



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 02:59 AM EST

PDB ID : 1CCU
Title : STRUCTURE-ASSISTED REDESIGN OF A PROTEIN-ZINC BINDING
SITE WITH FEMTOMOLAR AFFINITY
Authors : Ippolito, J.A.; Christianson, D.W.
Deposited on : unknown
Resolution : 2.25 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) : rb-20030345

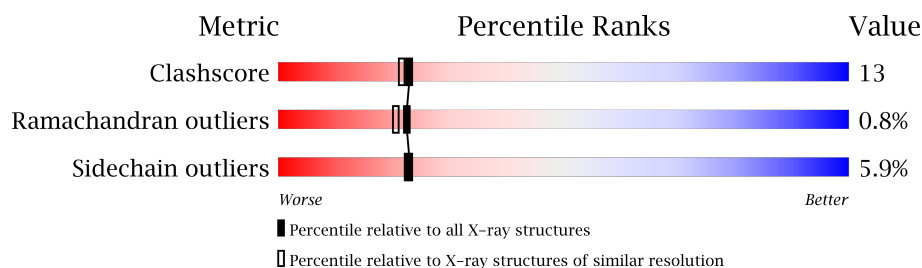
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)

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 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	259	

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
3	SO4	A	263	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2159 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
			2032	1305	349	376	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	HIS	THR	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 SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

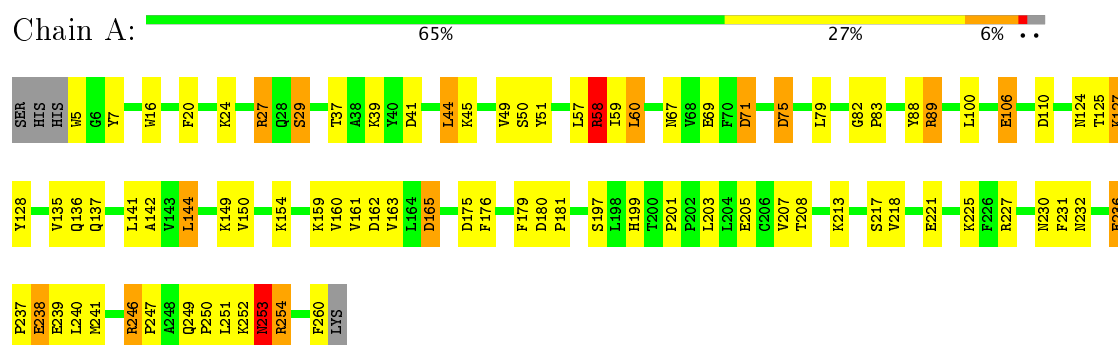
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	121	Total	O	0	0
			121	121		

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, α , β , γ	42.70 Å 41.70 Å 73.00 Å 90.00° 104.60° 90.00°	Depositor
Resolution (Å)	7.00 – 2.25	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.178 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2159	wwPDB-VP
Average B, all atoms (Å ²)	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, SO4

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	1.43	2/2093 (0.1%)	1.81	32/2841 (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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	GLU	CD-OE2	-6.26	1.18	1.25
1	A	50	SER	CB-OG	6.09	1.50	1.42

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	ARG	NE-CZ-NH2	-14.65	112.98	120.30
1	A	175	ASP	CB-CG-OD1	10.22	127.50	118.30
1	A	58	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	A	71	ASP	CB-CG-OD1	8.27	125.74	118.30
1	A	162	ASP	CB-CG-OD2	-7.88	111.21	118.30
1	A	37	THR	CA-CB-CG2	7.37	122.71	112.40
1	A	149	LYS	N-CA-CB	6.89	123.00	110.60
1	A	88	TYR	CG-CD2-CE2	6.60	126.58	121.30
1	A	7	TYR	CB-CG-CD1	6.55	124.93	121.00
1	A	100	LEU	CA-CB-CG	6.12	129.39	115.30
1	A	142	ALA	N-CA-CB	6.08	118.60	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	LEU	CB-CA-C	5.85	121.32	110.20
1	A	89	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	75	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	51	TYR	CB-CG-CD1	5.75	124.45	121.00
1	A	238	GLU	CG-CD-OE1	-5.63	107.03	118.30
1	A	236	GLU	CG-CD-OE1	5.62	129.55	118.30
1	A	197	SER	O-C-N	5.55	131.58	122.70
1	A	110	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	144	LEU	CA-CB-CG	5.44	127.82	115.30
1	A	27	ARG	CG-CD-NE	5.44	123.22	111.80
1	A	232	ASN	CA-C-N	-5.42	105.36	116.20
1	A	16	TRP	CE3-CZ3-CH2	5.39	127.13	121.20
1	A	44	LEU	CA-CB-CG	5.35	127.60	115.30
1	A	165	ASP	CB-CG-OD1	-5.26	113.57	118.30
1	A	141	LEU	CA-CB-CG	5.25	127.37	115.30
1	A	7	TYR	CB-CG-CD2	-5.23	117.86	121.00
1	A	27	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	159	LYS	N-CA-CB	5.12	119.81	110.60
1	A	208	THR	O-C-N	5.10	130.86	122.70
1	A	207	VAL	CA-C-O	5.05	130.70	120.10
1	A	227	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	246	ARG	Sidechain
1	A	254	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	2032	0	1982	52	0
2	A	1	0	0	0	0
3	A	5	0	0	2	0
4	A	121	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2159	0	1982	52	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 13.

All (52) 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:161:VAL:HG12	1:A:225:LYS:HD2	1.48	0.94
1:A:58:ARG:HD2	1:A:69:GLU:OE1	1.73	0.89
1:A:29:SER:HB2	1:A:199:HIS:NE2	1.90	0.86
1:A:199:HIS:HB2	3:A:263:SO4:O3	1.81	0.80
1:A:5:TRP:HA	4:A:354:HOH:O	1.83	0.79
1:A:161:VAL:CG1	1:A:225:LYS:HD2	2.12	0.78
1:A:253:ASN:HD22	1:A:254:ARG:N	1.80	0.78
1:A:253:ASN:ND2	1:A:254:ARG:N	2.34	0.76
1:A:253:ASN:HD22	1:A:253:ASN:C	1.94	0.69
1:A:236:GLU:HB3	1:A:237:PRO:HD2	1.73	0.69
1:A:29:SER:HB2	1:A:199:HIS:CD2	2.31	0.66
1:A:136:GLN:HB2	4:A:367:HOH:O	2.00	0.61
1:A:127:LYS:HE3	1:A:128:TYR:CZ	2.34	0.61
1:A:57:LEU:HD11	1:A:71:ASP:HB2	1.86	0.57
1:A:39:LYS:HD3	4:A:317:HOH:O	2.05	0.56
1:A:45:LYS:O	1:A:82:GLY:HA2	2.06	0.55
1:A:253:ASN:C	1:A:253:ASN:ND2	2.58	0.55
1:A:60:LEU:HD22	1:A:69:GLU:OE2	2.09	0.52
1:A:29:SER:O	1:A:246:ARG:NH1	2.40	0.52
1:A:127:LYS:HE3	1:A:128:TYR:OH	2.08	0.52
1:A:252:LYS:O	1:A:253:ASN:CB	2.58	0.51
1:A:252:LYS:O	1:A:253:ASN:CG	2.48	0.51
1:A:201:PRO:HA	1:A:203:LEU:HG	1.93	0.51
1:A:199:HIS:HB2	3:A:263:SO4:S	2.51	0.50
1:A:27:ARG:CG	1:A:205:GLU:HB3	2.41	0.50
1:A:29:SER:CB	1:A:199:HIS:NE2	2.71	0.50
1:A:27:ARG:HG3	1:A:205:GLU:HB3	1.94	0.50
1:A:106:GLU:OE1	1:A:199:HIS:ND1	2.38	0.49
1:A:213:LYS:HD3	1:A:260:PHE:CZ	2.48	0.49
1:A:160:VAL:O	1:A:163:VAL:HG12	2.14	0.48
1:A:59:ILE:HA	1:A:67:ASN:O	2.14	0.48
1:A:161:VAL:HG13	1:A:225:LYS:HB2	1.96	0.48
1:A:75:ASP:OD1	1:A:89:ARG:NH2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:VAL:HG23	1:A:49:VAL:O	2.16	0.46
1:A:89:ARG:HG3	1:A:125:THR:CG2	2.46	0.45
1:A:20:PHE:CE2	1:A:201:PRO:HB3	2.52	0.44
1:A:163:VAL:HG11	1:A:176:PHE:CE1	2.52	0.44
1:A:240:LEU:HA	1:A:240:LEU:HD23	1.88	0.42
1:A:179:PHE:HA	4:A:316:HOH:O	2.19	0.42
1:A:41:ASP:OD1	1:A:41:ASP:C	2.57	0.42
1:A:231:PHE:CE1	1:A:241:MET:HG3	2.54	0.42
1:A:150:VAL:HA	1:A:218:VAL:O	2.20	0.42
1:A:154:LYS:HD2	4:A:333:HOH:O	2.20	0.42
1:A:58:ARG:HD2	1:A:69:GLU:CD	2.38	0.42
1:A:180:ASP:HA	1:A:181:PRO:HD2	1.94	0.42
1:A:231:PHE:HD2	1:A:239:GLU:HG2	1.85	0.41
1:A:124:ASN:HB3	1:A:128:TYR:CD2	2.56	0.41
1:A:249:GLN:HB3	1:A:250:PRO:CD	2.50	0.41
1:A:213:LYS:HD3	1:A:260:PHE:CE2	2.55	0.41
1:A:246:ARG:HA	1:A:247:PRO:HD3	1.94	0.41
1:A:128:TYR:CE1	1:A:137:GLN:HG3	2.56	0.40
1:A:230:ASN:ND2	1:A:238:GLU:HG3	2.36	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	253/259 (98%)	240 (95%)	11 (4%)	2 (1%)	22 20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	135	VAL

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	220/224 (98%)	207 (94%)	13 (6%)	23	23

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	29	SER
1	A	44	LEU
1	A	58	ARG
1	A	60	LEU
1	A	79	LEU
1	A	83	PRO
1	A	127	LYS
1	A	144	LEU
1	A	165	ASP
1	A	217	SER
1	A	221	GLU
1	A	253	ASN

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	136	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 2 ligands modelled in this entry, 1 is 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	$\# Z > 2$
3	SO4	A	263	2	4,4,4	0.70	0	6,6,6	0.44	0

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
3	SO4	A	263	2	-	0/0/0/0	0/0/0/0

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	263	SO4	2	0

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.