Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 11:40 PM EDT

PDB ID	:	3LY9
Title	:	Crystal structure of mutant D471N of the periplasmic domain of CadC
Authors	:	Eichinger, A.; Skerra, A.
Deposited on	:	2010-02-26
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

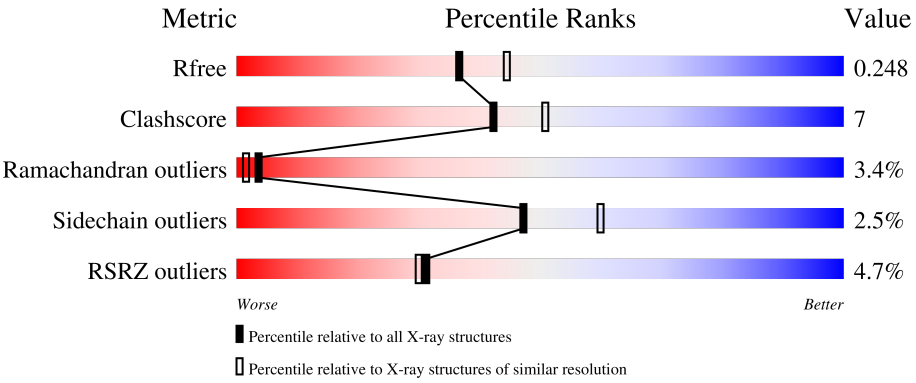
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	372	4% 73% 12% · 13%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2670 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 Transcriptional activator cadC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	322	2556	1621	434	491	10	288	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	GLY	-	expression tag	UNP P23890
A	142	SER	-	expression tag	UNP P23890
A	143	GLY	-	expression tag	UNP P23890
A	144	MET	-	expression tag	UNP P23890
A	145	LYS	-	expression tag	UNP P23890
A	146	GLU	-	expression tag	UNP P23890
A	147	THR	-	expression tag	UNP P23890
A	148	ALA	-	expression tag	UNP P23890
A	149	ALA	-	expression tag	UNP P23890
A	150	ALA	-	expression tag	UNP P23890
A	151	LYS	-	expression tag	UNP P23890
A	152	PHE	-	expression tag	UNP P23890
A	153	GLU	-	expression tag	UNP P23890
A	154	ARG	-	expression tag	UNP P23890
A	155	GLN	-	expression tag	UNP P23890
A	156	HIS	-	expression tag	UNP P23890
A	157	MET	-	expression tag	UNP P23890
A	158	ASP	-	expression tag	UNP P23890
A	159	SER	-	expression tag	UNP P23890
A	160	PRO	-	expression tag	UNP P23890
A	161	ASP	-	expression tag	UNP P23890
A	162	LEU	-	expression tag	UNP P23890
A	163	GLY	-	expression tag	UNP P23890
A	164	THR	-	expression tag	UNP P23890
A	165	ASP	-	expression tag	UNP P23890
A	166	ASP	-	expression tag	UNP P23890
A	167	ASP	-	expression tag	UNP P23890

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Chain	Residue	Modelled	Actual	Comment	Reference
A	168	ASP	-	expression tag	UNP P23890
A	169	LYS	-	expression tag	UNP P23890
A	170	ALA	-	expression tag	UNP P23890
A	171	MET	-	expression tag	UNP P23890
A	172	ALA	-	expression tag	UNP P23890
A	173	HIS	-	expression tag	UNP P23890
A	174	HIS	-	expression tag	UNP P23890
A	175	HIS	-	expression tag	UNP P23890
A	176	HIS	-	expression tag	UNP P23890
A	177	HIS	-	expression tag	UNP P23890
A	178	HIS	-	expression tag	UNP P23890
A	179	SER	-	expression tag	UNP P23890
A	180	SER	-	expression tag	UNP P23890
A	181	GLY	-	expression tag	UNP P23890
A	182	HIS	-	expression tag	UNP P23890
A	183	ILE	-	expression tag	UNP P23890
A	184	GLU	-	expression tag	UNP P23890
A	185	GLY	-	expression tag	UNP P23890
A	186	ARG	-	expression tag	UNP P23890
A	187	HIS	-	expression tag	UNP P23890
A	471	ASN	ASP	engineered mutation	UNP P23890

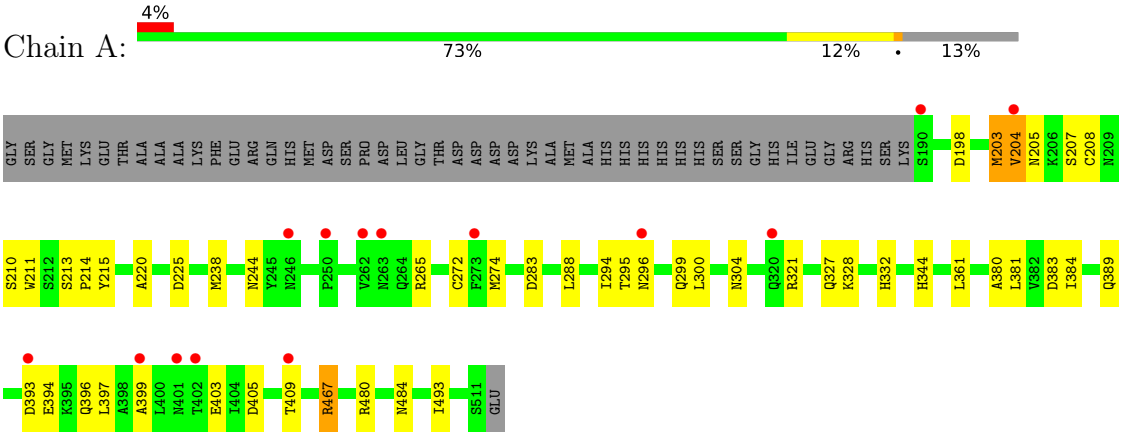
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	114	Total	O	0	0
			114	114		

3 Residue-property plots (i)

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

• Molecule 1: Transcriptional activator cadC



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	79.73Å 79.73Å 126.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	69.05 – 2.20 19.93 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (69.05-2.20) 99.8 (19.93-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 2.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.228 , 0.279 0.198 , 0.248	Depositor DCC
R_{free} test set	1228 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	35.7	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.039 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2670	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.84	0/2606	0.76	3/3540 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	321	ARG	NE-CZ-NH2	-8.87	115.86	120.30
1	A	321	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	288	LEU	CA-CB-CG	5.74	128.51	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2556	0	2538	31	1
2	A	114	0	0	1	0
All	All	2670	0	2538	31	1

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 7.

All (31) 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:467:ARG:H	1:A:467:ARG:CD	1.59	1.13
1:A:467:ARG:H	1:A:467:ARG:HD3	1.36	0.91
1:A:467:ARG:H	1:A:467:ARG:HD2	1.36	0.90
1:A:204:VAL:HG23	1:A:205:ASN:H	1.38	0.87
1:A:467:ARG:CD	1:A:467:ARG:N	2.41	0.83
1:A:480:ARG:HH12	1:A:484:ASN:HD22	1.26	0.82
1:A:295:THR:O	1:A:296:ASN:HB3	1.81	0.80
1:A:274:MET:CE	1:A:294:ILE:HD11	2.14	0.76
1:A:389:GLN:HE21	1:A:493:ILE:H	1.37	0.72
1:A:204:VAL:HG23	1:A:205:ASN:N	2.05	0.71
1:A:274:MET:HE3	1:A:294:ILE:HD11	1.77	0.66
1:A:274:MET:HE1	1:A:294:ILE:HD11	1.77	0.65
1:A:204:VAL:CG2	1:A:205:ASN:N	2.60	0.64
1:A:467:ARG:HD2	1:A:467:ARG:N	2.12	0.62
1:A:295:THR:O	1:A:296:ASN:CB	2.49	0.61
1:A:225:ASP:OD2	1:A:344:HIS:HE1	1.86	0.58
1:A:467:ARG:HD3	1:A:467:ARG:N	2.12	0.58
1:A:328:LYS:NZ	2:A:99:HOH:O	2.33	0.57
1:A:296:ASN:HA	1:A:299:GLN:HE22	1.77	0.49
1:A:244:ASN:CG	1:A:244:ASN:O	2.54	0.47
1:A:203:MET:HG3	1:A:204:VAL:N	2.29	0.46
1:A:220:ALA:HB2	1:A:274:MET:HE2	1.96	0.46
1:A:300:LEU:HD13	1:A:332:HIS:O	2.15	0.46
1:A:405:ASP:O	1:A:409:THR:HG23	2.17	0.45
1:A:283:ASP:OD2	1:A:283:ASP:C	2.55	0.45
1:A:296:ASN:HA	1:A:299:GLN:NE2	2.33	0.43
1:A:383:ASP:OD2	1:A:403:GLU:OE2	2.36	0.43
1:A:198:ASP:OD2	1:A:238:MET:HB2	2.19	0.43
1:A:380:ALA:O	1:A:384:ILE:HG12	2.19	0.42
1:A:393:ASP:OD1	1:A:394:GLU:N	2.53	0.41
1:A:381:LEU:O	1:A:384:ILE:HG13	2.21	0.41

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:MET:SD	1:A:238:MET:SD[4_555]	2.04	0.16

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	320/372 (86%)	295 (92%)	14 (4%)	11 (3%)	3 1

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	SER
1	A	208	CYS
1	A	213	SER
1	A	214	PRO
1	A	396	GLN
1	A	397	LEU
1	A	399	ALA
1	A	211	TRP
1	A	265	ARG
1	A	210	SER
1	A	215	TYR

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	284/324 (88%)	277 (98%)	7 (2%)	47 60

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

Mol	Chain	Res	Type
1	A	203	MET
1	A	204	VAL
1	A	272	CYS
1	A	304	ASN
1	A	327	GLN
1	A	361	LEU
1	A	467	ARG

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

Mol	Chain	Res	Type
1	A	344	HIS
1	A	389	GLN
1	A	484	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	301/372 (80%)	-0.31	14 (4%) 31 30	18, 30, 49, 57	38 (12%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	273	PHE	3.9
1	A	190	SER	3.7
1	A	296	ASN	3.5
1	A	262	VAL	3.5
1	A	402	THR	3.1
1	A	399	ALA	3.1
1	A	246	ASN	2.7
1	A	204	VAL	2.6
1	A	320	GLN	2.5
1	A	250	PRO	2.4
1	A	401	ASN	2.3
1	A	409	THR	2.3
1	A	263	ASN	2.2
1	A	393	ASP	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.