wwPDB X-ray Structure Validation Summary Report (i)

May 22, 2020 – 01:33 am BST

PDB ID	:	3BCG
Title	:	Conformational changes of the AcrR regulator reveal a mechanism of induction
Authors	:	Gu, R.; Li, M.; Su, C.C.; Long, F.; Yang, F.; McDermott, G.; Yu, E.Y.
Deposited on	:	2007-11-12
Resolution	:	2.48 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

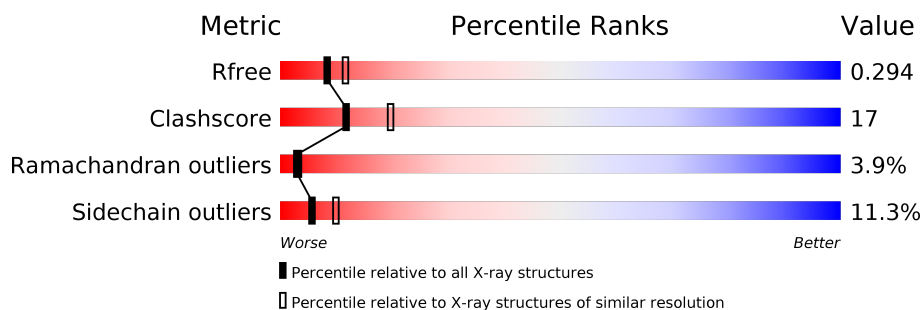|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.48 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		0.294
Clashscore		17
Ramachandran outliers		3.9%
Sidechain outliers		11.3%

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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)

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 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%

Mol	Chain	Length	Quality of chain
1	A	215	57% · · · 35% · ·
1	B	215	56% · · · 34% · · 6% ·

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3428 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 HTH-type transcriptional regulator acrR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total 1672	C 1065	N 287	O 309	S 11	0	0	0
1	B	207	Total 1672	C 1065	N 287	O 309	S 11	0	0	0

- Molecule 2 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	42	Total 42	O 42	0	0
2	B	42	Total 42	O 42	0	0

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: HTH-type transcriptional regulator acrR

Chain A:

• Molecule 1: HTH-type transcriptional regulator acrR

Chain B:
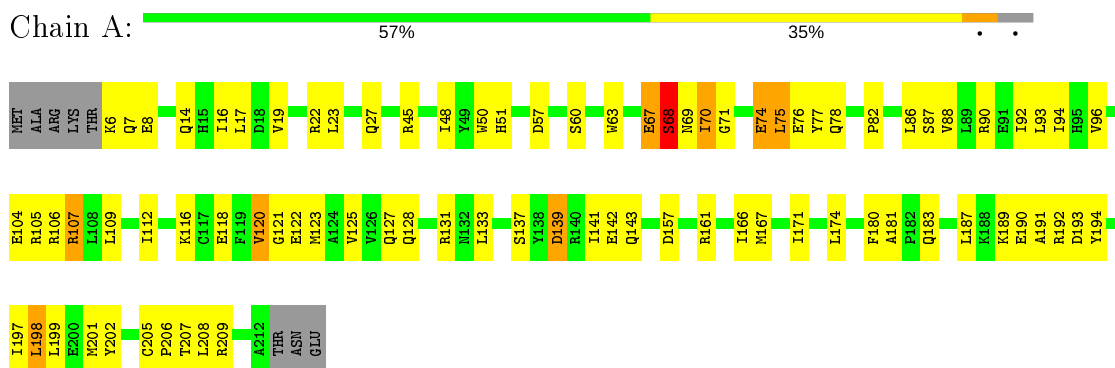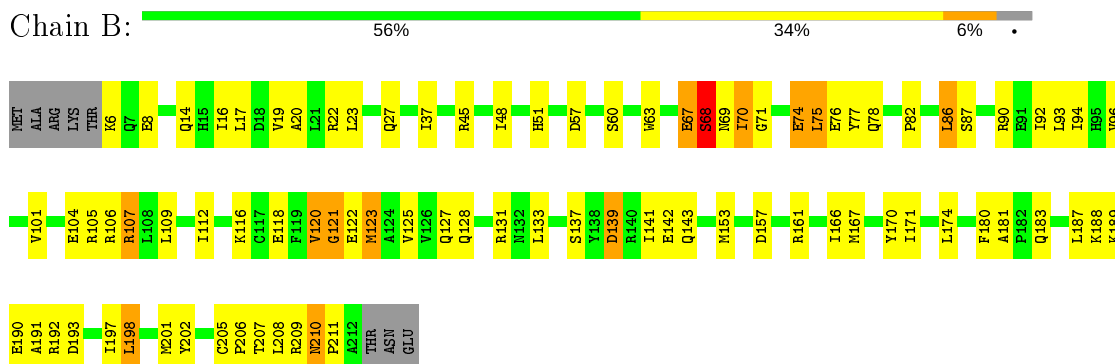
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	46.66Å 46.66Å 166.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.48 40.41 – 2.69	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.48) 97.7 (40.41-2.69)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$<I/\sigma(I)>$ [1]	12.14 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.268 0.305 , 0.294	Depositor DCC
R_{free} test set	523 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å^2)	64.6	Xtriage
Anisotropy	0.641	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 50.6	EDS
L-test for twinning [2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.479 for -h,-k,l 0.088 for h,-h-k,-l 0.086 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	3428	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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 (i)

5.1 Standard geometry (i)

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	0.35	0/1702	0.56	0/2295
1	B	0.35	0/1702	0.56	0/2295
All	All	0.35	0/3404	0.56	0/4590

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
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	68	SER	Peptide
1	B	68	SER	Peptide

5.2 Too-close contacts (i)

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	1672	0	1688	72	0
1	B	1672	0	1688	66	0
2	A	42	0	0	0	0
2	B	42	0	0	0	0
All	All	3428	0	3376	117	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 17.

The worst 5 of 117 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:201:MET:CE	1:B:201:MET:CE	1.97	1.40
1:A:201:MET:CE	1:B:201:MET:HE2	1.52	1.32
1:A:201:MET:HE2	1:B:201:MET:CE	1.53	1.27
1:A:201:MET:HE1	1:B:201:MET:CE	1.88	1.02
1:A:201:MET:CE	1:B:201:MET:HE1	1.91	0.96

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	205/215 (95%)	182 (89%)	16 (8%)	7 (3%)	3	4
1	B	205/215 (95%)	180 (88%)	16 (8%)	9 (4%)	2	2
All	All	410/430 (95%)	362 (88%)	32 (8%)	16 (4%)	3	3

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	SER

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Mol	Chain	Res	Type
1	A	70	ILE
1	A	74	GLU
1	B	68	SER
1	B	70	ILE

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	181/188 (96%)	161 (89%)	20 (11%)	6	10
1	B	181/188 (96%)	160 (88%)	21 (12%)	5	9
All	All	362/376 (96%)	321 (89%)	41 (11%)	6	10

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	GLU
1	B	19	VAL
1	B	183	GLN
1	A	198	LEU
1	B	6	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	B	51	HIS

5.3.3   RNA ⓘ

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 carbohydrates 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 (i)

6.1   Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3   Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4   Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5   Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.