



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:22 PM UTC

PDB ID : 4UDO / pdb_00004udo
Title : structure of Mn-bound periplasmic metal binding protein from candidatus liberibacter asiaticus
Authors : Sharma, N.; Selvakumar, P.; Kumar, P.; Sharma, A.K.
Deposited on : 2014-12-10
Resolution : 2.22 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries

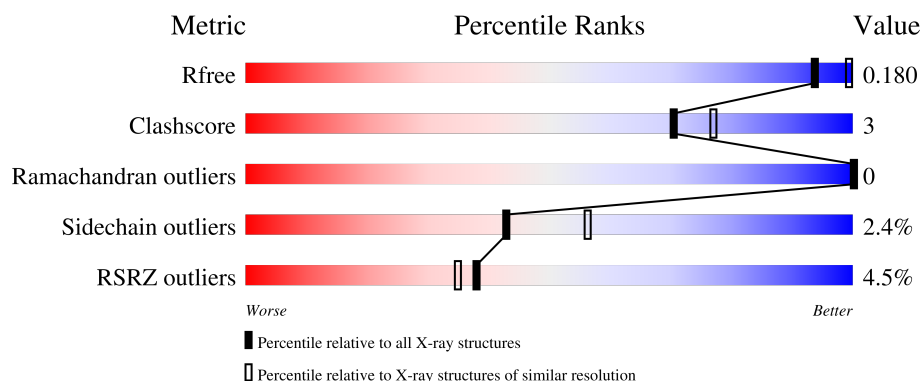
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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}	180053	7682 (2.24-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2388 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.

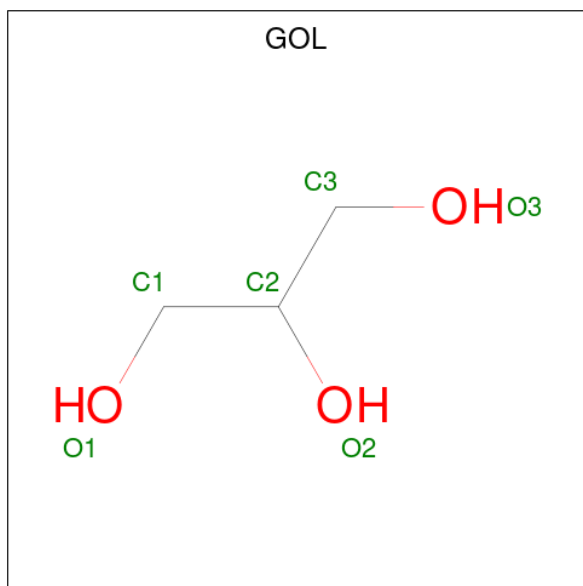
- Molecule 1 is a protein called PERIPLASMIC SOLUTE BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	7	0
			2154	1370	358	418	8			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

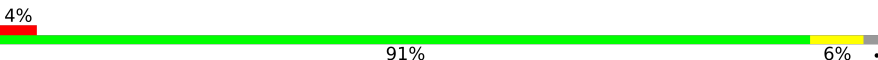
- Molecule 6 is water.

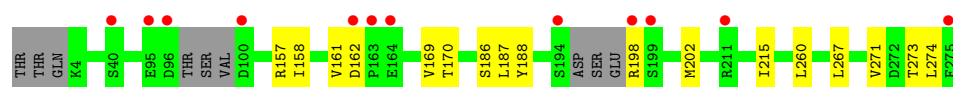
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	192	Total	O	0	0
			192	192		

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: PERIPLASMIC SOLUTE BINDING PROTEIN

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	94.32Å 94.32Å 94.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.20 – 2.22 47.20 – 2.22	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.20-2.22) 99.8 (47.20-2.22)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.164 , 0.196 (Not available) , 0.180	Depositor DCC
R_{free} test set	1244 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$	

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ACT, MN, GOL

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	0.52	0/2198	0.70	0/2976

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157[B]:ARG:HH11	1:A:157[B]:ARG:CG	1.88	0.84
1:A:158:ILE:CG1	1:A:271:VAL:HG12	2.11	0.81
1:A:158:ILE:HG13	1:A:271:VAL:HG12	1.61	0.81
1:A:157[B]:ARG:HH11	1:A:157[B]:ARG:HG3	1.62	0.61
1:A:157[B]:ARG:HH11	1:A:157[B]:ARG:HG2	1.65	0.61
1:A:158:ILE:HG13	1:A:271:VAL:CG1	2.31	0.60
1:A:267:LEU:O	1:A:271:VAL:HG13	2.06	0.56
1:A:157[B]:ARG:HG2	1:A:157[B]:ARG:NH1	2.18	0.56
1:A:157[B]:ARG:CG	1:A:157[B]:ARG:NH1	2.56	0.56
1:A:169:VAL:HG21	1:A:215:ILE:HG21	1.88	0.55
1:A:169:VAL:HG22	1:A:187:LEU:HB2	1.90	0.52
1:A:161:VAL:HG21	1:A:274:LEU:HD13	1.96	0.47
1:A:260:LEU:HD23	1:A:260		

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	214/247 (87%)	208 (97%)	6 (3%)	38 50

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

Mol	Chain	Res	Type
1	A	162	ASP
1	A	186[A]	SER
1	A	186[B]	SER
1	A	198	ARG
1	A	202	MET
1	A	273	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	1277	-	4,4,4	0.42	0	6,6,6	0.23	0
2	SO4	A	1276	-	4,4,4	0.43	0	6,6,6	0.39	0
5	ACT	A	1284	-	3,3,3	0.74	0	3,3,3	0.93	0
2	SO4	A	1279	-	4,4,4	0.36	0	6,6,6	0.14	0
2	SO4	A	1280	-	4,4,4	0.44	0	6,6,6	0.18	0
3	GOL	A	1281	-	5,5,5	0.24	0	5,5,5	0.44	0
3	GOL									

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, 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	266/275 (96%)	-0.26	12 (4%) 38 35	7, 20, 49, 87	7 (2%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	SER	4.2
1	A	275	PHE	3.7
1	A	198	ARG	3.7
1	A	96	ASP	3.6
1	A</			

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($\text{\AA}^2$)	Q<0.9
3	GOL	A	1281	6/6	0.75	0.24	50,53,57,64	0
3	GOL	A	1283	6/6	0.77	0.20	56,65,70,70	0
5	ACT	A	1284	4/4	0.78	0.20	46,59,59,66	0
2	SO4	A	1280	5/5	0.87	0.15	60,65,69,81	0
2	SO4	A	1279	5/5	0.89	0.14	24,33,35,35	5
2	SO4	A	1278	5/5	0.92	0.15	46,51,54,57	5
2	SO4	A	1277	5/5	0.93	0.18	30,33,34,38	5
2	SO4	A						