



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 04:34 AM GMT

PDB ID : 2B0R
Title : Crystal Structure of Cyclase-Associated Protein from *Cryptosporidium parvum*
Authors : Tempel, W.; Dong, A.; Zhao, Y.; Lew, J.; Kozieradzki, I.; Alam, Z.; Melone, M.; Wasney, G.; Vedadi, M.; Arrowsmith, C.; Edwards, A.; Weigelt, J.; Sundstrom, M.; Hui, R.; Bochkarev, A.; Artz, J.; Structural Genomics Consortium (SGC)
Deposited on : 2005-09-14
Resolution : 2.60 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>

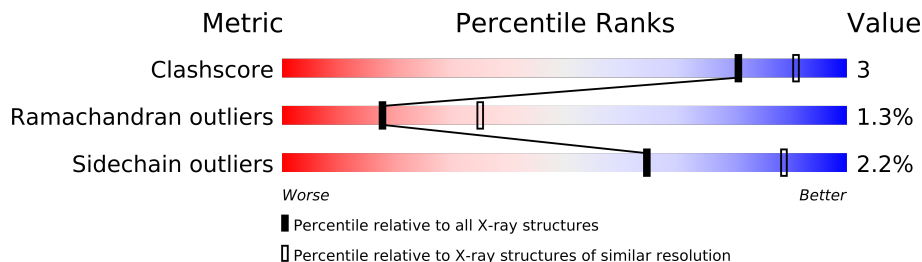
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	FAILED
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 2.60 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	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)

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 failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	202	
1	B	202	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2433 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 possible adenyl cyclase-associated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1232	776	201	247	8			
1	B	158	Total	C	N	O	S	0	0	0
			1200	755	197	240	8			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	GB 46227316
A	2	GLY	-	CLONING ARTIFACT	GB 46227316
A	3	SER	-	CLONING ARTIFACT	GB 46227316
A	4	SER	-	CLONING ARTIFACT	GB 46227316
A	5	HIS	-	EXPRESSION TAG	GB 46227316
A	6	HIS	-	EXPRESSION TAG	GB 46227316
A	7	HIS	-	EXPRESSION TAG	GB 46227316
A	8	HIS	-	EXPRESSION TAG	GB 46227316
A	9	HIS	-	EXPRESSION TAG	GB 46227316
A	10	HIS	-	EXPRESSION TAG	GB 46227316
A	11	SER	-	CLONING ARTIFACT	GB 46227316
A	12	SER	-	CLONING ARTIFACT	GB 46227316
A	13	GLY	-	CLONING ARTIFACT	GB 46227316
A	14	LEU	-	CLONING ARTIFACT	GB 46227316
A	15	VAL	-	CLONING ARTIFACT	GB 46227316
A	16	PRO	-	CLONING ARTIFACT	GB 46227316
A	17	ARG	-	CLONING ARTIFACT	GB 46227316
A	18	GLY	-	CLONING ARTIFACT	GB 46227316
A	19	SER	-	CLONING ARTIFACT	GB 46227316
B	1	MET	-	CLONING ARTIFACT	GB 46227316
B	2	GLY	-	CLONING ARTIFACT	GB 46227316
B	3	SER	-	CLONING ARTIFACT	GB 46227316
B	4	SER	-	CLONING ARTIFACT	GB 46227316
B	5	HIS	-	EXPRESSION TAG	GB 46227316
B	6	HIS	-	EXPRESSION TAG	GB 46227316

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Chain	Residue	Modelled	Actual	Comment	Reference
B	7	HIS	-	EXPRESSION TAG	GB 46227316
B	8	HIS	-	EXPRESSION TAG	GB 46227316
B	9	HIS	-	EXPRESSION TAG	GB 46227316
B	10	HIS	-	EXPRESSION TAG	GB 46227316
B	11	SER	-	CLONING ARTIFACT	GB 46227316
B	12	SER	-	CLONING ARTIFACT	GB 46227316
B	13	GLY	-	CLONING ARTIFACT	GB 46227316
B	14	LEU	-	CLONING ARTIFACT	GB 46227316
B	15	VAL	-	CLONING ARTIFACT	GB 46227316
B	16	PRO	-	CLONING ARTIFACT	GB 46227316
B	17	ARG	-	CLONING ARTIFACT	GB 46227316
B	18	GLY	-	CLONING ARTIFACT	GB 46227316
B	19	SER	-	CLONING ARTIFACT	GB 46227316

- Molecule 2 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

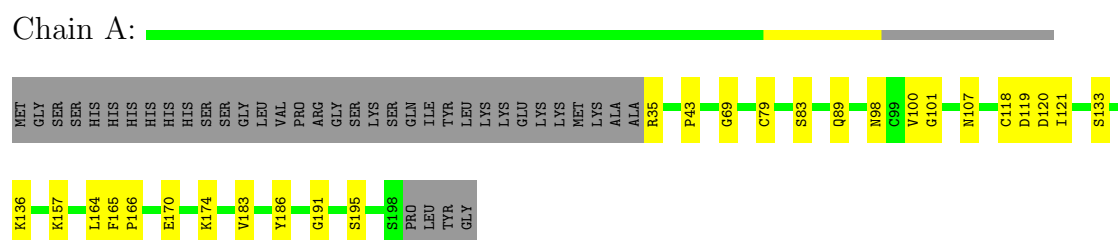
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total X 1 1	0	0

3 Residue-property plots

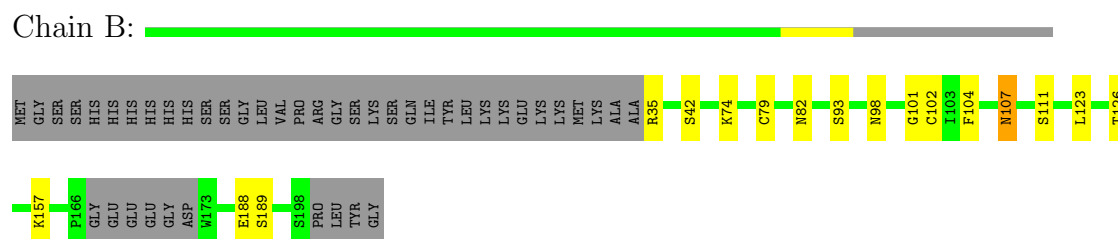
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 failed to run properly.

- Molecule 1: possible adenyl cyclase-associated protein



- Molecule 1: possible adenyl cyclase-associated protein



4 Data and refinement statistics i

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.26Å 58.86Å 65.81Å 90.00° 115.47° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	98.6 (20.00-2.60)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.216 , 0.267	Depositor
Wilson B-factor (Å ²)	59.9	Xtriage
Anisotropy	0.245	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 15674 reflections	Xtriage
Total number of atoms	2433	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.79	1/1247 (0.1%)	0.69	0/1691
1	B	0.80	2/1214 (0.2%)	0.69	0/1645
All	All	0.79	3/2461 (0.1%)	0.69	0/3336

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	102	CYS	CB-SG	-5.97	1.72	1.81
1	B	79	CYS	CB-SG	-5.39	1.73	1.81
1	A	79	CYS	CB-SG	-5.00	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1232	0	1205	11	0
1	B	1200	0	1189	6	0
2	A	1	0	0	0	0
All	All	2433	0	2394	16	0

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 3.

All (16) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:74:LYS:HG2	1:B:93:SER:OG	1.99	0.62
1:A:35:ARG:NH2	1:A:98:ASN:OD1	2.34	0.60
1:B:35:ARG:NH2	1:B:98:ASN:OD1	2.36	0.58
1:A:118:CYS:HB3	1:A:121:ILE:HG13	1.87	0.57
1:B:104:PHE:HB2	1:B:123:LEU:HD12	1.85	0.56
1:A:136:LYS:HA	1:A:157:LYS:O	2.05	0.56
1:B:107:ASN:HA	1:B:126:THR:HB	1.87	0.55
1:A:183:VAL:O	1:A:195:SER:HA	2.08	0.53
1:A:157:LYS:HA	1:B:157:LYS:HA	1.92	0.51
1:A:69:GLY:O	1:A:89:GLN:HG3	2.12	0.48
1:A:101:GLY:HA2	1:A:120:ASP:O	2.15	0.47
1:A:186:TYR:OH	1:A:191:GLY:HA2	2.16	0.46
1:A:164:LEU:HA	1:A:174:LYS:O	2.16	0.45
1:A:100:VAL:HA	1:A:119:ASP:O	2.18	0.43
1:B:82:ASN:HA	1:B:101:GLY:O	2.18	0.43
1:A:165:PHE:HA	1:A:166:PRO:HD3	1.92	0.40

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	162/202 (80%)	150 (93%)	10 (6%)	2 (1%)	19	39
1	B	154/202 (76%)	145 (94%)	7 (4%)	2 (1%)	18	35
All	All	316/404 (78%)	295 (93%)	17 (5%)	4 (1%)	18	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	189	SER

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Mol	Chain	Res	Type
1	B	107	ASN
1	A	107	ASN
1	A	43	PRO

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	139/185 (75%)	136 (98%)	3 (2%)	64	89
1	B	140/185 (76%)	137 (98%)	3 (2%)	66	90
All	All	279/370 (75%)	273 (98%)	6 (2%)	64	89

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	SER
1	A	133	SER
1	A	170	GLU
1	B	42	SER
1	B	111	SER
1	B	188	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 unknown - 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 failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.