



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2020 – 10:21 AM BST

PDB ID : 1FX4  
Title : STRUCTURE ANALYSIS OF ADENYLATE CYCLASES FROM TRY-  
PANOSOMA BRUCEI IN THEIR MONOMERIC STATE  
Authors : Bieger, B.; Essen, L.O.  
Deposited on : 2000-09-25  
Resolution : 1.90 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](mailto: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.

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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	:	2.13
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)	:	2.13

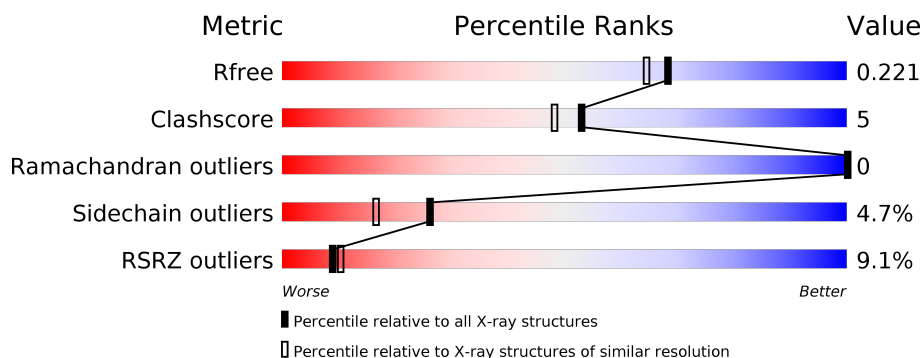
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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  $\geq 3$ , 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	231	<div> <div>9%</div> <div>86%</div> <div>13%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2063 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 RECEPTOR-TYPE ADENYLATE CYCLASE GRESAG 4.3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	231	1798	1124	313	351	10	10	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	959	CYS	ARG	CONFLICT	UNP Q99280
A	970	VAL	LEU	CONFLICT	UNP Q99280
A	994	SER	HIS	CONFLICT	UNP Q99280
A	995	LEU	MET	CONFLICT	UNP Q99280

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

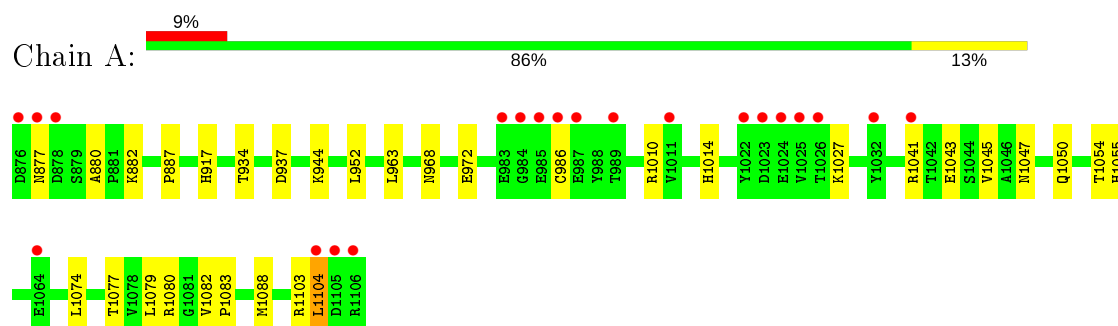
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	264	Total	O	0	0
			264	264		

### 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: RECEPTOR-TYPE ADENYLATE CYCLASE GRESAG 4.3



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00 Å 90.00 Å 66.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.67 – 1.90 23.39 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (18.67-1.90) 99.6 (23.39-1.90)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.67 (at 1.90 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.202 , 0.232 0.194 , 0.221	Depositor DCC
$R_{free}$ test set	688 reflections (3.27%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.6	Xtriage
Anisotropy	0.765	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2063	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: MG

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	0.41	0/1837	0.67	0/2503

There are no bond length outliers.

There are no bond angle outliers.

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	1798	0	1724	19	0
2	A	1	0	0	0	0
3	A	264	0	0	5	0
All	All	2063	0	1724	19	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 5.

All (19) 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:1047:ASN:H	1:A:1050:GLN:HE21	1.30	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:877:ASN:ND2	1:A:1027:LYS:O	2.35	0.59
1:A:1077:THR:HG23	1:A:1104:LEU:HD21	1.84	0.59
1:A:1014:HIS:HD2	1:A:1054:THR:OG1	1.86	0.57
1:A:1041:ARG:HD2	1:A:1080:ARG:O	2.05	0.56
1:A:1010:ARG:HD2	1:A:1043:GLU:OE1	2.05	0.56
1:A:1014:HIS:HE1	3:A:80:HOH:O	1.89	0.55
1:A:880:ALA:O	1:A:882:LYS:HG3	2.07	0.55
1:A:1047:ASN:HD22	1:A:1050:GLN:HE22	1.59	0.50
1:A:1047:ASN:H	1:A:1050:GLN:NE2	2.03	0.49
1:A:1055:HIS:HD2	3:A:164:HOH:O	1.96	0.48
1:A:1055:HIS:HE1	3:A:192:HOH:O	1.98	0.46
1:A:968:ASN:O	1:A:972:GLU:HG3	2.16	0.46
1:A:1045:VAL:HA	1:A:1103:ARG:HB2	1.97	0.45
1:A:887:PRO:HD2	3:A:247:HOH:O	2.16	0.44
1:A:1010:ARG:NH2	1:A:1103:ARG:NH1	2.66	0.44
1:A:952:LEU:HD23	1:A:952:LEU:C	2.39	0.43
1:A:944:LYS:NZ	3:A:209:HOH:O	2.52	0.41
1:A:1082:VAL:HA	1:A:1083:PRO:HD3	1.94	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	229/231 (99%)	224 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	191/195 (98%)	182 (95%)	9 (5%)	26	16

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	917	HIS
1	A	934	THR
1	A	937	ASP
1	A	963	LEU
1	A	986	CYS
1	A	1074	LEU
1	A	1079	LEU
1	A	1088	MET
1	A	1104	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1014	HIS
1	A	1050	GLN
1	A	1090	GLN
1	A	1092	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 monosaccharides 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.

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	231/231 (100%)	0.60	21 (9%) <b>9</b> <b>10</b>	17, 28, 54, 67	2 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	986	CYS	9.9
1	A	1106	ARG	9.5
1	A	1025	VAL	7.4
1	A	1104	LEU	7.0
1	A	1105	ASP	6.0
1	A	983	GLU	5.0
1	A	984	GLY	4.9
1	A	985	GLU	4.3
1	A	1026	THR	3.9
1	A	989	THR	3.8
1	A	878	ASP	3.8
1	A	987	GLU	3.8
1	A	1041	ARG	3.1
1	A	876	ASP	3.1
1	A	1032	TYR	2.9
1	A	1024	GLU	2.9
1	A	1022	TYR	2.7
1	A	1064	GLU	2.6
1	A	1023	ASP	2.4
1	A	877	ASN	2.1
1	A	1011	VAL	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	MG	A	2001	1/1	0.98	0.07	22,22,22,22	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.