WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 6, 2024 – 01:02 AM EST

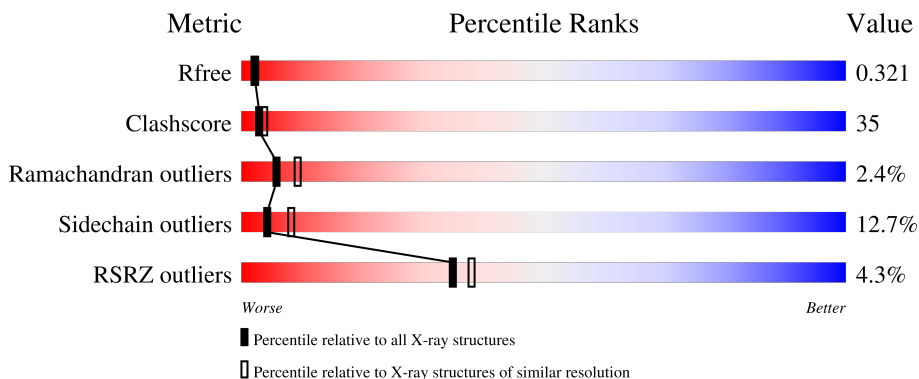|		
PDB ID	:	1YRU
Title	:	Crystal Structure analysis of the adenylyl cyclaes catalytic domain of adenylyl cyclase toxin of Bordetella pertussis in presence of c-terminal calmodulin and 1mM calcium chloride
Authors	:	Guo, Q.; Shen, Y.; Tang, W.J.
Deposited on	:	2005-02-04
Resolution	:	2.50 Å(reported)

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 2.50 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	Percentile Ranks	Value
Rfree		0.321
Clashscore		35
Ramachandran outliers		2.4%
Sidechain outliers		12.7%
RSRZ outliers		4.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	364	5% — 54% / 32% / 8% · ·
2	B	74	53% / 34% / 7% / 7%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 3307 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 Bifunctional hemolysin-adenylate cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total 2684	C 1664	N 495	O 519	S 6	0	0	0

- Molecule 2 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	69	Total 551	C 335	N 90	O 122	S 4	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	Ca 2	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	56	Total 56	O 56	0	0
4	B	14	Total 14	O 14	0	0

3 Residue-property plots ⓘ

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: Bifunctional hemolysin-adenylate cyclase

Chain A:
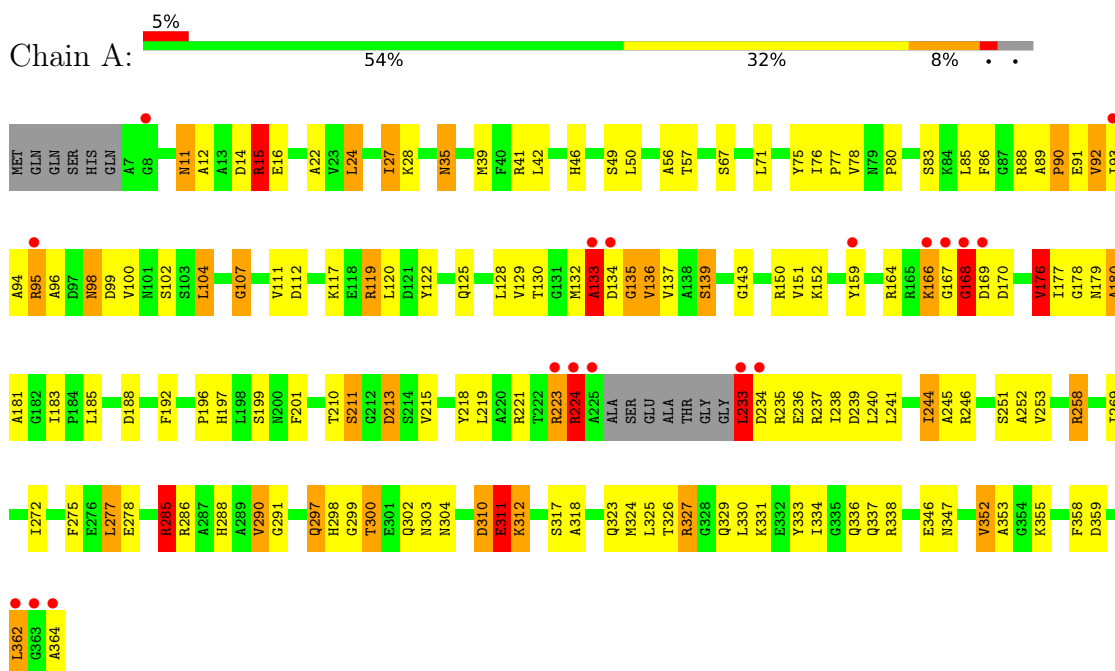
• Molecule 2: Calmodulin

Chain B:
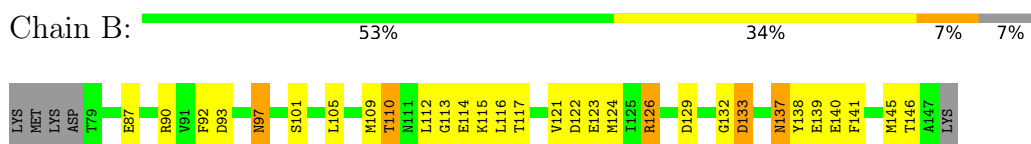
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	79.44Å 79.44Å 139.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 38.20 – 2.44	Depositor EDS
% Data completeness (in resolution range)	92.9 (30.00-2.50) 94.2 (38.20-2.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.52 (at 2.45Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.308 0.240 , 0.321	Depositor DCC
R_{free} test set	1441 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.0	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	3307	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	1.06	3/2728 (0.1%)	1.16	10/3682 (0.3%)
2	B	1.17	1/556 (0.2%)	1.31	6/746 (0.8%)
All	All	1.08	4/3284 (0.1%)	1.19	16/4428 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	311	GLU	C-N	-6.57	1.19	1.34
1	A	176	VAL	CB-CG2	-5.66	1.41	1.52
2	B	141	PHE	CE1-CZ	5.22	1.47	1.37
1	A	312	LYS	N-CA	-5.06	1.36	1.46

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	110	THR	N-CA-CB	-16.18	79.55	110.30
1	A	233	LEU	C-N-CA	-10.82	94.64	121.70
1	A	285	ARG	NE-CZ-NH1	-8.40	116.10	120.30
1	A	133	ALA	N-CA-C	-7.53	90.67	111.00
1	A	258	ARG	NE-CZ-NH2	-7.32	116.64	120.30

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	2684	0	2623	199	0
2	B	551	0	503	35	0
3	B	2	0	0	0	0
4	A	56	0	0	4	0
4	B	14	0	0	1	0
All	All	3307	0	3126	221	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 35.

The worst 5 of 221 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:89:ALA:HB1	1:A:90:PRO:HD2	1.26	1.11
1:A:85:LEU:HD22	1:A:88:ARG:HG3	1.31	1.11
1:A:166:LYS:CD	1:A:166:LYS:O	2.04	1.06
1:A:166:LYS:O	1:A:166:LYS:HD3	1.55	1.06
1:A:311:GLU:O	1:A:311:GLU:HG3	1.31	1.05

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	347/364 (95%)	309 (89%)	29 (8%)	9 (3%)	5	8
2	B	67/74 (90%)	59 (88%)	7 (10%)	1 (2%)	10	18
All	All	414/438 (94%)	368 (89%)	36 (9%)	10 (2%)	6	9

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	97	ASN
1	A	134	ASP
1	A	168	GLY
1	A	135	GLY
1	A	107	GLY

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	271/280 (97%)	232 (86%)	39 (14%)	3	6
2	B	59/64 (92%)	56 (95%)	3 (5%)	24	45
All	All	330/344 (96%)	288 (87%)	42 (13%)	4	8

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	285	ARG
1	A	327	ARG
1	A	297	GLN
1	A	310	ASP
1	A	359	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	HIS
2	B	135	GLN
1	A	302	GLN
2	B	137	ASN
2	B	107	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are 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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	311:GLU	C	312:LYS	N	1.18

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, 95th 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(Å²)	Q<0.9
1	A	351/364 (96%)	0.04	18 (5%)	28	29	11, 34, 59, 72	0
2	B	69/74 (93%)	-0.21	0	100	100	18, 30, 47, 56	0
All	All	420/438 (95%)	-0.00	18 (4%)	35	38	11, 33, 58, 72	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	363	GLY	8.6
1	A	364	ALA	5.3
1	A	133	ALA	3.9
1	A	233	LEU	3.7
1	A	224	ARG	3.5

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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	B	800	1/1	0.96	0.10	31,31,31,31	0
3	CA	B	801	1/1	0.96	0.05	39,39,39,39	0

6.5   Other polymers ⓘ

There are no such residues in this entry.