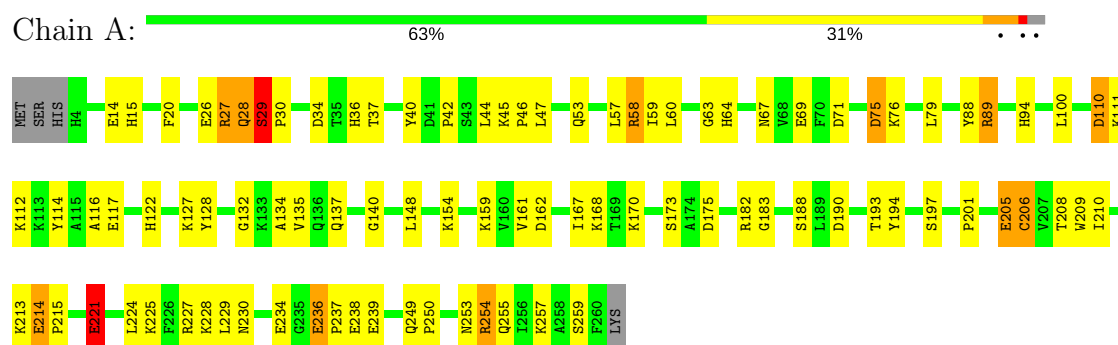
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	76	Total	O	0	0
			76	76		

3 Residue-property plots [i](#)

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, α , β , γ	42.70 Å 41.70 Å 73.00 Å 90.00° 104.60° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2150	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

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: EG3, ZN, HG

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	1.48	14/2100 (0.7%)	1.75	32/2851 (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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	239	GLU	CD-OE2	9.74	1.36	1.25
1	A	234	GLU	CD-OE1	8.82	1.35	1.25
1	A	205	GLU	CD-OE2	7.63	1.34	1.25
1	A	234	GLU	CD-OE2	-7.28	1.17	1.25
1	A	236	GLU	CD-OE2	7.26	1.33	1.25
1	A	117	GLU	CD-OE2	7.09	1.33	1.25
1	A	29	SER	C-O	-6.90	1.10	1.23
1	A	221	GLU	CD-OE1	6.75	1.33	1.25
1	A	239	GLU	CD-OE1	-6.72	1.18	1.25
1	A	26	GLU	CD-OE2	6.31	1.32	1.25
1	A	28	GLN	C-N	-5.67	1.21	1.34
1	A	29	SER	N-CA	-5.37	1.35	1.46
1	A	253	ASN	C-O	5.06	1.32	1.23
1	A	188	SER	CA-CB	5.03	1.60	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	GLN	C-N-CA	22.76	178.59	121.70
1	A	27	ARG	NE-CZ-NH1	13.35	126.97	120.30
1	A	29	SER	O-C-N	13.18	146.15	121.10
1	A	182	ARG	NE-CZ-NH2	-10.94	114.83	120.30
1	A	30	PRO	CA-N-CD	-10.52	96.77	111.50
1	A	29	SER	CA-C-O	-10.13	98.82	120.10
1	A	30	PRO	N-CA-CB	9.60	114.81	103.30
1	A	227	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	A	175	ASP	CB-CG-OD1	8.48	125.93	118.30
1	A	214	GLU	OE1-CD-OE2	-8.38	113.24	123.30
1	A	30	PRO	N-CD-CG	8.24	115.56	103.20
1	A	194	TYR	CB-CG-CD2	7.74	125.64	121.00
1	A	34	ASP	CB-CG-OD2	7.27	124.84	118.30
1	A	194	TYR	CB-CG-CD1	-7.23	116.66	121.00
1	A	29	SER	N-CA-C	7.00	129.89	111.00
1	A	44	LEU	CA-CB-CG	6.59	130.46	115.30
1	A	254	ARG	NE-CZ-NH1	-6.48	117.06	120.30
1	A	28	GLN	CA-C-N	-6.03	103.93	117.20
1	A	148	LEU	CA-CB-CG	5.91	128.89	115.30
1	A	239	GLU	CA-CB-CG	5.89	126.35	113.40
1	A	182	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	27	ARG	CD-NE-CZ	5.64	131.49	123.60
1	A	234	GLU	CG-CD-OE2	5.62	129.53	118.30
1	A	221	GLU	CA-CB-CG	5.59	125.70	113.40
1	A	110	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	116	ALA	O-C-N	5.49	131.48	122.70
1	A	208	THR	CA-C-O	-5.33	108.91	120.10
1	A	259	SER	N-CA-CB	5.29	118.43	110.50
1	A	162	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	75	ASP	CB-CG-OD2	-5.18	113.63	118.30
1	A	214	GLU	CG-CD-OE2	5.16	128.62	118.30
1	A	28	GLN	O-C-N	5.06	130.79	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	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	2039	0	1988	48	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	33	0	30	0	0
5	A	76	0	0	3	0
All	All	2150	0	2018	48	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 12.

All (48) 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:137:GLN:O	1:A:206:CYS:HB3	1.68	0.93
1:A:58:ARG:HD2	1:A:69:GLU:OE1	1.80	0.82
1:A:190:ASP:OD2	1:A:213:LYS:NZ	2.17	0.77
1:A:29:SER:HB2	1:A:197:SER:OG	1.86	0.76
1:A:159:LYS:HG3	5:A:372:HOH:O	1.90	0.70
1:A:137:GLN:O	1:A:206:CYS:CB	2.43	0.66
1:A:221:GLU:HA	1:A:224:LEU:HD12	1.81	0.63
1:A:190:ASP:HB2	1:A:213:LYS:HE2	1.80	0.62
1:A:63:GLY:HA3	1:A:170:LYS:HZ2	1.65	0.62
1:A:36:HIS:HD2	5:A:282:HOH:O	1.83	0.62
1:A:59:ILE:HG12	1:A:167:ILE:HD13	1.83	0.59
1:A:168:LYS:NZ	1:A:228:LYS:O	2.33	0.59
1:A:40:TYR:CE2	1:A:42:PRO:HG3	2.37	0.58
1:A:89:ARG:O	1:A:122:HIS:HA	2.05	0.56
1:A:58:ARG:HD2	1:A:69:GLU:CD	2.27	0.55
1:A:161:VAL:HG13	1:A:225:LYS:HD2	1.88	0.55
1:A:14:GLU:HG2	1:A:15:HIS:CD2	2.42	0.54
1:A:236:GLU:HB3	1:A:237:PRO:CD	2.38	0.54
1:A:63:GLY:HA3	1:A:170:LYS:NZ	2.23	0.54
1:A:28:GLN:O	1:A:254:ARG:NH2	2.26	0.54
1:A:67:ASN:ND2	1:A:94:HIS:HB3	2.24	0.52
1:A:64:HIS:ND1	5:A:332:HOH:O	2.17	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:VAL:CG1	1:A:225:LYS:HD2	2.43	0.49
1:A:154:LYS:HE3	1:A:183:GLY:O	2.12	0.49
1:A:29:SER:CB	1:A:197:SER:H	2.26	0.49
1:A:230:ASN:OD1	1:A:238:GLU:HG3	2.13	0.48
1:A:29:SER:HB2	1:A:197:SER:H	1.79	0.48
1:A:45:LYS:HB3	1:A:46:PRO:CD	2.44	0.48
1:A:110:ASP:O	1:A:111:LYS:HB2	2.14	0.47
1:A:193:THR:HA	1:A:209:TRP:O	2.14	0.47
1:A:27:ARG:HG3	1:A:205:GLU:HB3	1.97	0.46
1:A:88:TYR:HB3	1:A:122:HIS:HB3	1.97	0.46
1:A:45:LYS:HB3	1:A:46:PRO:HD2	1.97	0.46
1:A:214:GLU:HA	1:A:215:PRO:HD3	1.66	0.46
1:A:60:LEU:CD1	1:A:173:SER:HB3	2.47	0.45
1:A:112:LYS:HE3	1:A:114:TYR:CZ	2.52	0.45
1:A:255:GLN:OE1	1:A:257:LYS:NZ	2.40	0.44
1:A:132:GLY:O	1:A:135:VAL:HG22	2.18	0.44
1:A:128:TYR:CE1	1:A:137:GLN:HG3	2.53	0.43
1:A:53:GLN:HB3	1:A:76:LYS:O	2.18	0.43
1:A:47:LEU:HD21	1:A:210:ILE:HG21	1.99	0.43
1:A:57:LEU:HD11	1:A:71:ASP:HB2	1.99	0.42
1:A:20:PHE:CD2	1:A:201:PRO:HB3	2.54	0.42
1:A:249:GLN:HB3	1:A:250:PRO:HD2	2.02	0.41
1:A:134:ALA:O	1:A:140:GLY:HA3	2.21	0.41
1:A:112:LYS:HE3	1:A:114:TYR:CE1	2.56	0.41
1:A:60:LEU:HD12	1:A:173:SER:HB3	2.03	0.41
1:A:20:PHE:CE2	1:A:201:PRO:HB3	2.56	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	254/260 (98%)	241 (95%)	11 (4%)	2 (1%)	22 26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	SER
1	A	75	ASP

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	221/225 (98%)	213 (96%)	8 (4%)	40 55

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

Mol	Chain	Res	Type
1	A	37	THR
1	A	58	ARG
1	A	79	LEU
1	A	100	LEU
1	A	127	LYS
1	A	206	CYS
1	A	221	GLU
1	A	229	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	36	HIS
1	A	53	GLN
1	A	67	ASN
1	A	253	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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z > 2$
4	EG3	A	555	2	34,34,34	2.97	10 (29%)	44,44,44	2.75	13 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EG3	A	555	2	-	0/31/31/31	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	555	EG3	C1-C7	-6.98	1.35	1.50
4	A	555	EG3	S-N1	-5.83	1.48	1.60
4	A	555	EG3	C4-S	-2.69	1.72	1.77
4	A	555	EG3	O4-C9	-2.56	1.31	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	555	EG3	C22-C17	-2.20	1.34	1.38
4	A	555	EG3	O5-C12	2.30	1.51	1.42
4	A	555	EG3	C8-N2	2.32	1.51	1.46
4	A	555	EG3	O4-C10	3.72	1.58	1.42
4	A	555	EG3	C7-N2	7.68	1.50	1.33
4	A	555	EG3	C14-N3	9.37	1.52	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	555	EG3	O3-C7-N2	-8.70	104.62	122.59
4	A	555	EG3	C13-N3-C14	-7.04	109.46	122.59
4	A	555	EG3	O2-S-O1	-4.01	111.34	118.70
4	A	555	EG3	C5-C6-C1	-3.19	117.22	120.79
4	A	555	EG3	O1-S-N1	-3.09	102.48	107.34
4	A	555	EG3	C4-S-N1	-2.77	104.41	108.41
4	A	555	EG3	C8-N2-C7	-2.40	116.62	122.11
4	A	555	EG3	C6-C5-C4	2.21	121.85	119.46
4	A	555	EG3	C16-C15-C14	3.02	113.90	108.37
4	A	555	EG3	O2-S-N1	3.50	112.84	107.34
4	A	555	EG3	C1-C7-N2	3.69	125.08	117.12
4	A	555	EG3	O3-C7-C1	5.24	130.25	120.94
4	A	555	EG3	O1-S-C4	7.63	116.32	107.39

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.