



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2024 – 09:29 pm BST

PDB ID : 4UDS
Title : Crystal structure of MbdR regulator from Azoarcus sp. CIB
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Deposited on : 2014-12-11
Resolution : 1.76 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
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

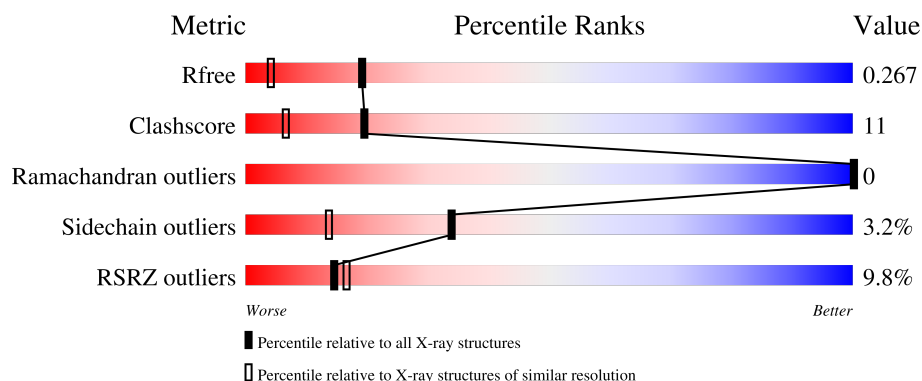
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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}	164625	2888 (1.76-1.76)
Clashscore	180529	3097 (1.76-1.76)
Ramachandran outliers	177936	3072 (1.76-1.76)
Sidechain outliers	177891	3072 (1.76-1.76)
RSRZ outliers	164620	2887 (1.76-1.76)

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 $\leq 5\%$. 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	214	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1677 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 MBDR REGULATOR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	Se	0	0	0
			1469	942	246	273	1	7			

- Molecule 2 is water.

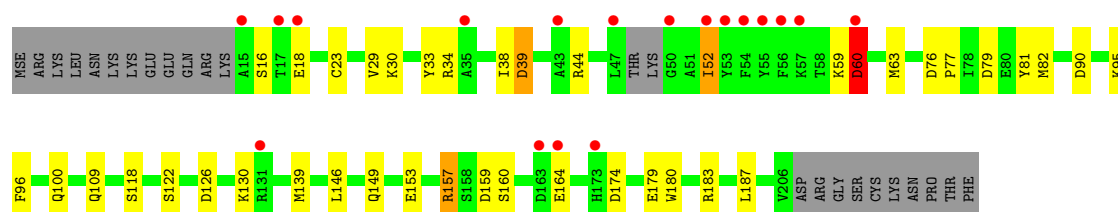
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	208	Total	O	0	0
			208	208		

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: MBDR REGULATOR

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	47.03Å 56.21Å 143.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.35 – 1.76 52.35 – 1.76	Depositor EDS
% Data completeness (in resolution range)	94.1 (52.35-1.76) 94.1 (52.35-1.76)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.55 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.6.0111	Depositor
R, R_{free}	0.191 , 0.249 0.218 , 0.267	Depositor DCC
R_{free} test set	937 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	1677	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [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	1.31	5/1483 (0.3%)	1.04	9/1990 (0.5%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	ASP	CB-CG	-5.86	1.39	1.51
1	A	118	SER	CB-OG	-5.83	1.34	1.42
1	A	179	GLU	CD-OE1	-5.50	1.19	1.25
1	A	59	LYS	C-N	-5.33	1.21	1.34
1	A	63	MSE	C-N	-5.18	1.22	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	ARG	NE-CZ-NH1	10.59	125.59	120.30
1	A	183	ARG	NE-CZ-NH2	-8.95	115.82	120.30
1	A	157	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	A	90	ASP	CB-CG-OD1	6.72	124.35	118.30
1	A	183	ARG	CG-CD-NE	-6.59	97.96	111.80
1	A	34	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	A	183	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	174	ASP	CB-CG-OD1	6.19	123.87	118.30
1	A	60	ASP	CB-CG-OD1	-6.14	112.77	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	60	ASP	Mainchain

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	1469	0	1507	34	2
2	A	208	0	0	15	5
All	All	1677	0	1507	34	6

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 11.

All (34) 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:82:MSE:CE	1:A:146:LEU:HD22	1.59	1.32
1:A:82:MSE:HG3	2:A:2068:HOH:O	1.32	1.28
1:A:82:MSE:HE1	1:A:146:LEU:CD2	1.86	1.06
1:A:82:MSE:HE1	1:A:146:LEU:HD22	0.97	0.97
1:A:33:TYR:OH	1:A:60:ASP:OD1	1.86	0.93
1:A:157:ARG:HD3	1:A:159:ASP:OD1	1.68	0.93
1:A:122:SER:OG	2:A:2120:HOH:O	1.95	0.83
1:A:164:GLU:OE1	2:A:2169:HOH:O	1.99	0.81
1:A:82:MSE:HE2	1:A:146:LEU:HD22	1.63	0.79
1:A:18:GLU:HG3	2:A:2004:HOH:O	1.89	0.72
1:A:82:MSE:HE2	2:A:2068:HOH:O	1.93	0.68
1:A:109:GLN:HG3	2:A:2118:HOH:O	1.93	0.68
1:A:38:ILE:CG2	1:A:52:ILE:HG21	2.25	0.67
1:A:100:GLN:NE2	1:A:139:MSE:HE1	2.19	0.57
1:A:82:MSE:CG	2:A:2068:HOH:O	2.13	0.56
1:A:82:MSE:CE	2:A:2068:HOH:O	2.54	0.54
1:A:130:LYS:HD2	2:A:2133:HOH:O	2.10	0.51
1:A:96:PHE:HZ	1:A:139:MSE:HE2	1.76	0.51
1:A:126:ASP:HB2	2:A:2129:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LYS:HD3	2:A:2020:HOH:O	2.12	0.50
1:A:23:CYS:HB3	1:A:44:ARG:HG2	1.94	0.49
1:A:180:TRP:HD1	1:A:187:LEU:HD12	1.78	0.49
1:A:82:MSE:SE	2:A:2068:HOH:O	2.81	0.48
1:A:76:ASP:N	1:A:77:PRO:CD	2.78	0.47
1:A:39:ASP:OD1	2:A:2032:HOH:O	2.21	0.46
1:A:96:PHE:CZ	1:A:139:MSE:HE2	2.51	0.45
1:A:38:ILE:HG23	1:A:52:ILE:HG21	1.98	0.45
1:A:76:ASP:HB2	1:A:77:PRO:HD3	1.98	0.45
1:A:180:TRP:HA	1:A:187:LEU:HD11	1.98	0.45
1:A:149:GLN:O	1:A:153:GLU:HG3	2.18	0.42
1:A:30:LYS:HD3	1:A:30:LYS:HA	1.86	0.42
1:A:29:VAL:HG12	1:A:30:LYS:NZ	2.35	0.41
1:A:30:LYS:CE	2:A:2020:HOH:O	2.68	0.41
1:A:164:GLU:CD	2:A:2169:HOH:O	2.54	0.41

All (6) 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)
2:A:2055:HOH:O	2:A:2055:HOH:O[4_555]	1.16	1.04
2:A:2086:HOH:O	2:A:2087:HOH:O[2_655]	1.76	0.44
1:A:95:LYS:NZ	1:A:164:GLU:OE2[7_555]	1.77	0.43
2:A:2086:HOH:O	2:A:2086:HOH:O[2_655]	1.78	0.42
2:A:2166:HOH:O	2:A:2196:HOH:O[2_555]	1.87	0.33
1:A:79:ASP:OD1	2:A:2086:HOH:O[2_655]	2.06	0.14

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	186/214 (87%)	184 (99%)	2 (1%)	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	154/169 (91%)	149 (97%)	5 (3%)	34 14

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	39	ASP
1	A	52	ILE
1	A	81	TYR
1	A	160	SER

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

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 oligosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	81:TYR	C	82:MSE	N	1.16
1	A	64:LEU	C	65:MSE	N	1.15

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, 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(Å ²)	Q<0.9
1	A	183/214 (85%)	0.66	18 (9%) 14 16	13, 20, 41, 54	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	54	PHE	6.5
1	A	15	ALA	4.3
1	A	47	LEU	4.2
1	A	60	ASP	3.0
1	A	173	HIS	3.0
1	A	55	TYR	2.9
1	A	57	LYS	2.9
1	A	163	ASP	2.7
1	A	52	ILE	2.6
1	A	18	GLU	2.5
1	A	164	GLU	2.5
1	A	56	PHE	2.4
1	A	50	GLY	2.4
1	A	131	ARG	2.3
1	A	35	ALA	2.3
1	A	53	TYR	2.2
1	A	43	ALA	2.1
1	A	17	THR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.