WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Aug 7, 2023 – 04:46 PM EDT

PDB ID : 1QAK
Title : THE ACTIVE SITE BASE CONTROLS COFACTOR REACTIVITY IN ES-
CHERICHIA COLI AMINE OXIDASE : X-RAY CRYSTALLOGRAPHIC
STUDIES WITH MUTATIONAL VARIANTS
Authors : Murray, J.M.; Wilmot, C.M.; Saysell, C.G.; Jaeger, J.; Knowles, P.F.; Phillips,
S.E.; McPherson, M.J.
Deposited on : 1999-03-15
Resolution : 2.00 Å(reported)

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

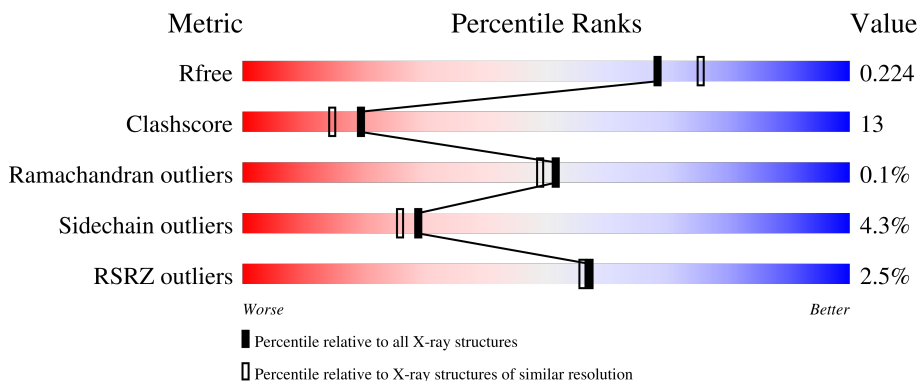|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

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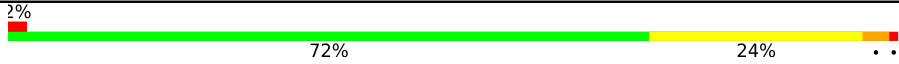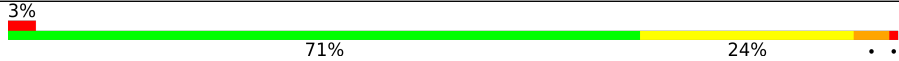*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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		0.224
Clashscore		13
Ramachandran outliers		0.1%
Sidechain outliers		4.3%
RSRZ outliers		2.5%

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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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% 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	722	2% / 72% / 24% / · ·
1	B	722	3% / 71% / 24% / · ·

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 12895 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 COPPER AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	720	Total 5686	C 3616	N 969	O 1079	S 22	0	1	1
1	B	722	Total 5712	C 3632	N 973	O 1085	S 22	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	383	ALA	ASP	engineered mutation	UNP P46883
A	466	TPQ	TYR	modified residue	UNP P46883
B	383	ALA	ASP	engineered mutation	UNP P46883
B	466	TPQ	TYR	modified residue	UNP P46883

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Cu 1	0	0
2	B	1	Total 1	Cu 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Ca 2	0	0
3	B	2	Total 2	Ca 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	791	Total 791	O 791	0	0
4	B	700	Total 700	O 700	0	0

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 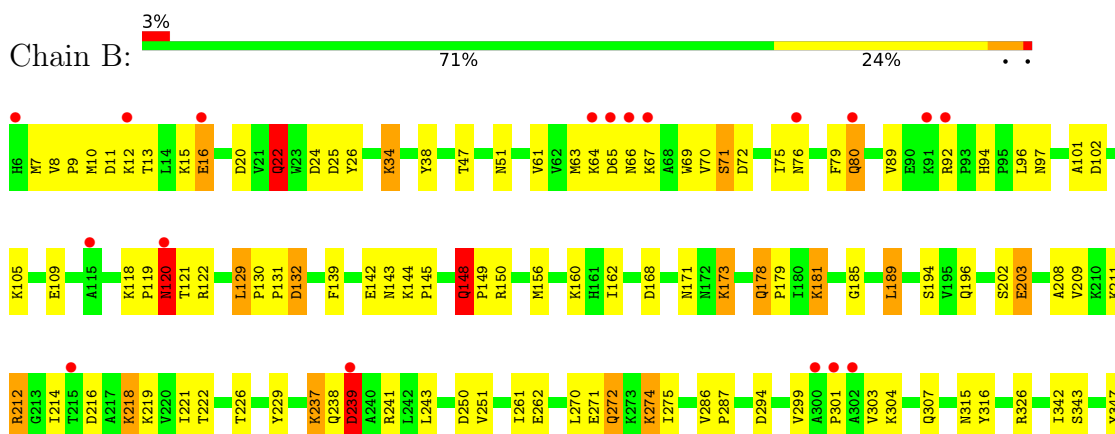for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: COPPER AMINE OXIDASE

• Molecule 1: COPPER AMINE OXIDASE

E359 I366 V367 P368 Y369 G370 Y377 Y381 L382 R398 G399 K400 A406 D415 Y416 M421 R432 Y438 K439 H440 M443 S449 R452 R453 N465 Y466 D467 Y468 I469 F470 D471 W472 N477 I489 E490 A497 K498 H501 D502 E503 K506

R510 D516 H517 N518 I519 H524 Q525 H526 V536 E539 N540 N541 A545 N553 T554 A555 P558 R559 Q567 N572 E573 Q574 D575 Q578 K579 F580 D581 P582 R586 L587 L588 N592 N595 R596 S602 Y608 A609 G610 H613 P614 V615 A616 K617

Q620 F621 D624 I627 R630 M634 D635 K636 Q637 R642 R648 R657 K669 D670 N671 E672 N676 A679 T688 H689 V690 A691 R692 E695 V704 T717 L720 K725 D726 K727

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	134.66Å 166.17Å 79.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.94 – 1.99	Depositor EDS
% Data completeness (in resolution range)	97.4 (20.00-2.00) 90.0 (19.94-1.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.36 (at 1.99Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.176 , 0.244 0.170 , 0.224	Depositor DCC
R_{free} test set	3766 reflections (3.43%)	wwPDB-VP
Wilson B-factor (Å^2)	22.6	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 64.8	EDS
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12895	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 2.71% 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 ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CU, CA, 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	A	0.53	0/5802	1.71	80/7899 (1.0%)
1	B	0.51	0/5828	1.65	89/7930 (1.1%)
All	All	0.52	0/11630	1.68	169/15829 (1.1%)

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.

The worst 5 of 169 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	692	ARG	NE-CZ-NH2	-20.10	110.25	120.30
1	A	596	ARG	CD-NE-CZ	19.41	150.78	123.60
1	A	648	ARG	NE-CZ-NH1	16.45	128.52	120.30
1	A	692	ARG	NE-CZ-NH2	-16.04	112.28	120.30
1	A	648	ARG	NE-CZ-NH2	-12.50	114.05	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	466[B]	TPQ	Mainchain

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Mol	Chain	Res	Type	Group
1	B	466[B]	TPQ	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	5686	0	5553	148	0
1	B	5712	0	5583	161	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	791	0	0	23	0
4	B	700	0	0	21	0
All	All	12895	0	11136	288	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 13.

The worst 5 of 288 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:B:466[A]:TPQ:H6	4:B:1351:HOH:O	1.25	1.29
1:B:466[A]:TPQ:C6	4:B:1351:HOH:O	1.92	1.00
1:B:67:LYS:HG3	1:B:69:TRP:HE1	1.27	0.98
1:B:272:GLN:HE21	1:B:274:LYS:HD3	1.30	0.93
1:A:466[A]:TPQ:O5	4:A:1575:HOH:O	1.86	0.93

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	717/722 (99%)	694 (97%)	23 (3%)	0	100	100
1	B	719/722 (100%)	693 (96%)	25 (4%)	1 (0%)	51	49
All	All	1436/1444 (99%)	1387 (97%)	48 (3%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	726	ASP

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	609/612 (100%)	587 (96%)	22 (4%)	35	34
1	B	612/612 (100%)	581 (95%)	31 (5%)	24	19
All	All	1221/1224 (100%)	1168 (96%)	53 (4%)	29	26

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	71	SER
1	B	181	LYS
1	B	617	LYS
1	B	80	GLN
1	B	148	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	671	ASN

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Mol	Chain	Res	Type
1	B	572	ASN
1	B	148	GLN
1	B	567	GLN
1	B	613	HIS

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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	TPQ	A	466[A]	1	13,14,15	2.15	6 (46%)	15,19,21	4.23	5 (33%)
1	TPQ	B	466[B]	1	13,14,15	2.31	6 (46%)	15,19,21	5.29	5 (33%)
1	TPQ	B	466[A]	1	13,14,15	2.88	6 (46%)	15,19,21	3.34	2 (13%)
1	TPQ	A	466[B]	1	13,14,15	2.34	5 (38%)	15,19,21	5.84	7 (46%)

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	TPQ	A	466[A]	1	-	2/5/22/24	0/1/1/1
1	TPQ	B	466[B]	1	-	2/5/22/24	0/1/1/1
1	TPQ	B	466[A]	1	-	0/5/22/24	0/1/1/1
1	TPQ	A	466[B]	1	-	2/5/22/24	0/1/1/1

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	466[B]	TPQ	C1-C2	-5.52	1.40	1.49
1	A	466[B]	TPQ	C1-C2	-5.35	1.41	1.49
1	B	466[A]	TPQ	C1-C2	-5.11	1.41	1.49
1	B	466[A]	TPQ	O5-C5	-5.08	1.11	1.24
1	A	466[A]	TPQ	C1-C2	-5.00	1.41	1.49

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	466[B]	TPQ	CB-CA-C	-20.84	72.41	111.47
1	B	466[B]	TPQ	CB-CA-C	-18.55	76.69	111.47
1	A	466[A]	TPQ	CB-CA-C	-14.18	84.89	111.47
1	B	466[A]	TPQ	CB-CA-C	-11.92	89.13	111.47
1	B	466[B]	TPQ	CB-C1-C2	6.34	129.93	118.57

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	466[A]	TPQ	N-CA-CB-C1
1	A	466[A]	TPQ	C-CA-CB-C1
1	B	466[B]	TPQ	C-CA-CB-C1
1	A	466[B]	TPQ	N-CA-CB-C1
1	B	466[B]	TPQ	N-CA-CB-C1

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	466[A]	TPQ	4	0
1	B	466[A]	TPQ	3	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 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 ⓘ

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 ⓘ

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	719/722 (99%)	-0.34	13 (1%)	68	66	12, 23, 45, 70	0
1	B	721/722 (99%)	-0.26	23 (3%)	47	46	15, 24, 48, 95	0
All	All	1440/1444 (99%)	-0.30	36 (2%)	57	56	12, 24, 47, 95	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	727	LYS	7.3
1	B	301	PRO	5.6
1	B	302	ALA	5.0
1	B	6	HIS	4.3
1	B	215	THR	4.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, 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(Å^2)	Q<0.9
1	TPQ	A	466[A]	14/15	0.87	0.21	24,45,47,48	14
1	TPQ	A	466[B]	14/15	0.87	0.21	15,43,53,53	14
1	TPQ	B	466[A]	14/15	0.89	0.19	22,50,57,57	14
1	TPQ	B	466[B]	14/15	0.89	0.19	20,40,50,54	14

6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, 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(Å^2)	Q<0.9
3	CA	B	803	1/1	0.95	0.06	49,49,49,49	0
3	CA	A	803	1/1	0.98	0.12	42,42,42,42	0
3	CA	A	802	1/1	0.99	0.09	21,21,21,21	0
2	CU	B	801	1/1	1.00	0.04	23,23,23,23	0
3	CA	B	802	1/1	1.00	0.07	22,22,22,22	0
2	CU	A	801	1/1	1.00	0.05	26,26,26,26	0

6.5   Other polymers ⓘ

There are no such residues in this entry.