Full wwPDB X-ray Structure Validation Report (i)

Mar 1, 2014 – 03:13 AM GMT

PDB ID	:	1CVH
Title	:	STRUCTURAL CONSEQUENCES OF REDESIGNING A PROTEIN-ZINC BINDING SITE
Authors	:	Ippolito, J.A.; Christianson, D.W.
Deposited on	:	1994-11-16
Resolution	:	2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html

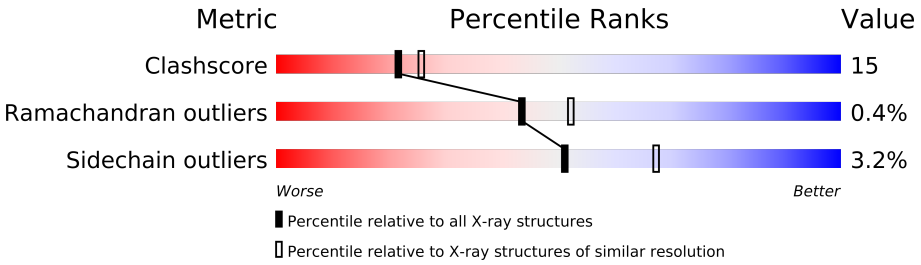
The following versions of software and data (see references) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	255	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2137 atoms, of which 0 are hydrogen and 0 are deuterium.

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	96	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	111	Total	O	0	0
			111	111		

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 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.

Note EDS was not executed.

• Molecule 1: CARBONIC ANHYDRASE II

Chain A:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	42.70Å 41.70Å 73.00Å 90.00° 104.60° 90.00°	Depositor
Resolution (Å)	7.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2137	wwPDB-VP
Average B, all atoms (Å^2)	13.0	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	1.47	11/2084 (0.5%)	1.98	47/2829 (1.7%)

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 (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	239	GLU	CD-OE2	8.50	1.35	1.25
1	A	236	GLU	CD-OE1	-6.79	1.18	1.25
1	A	106	GLU	CD-OE1	-6.78	1.18	1.25
1	A	233	GLY	CA-C	5.54	1.60	1.51
1	A	254	ARG	CZ-NH1	5.43	1.40	1.33
1	A	214	GLU	CD-OE2	-5.31	1.19	1.25
1	A	14	GLU	CD-OE2	-5.22	1.20	1.25
1	A	114	TYR	CE1-CZ	5.13	1.45	1.38
1	A	152	SER	CB-OG	5.13	1.49	1.42
1	A	5	TRP	CD2-CE2	5.04	1.47	1.41
1	A	20	PHE	CE1-CZ	5.03	1.47	1.37

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	58	ARG	NE-CZ-NH1	17.56	129.08	120.30
1	A	89	ARG	NE-CZ-NH1	12.87	126.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	182	ARG	NE-CZ-NH2	12.00	126.30	120.30
1	A	58	ARG	NE-CZ-NH2	-11.63	114.49	120.30
1	A	58	ARG	CD-NE-CZ	11.46	139.65	123.60
1	A	227	ARG	NE-CZ-NH1	-10.86	114.87	120.30
1	A	227	ARG	NE-CZ-NH2	9.56	125.08	120.30
1	A	24	LYS	CA-CB-CG	9.00	133.20	113.40
1	A	71	ASP	CB-CG-OD1	8.97	126.37	118.30
1	A	72	ASP	CB-CG-OD2	8.78	126.20	118.30
1	A	182	ARG	NE-CZ-NH1	-8.62	115.99	120.30
1	A	34	ASP	CB-CG-OD1	8.02	125.52	118.30
1	A	197	SER	N-CA-CB	-8.01	98.48	110.50
1	A	89	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	A	32	ASP	CB-CG-OD2	7.71	125.23	118.30
1	A	51	TYR	CB-CG-CD1	7.63	125.58	121.00
1	A	254	ARG	NE-CZ-NH2	7.35	123.97	120.30
1	A	20	PHE	CB-CG-CD1	-7.34	115.66	120.80
1	A	208	THR	N-CA-CB	7.20	123.98	110.30
1	A	236	GLU	CG-CD-OE1	7.05	132.41	118.30
1	A	236	GLU	CG-CD-OE2	-6.94	104.42	118.30
1	A	106	GLU	CG-CD-OE1	6.73	131.75	118.30
1	A	253	ASN	O-C-N	6.62	133.28	122.70
1	A	158	GLN	O-C-N	6.39	132.93	122.70
1	A	37	THR	CA-CB-CG2	6.11	120.95	112.40
1	A	187	GLU	OE1-CD-OE2	6.09	130.61	123.30
1	A	75	ASP	CB-CG-OD1	6.03	123.72	118.30
1	A	27	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	230	ASN	CB-CG-OD1	-5.76	110.07	121.60
1	A	253	ASN	N-CA-CB	5.65	120.77	110.60
1	A	176	PHE	CB-CG-CD1	-5.56	116.91	120.80
1	A	109	VAL	CA-CB-CG2	5.53	119.20	110.90
1	A	175	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	251	LEU	CB-CA-C	5.32	120.30	110.20
1	A	140	GLY	CA-C-O	-5.30	111.05	120.60
1	A	19	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	238	GLU	CG-CD-OE2	5.28	128.86	118.30
1	A	253	ASN	CB-CG-OD1	-5.27	111.06	121.60
1	A	221	GLU	CA-CB-CG	5.25	124.94	113.40
1	A	239	GLU	CG-CD-OE2	-5.24	107.81	118.30
1	A	200	THR	N-CA-CB	5.22	120.21	110.30
1	A	106	GLU	CG-CD-OE2	-5.20	107.90	118.30
1	A	254	ARG	NH1-CZ-NH2	-5.17	113.72	119.40
1	A	174	ALA	O-C-N	5.15	130.94	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	7	TYR	CB-CG-CD1	5.12	124.07	121.00
1	A	49	VAL	O-C-N	5.11	130.88	122.70
1	A	239	GLU	CA-CB-CG	5.08	124.57	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	58	ARG	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2025	0	1980	61	4
2	A	1	0	0	0	0
3	A	111	0	0	4	3
All	All	2137	0	1980	61	4

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (61) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:58:ARG:HD2	1:A:69:GLU:OE1	1.53	1.08
1:A:96:CYS:SG	1:A:106:GLU:HG3	2.19	0.82
1:A:161:VAL:HG13	1:A:225:LYS:HD2	1.59	0.82
1:A:30:PRO:HG3	1:A:106:GLU:HB3	1.62	0.82
1:A:106:GLU:OE1	1:A:119:HIS:HE1	1.70	0.73
1:A:63:GLY:HA3	1:A:170:LYS:NZ	2.04	0.73
1:A:63:GLY:HA3	1:A:170:LYS:HZ3	1.54	0.72
1:A:89:ARG:O	1:A:122:HIS:HA	1.95	0.66
1:A:161:VAL:CG1	1:A:225:LYS:HD2	2.25	0.65
1:A:57:LEU:HD11	1:A:71:ASP:HB2	1.78	0.64
1:A:5:TRP:N	3:A:272:HOH:O	2.31	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:164:LEU:HB3	1:A:229:LEU:HD11	1.80	0.63
1:A:253:ASN:HD22	1:A:254:ARG:N	1.95	0.63
1:A:59:ILE:HA	1:A:67:ASN:O	2.00	0.62
1:A:213:LYS:HD3	1:A:260:PHE:CZ	2.34	0.61
1:A:40:TYR:CE2	1:A:42:PRO:HG3	2.35	0.61
1:A:45:LYS:O	1:A:82:GLY:HA2	2.04	0.58
1:A:58:ARG:CD	1:A:69:GLU:OE1	2.40	0.57
1:A:143:VAL:HG23	1:A:207:VAL:CG1	2.36	0.56
1:A:236:GLU:HB3	1:A:237:PRO:HD2	1.88	0.56
1:A:213:LYS:HD3	1:A:260:PHE:CE2	2.42	0.55
1:A:95:PHE:HA	1:A:117:GLU:O	2.08	0.53
1:A:253:ASN:ND2	1:A:254:ARG:N	2.57	0.53
1:A:146:ILE:HG12	1:A:212:LEU:HD12	1.91	0.52
1:A:161:VAL:HG13	1:A:225:LYS:CD	2.34	0.52
1:A:58:ARG:HD2	1:A:69:GLU:CD	2.26	0.51
1:A:29:SER:O	1:A:246:ARG:NH1	2.43	0.51
1:A:231:PHE:HD2	1:A:239:GLU:HG2	1.76	0.51
1:A:143:VAL:HG23	1:A:207:VAL:HG13	1.93	0.51
1:A:149:LYS:O	1:A:217:SER:HA	2.12	0.50
1:A:160:VAL:O	1:A:163:VAL:HG12	2.13	0.49
1:A:63:GLY:CA	1:A:170:LYS:HG3	2.43	0.48
1:A:47:LEU:HD11	1:A:210:ILE:HG21	1.94	0.48
1:A:100:LEU:HD12	3:A:308:HOH:O	2.14	0.48
1:A:207:VAL:CG1	1:A:208:THR:N	2.78	0.47
1:A:252:LYS:O	1:A:253:ASN:CG	2.54	0.47
1:A:243:ASP:HA	1:A:245:TRP:CD1	2.49	0.46
1:A:253:ASN:HD22	1:A:253:ASN:C	2.19	0.45
1:A:207:VAL:HG12	1:A:208:THR:N	2.31	0.45
1:A:230:ASN:HB3	1:A:232:ASN:OD1	2.16	0.45
1:A:147:PHE:HB2	1:A:215:PRO:HB3	2.00	0.44
1:A:29:SER:HB3	1:A:30:PRO:HA	1.99	0.44
1:A:154:LYS:HE3	1:A:183:GLY:O	2.16	0.44
1:A:99:SER:O	1:A:100:LEU:HD13	2.18	0.43
1:A:27:ARG:CG	1:A:205:GLU:HB3	2.49	0.43
1:A:60:LEU:HD22	1:A:69:GLU:OE2	2.19	0.42
1:A:60:LEU:N	1:A:60:LEU:HD23	2.34	0.42
1:A:154:LYS:HA	1:A:155:PRO:HD2	1.81	0.42
1:A:154:LYS:HE3	3:A:331:HOH:O	2.17	0.42
1:A:180:ASP:HA	1:A:181:PRO:HD2	1.95	0.42
1:A:89:ARG:HG3	1:A:125:THR:CG2	2.49	0.42
1:A:201:PRO:HA	1:A:203:LEU:HG	2.02	0.42
1:A:167:ILE:HA	1:A:172:LYS:HB2	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:252:LYS:O	1:A:253:ASN:CB	2.68	0.41
1:A:25:GLY:O	1:A:252:LYS:NZ	2.46	0.41
1:A:60:LEU:HA	1:A:173:SER:HA	2.03	0.41
1:A:113:LYS:NZ	3:A:361:HOH:O	2.52	0.41
1:A:40:TYR:HE2	1:A:42:PRO:HG3	1.83	0.41
1:A:154:LYS:HA	1:A:154:LYS:HD2	1.90	0.41
1:A:148:LEU:HD11	1:A:216:ILE:HD11	2.01	0.40
1:A:214:GLU:HA	1:A:215:PRO:HD3	1.91	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:162:ASP:OD2	3:A:320:HOH:O[2_445]	1.69	0.51
1:A:133:LYS:CG	3:A:371:HOH:O[1_565]	2.07	0.13
1:A:133:LYS:CE	3:A:371:HOH:O[1_565]	2.11	0.09
1:A:102:GLY:N	1:A:130:ASP:OD1[1_545]	2.17	0.03

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	253/255 (99%)	239 (94%)	13 (5%)	1 (0%)	43 52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	ASN

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	220/220 (100%)	213 (97%)	7 (3%)	51 67

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	53	GLN
1	A	58	ARG
1	A	79	LEU
1	A	100	LEU
1	A	144	LEU
1	A	253	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	136	GLN
1	A	253	ASN

5.3.3 RNA

There are no RNA chains 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 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.

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.