Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 06:50 AM JST

PDB ID	:	6L9C
Title	:	Neutron structure of copper amine oxidase from Arthrobacter glibiformis at pD 7.4
Authors	:	Murakawa, T.; Kurihara, K.; Shoji, M.; Shibazaki, C.; Sunami, T.; Tamada, T.; Yano, N.; Yamada, T.; Kusaka, K.; Suzuki, M.; Shigeta, Y.; Kuroki, R.; Hayashi, H.; Yano, Y.; Tanizawa, K.; Adachi, M.; Okajima, T.
Deposited on	:	2019-11-08
Resolution	:	1.14 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 (i) 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 (i)) were used in the production of this report:

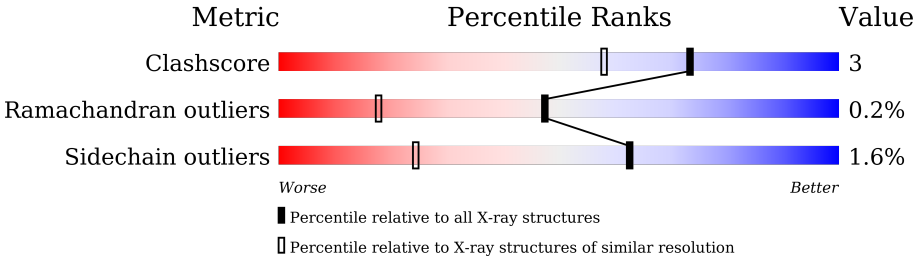
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION, NEUTRON DIFFRACTION

The reported resolution of this entry is 1.14 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	141614	1537 (1.18-1.10)
Ramachandran outliers	138981	1483 (1.18-1.10)
Sidechain outliers	138945	1480 (1.18-1.10)

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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	X	622	94% 5% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13687 atoms, of which 4809 are hydrogens and 2620 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 Phenylethylamine oxidase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	D	H	N	O	S			
1	X	621	11015	3317	1013	4809	891	971	14	0	587	0

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	X	1	1	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	D	O		
4	X	1063	2670	1607	1063	0	1

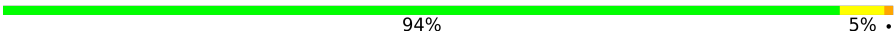
3 Residue-property plots (i)

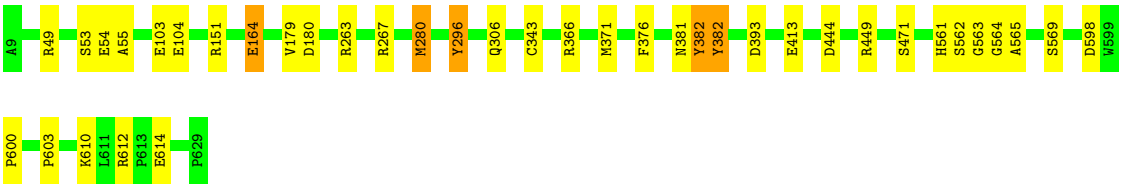
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

Note EDS failed to run properly.

- Molecule 1: Phenylethylamine oxidase

Chain X:





4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	157.55Å 61.78Å 92.33Å 90.00° 112.13° 90.00°	Depositor
Resolution (Å)	45.03 – 1.14	Depositor
% Data completeness (in resolution range)	99.3 (45.03-1.14)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 1.14Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.168 , 0.181	Depositor
Wilson B-factor (Å^2)	15.7	Xtriage
Anisotropy	0.386	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13687	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[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)

Bond lengths and bond angles in the following residue types are not validated in this section: ASA, NA, E9C, CU, TPQ

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	X	0.68	6/8789 (0.1%)	0.87	19/11953 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	343[A]	CYS	CB-SG	-7.66	1.69	1.82
1	X	343[B]	CYS	CB-SG	-7.66	1.69	1.82
1	X	151[B]	ARG	CB-CG	-6.11	1.36	1.52
1	X	151[A]	ARG	CB-CG	-6.11	1.36	1.52
1	X	104[A]	GLU	CD-OE2	5.25	1.31	1.25
1	X	104[B]	GLU	CD-OE2	5.25	1.31	1.25

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	449[A]	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	X	449[B]	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	X	151[B]	ARG	CG-CD-NE	-7.52	96.02	111.80
1	X	151[A]	ARG	CG-CD-NE	-7.52	96.02	111.80
1	X	151[B]	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	X	151[A]	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	X	612[A]	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	X	612[B]	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	X	598[A]	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	X	598[B]	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	X	612[A]	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	X	612[B]	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	X	49[A]	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	X	49[B]	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	X	366[A]	ARG	NE-CZ-NH1	5.57	123.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	366[B]	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	X	280[A]	MET	CG-SD-CE	-5.29	91.74	100.20
1	X	280[B]	MET	CG-SD-CE	-5.29	91.74	100.20
1	X	180[A]	ASP	CB-CG-OD2	-5.08	113.73	118.30

There are no chirality outliers.

There are no planarity outliers.

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	X	6206	4809	1132	29	0
2	X	1	0	0	0	0
3	X	1	0	0	0	0
4	X	2670	0	0	21	8
All	All	8878	4809	1132	34	8

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 3.

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:X:393[B]:ASP:OD2	4:X:801:HOH:O	1.73	1.06
1:X:164[A]:GLU:OE2	4:X:802:HOH:O	1.76	1.02
1:X:614[B]:GLU:OE1	4:X:803:HOH:O	1.80	0.98
1:X:614[A]:GLU:OE2	4:X:804:HOH:O	1.84	0.96
1:X:561[A]:HIS:ND1	1:X:562[A]:SER:O	2.13	0.80
1:X:413[A]:GLU:OE2	4:X:805:HOH:O	2.00	0.80
1:X:296[A]:TYR:OH	4:X:806:HOH:O	2.00	0.69
1:X:610[B]:LYS:NZ	4:X:809:HOH:O	2.18	0.54
1:X:562[C]:SER:O	4:X:814:HOH:O	2.24	0.47
1:X:471[A]:SER:OG	4:X:811:HOH:O	2.23	0.47
1:X:603[B]:PRO:HG2	4:X:992:HOH:O	2.12	0.43
1:X:565[B]:ALA:CB	4:X:1417:HOH:O	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:565[B]:ALA:HB1	4:X:1417:HOH:O	2.15	0.42
1:X:103[A]:GLU:HG3	4:X:842:HOH:O	2.15	0.42
1:X:610[B]:LYS:NZ	4:X:838:HOH:O	2.45	0.42
1:X:381[A]:ASN:HD22	1:X:381[A]:ASN:H	1.56	0.41
1:X:563[A]:GLY:HA2	4:X:871:HOH:O	2.15	0.41
1:X:564[B]:GLY:O	1:X:569[B]:SER:OG	2.37	0.41
1:X:296[A]:TYR:CG	1:X:382[A]:E9C:OAJ	2.75	0.40
1:X:614[B]:GLU:HB2	4:X:1039:HOH:O	2.15	0.40

All (8) 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)
4:X:1486:HOH:O	4:X:1486:HOH:O[2_556]	1.78	0.42
4:X:804:HOH:O	4:X:930:HOH:O[2_556]	1.86	0.34
4:X:930:HOH:O	4:X:1088:HOH:O[2_556]	2.00	0.20
4:X:1142:HOH:O	4:X:1538:HOH:O[2_556]	2.01	0.19
4:X:1287:HOH:O	4:X:1433:HOH:O[2_556]	2.11	0.09
4:X:808:HOH:O	4:X:1433:HOH:O[2_556]	2.12	0.08
4:X:1294:HOH:O	4:X:1521:HOH:O[2_556]	2.19	0.01
4:X:1810:HOH:O	4:X:1814:HOH:O[2_556]	2.19	0.01

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	X	1084/622 (174%)	1049 (97%)	33 (3%)	2 (0%)	47 18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	55[A]	ALA

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Mol	Chain	Res	Type
1	X	55[B]	ALA

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	X	907/513 (177%)	891 (98%)	16 (2%)	59 20

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	53[A]	SER
1	X	53[B]	SER
1	X	54[A]	GLU
1	X	54[B]	GLU
1	X	164[A]	GLU
1	X	164[B]	GLU
1	X	267[A]	ARG
1	X	267[B]	ARG
1	X	296[A]	TYR
1	X	296[B]	TYR
1	X	371[A]	MET
1	X	371[B]	MET
1	X	376[A]	PHE
1	X	376[B]	PHE
1	X	444[A]	ASP
1	X	444[B]	ASP

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)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	E9C	X	382[A]	1	12,14,15	2.02	3 (25%)	11,19,21	2.09	4 (36%)
1	TPQ	X	382[B]	1	13,14,15	0.95	1 (7%)	15,19,21	1.92	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	E9C	X	382[A]	1	-	1/5/22/24	0/1/1/1
1	TPQ	X	382[B]	1	-	1/5/22/24	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	382[A]	E9C	CD2-CG	-4.22	1.45	1.49
1	X	382[A]	E9C	CB-CG	-3.48	1.44	1.50
1	X	382[A]	E9C	CD1-CG	2.45	1.41	1.34
1	X	382[B]	TPQ	C1-C2	2.30	1.52	1.49

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	382[B]	TPQ	CB-CA-C	-5.74	100.72	111.47
1	X	382[A]	E9C	CB-CA-C	-4.53	102.98	111.47
1	X	382[B]	TPQ	C6-C1-C2	3.66	121.45	118.64
1	X	382[A]	E9C	CA-CB-CG	2.53	118.34	113.51
1	X	382[A]	E9C	OAI-CD2-CAE	-2.15	118.00	121.12
1	X	382[A]	E9C	CAE-CAD-CAC	2.10	120.44	116.63

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	X	382[A]	E9C	O-C-CA-CB
1	X	382[B]	TPQ	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	X	382[A]	E9C	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are 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 (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)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.