



wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 09:03 pm BST

PDB ID : 1XMH
Title : Structure of Co(II) reconstituted methane monooxygenase hydroxylase from
M. capsulatus (Bath)
Authors : Sazinsky, M.H.; Merckx, M.; Cadieux, E.; Tang, S.; Lippard, S.J.
Deposited on : 2004-10-02
Resolution : 2.32 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

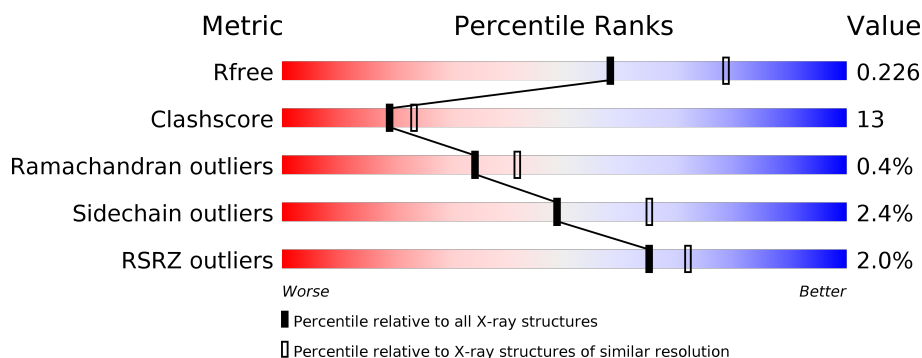
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 $\leq 5\%$. 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	527	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>24%</div> <div>• •</div> </div> </div>
1	B	527	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>28%</div> <div>• •</div> </div> </div>
2	C	388	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>17%</div> <div>•</div> </div> </div>
2	D	388	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>32%</div> <div>•</div> </div> </div>
3	E	169	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div>• •</div> </div> </div>
3	F	169	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18154 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 Methane monooxygenase component A alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			4138	2649	709	762	18			
1	B	511	Total	C	N	O	S	0	0	0
			4141	2648	712	763	18			

- Molecule 2 is a protein called Methane monooxygenase component A beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	388	Total	C	N	O	S	0	0	0
			3167	2038	545	576	8			
2	D	388	Total	C	N	O	S	0	0	0
			3151	2028	543	572	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	18	GLU	ALA	CONFLICT	UNP P18798
C	370	ARG	ALA	CONFLICT	UNP P18798
D	18	GLU	ALA	CONFLICT	UNP P18798
D	370	ARG	ALA	CONFLICT	UNP P18798

- Molecule 3 is a protein called Methane monooxygenase component A gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	167	Total	C	N	O	S	0	0	0
			1368	866	246	251	5			
3	F	166	Total	C	N	O	S	0	0	0
			1358	860	243	250	5			

- Molecule 4 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total 2	Co 2	0	0
4	A	2	Total 2	Co 2	0	0

- Molecule 5 is water.

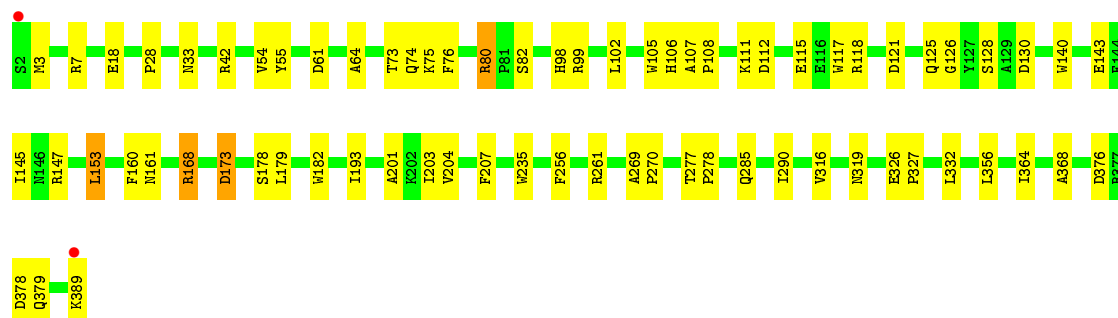
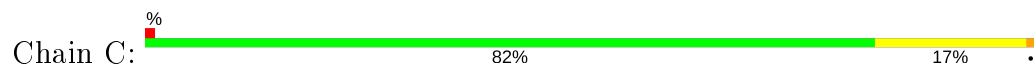
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	187	Total 187	O 187	0	0
5	B	189	Total 189	O 189	0	0
5	C	225	Total 225	O 225	0	0
5	D	97	Total 97	O 97	0	0
5	E	90	Total 90	O 90	0	0
5	F	39	Total 39	O 39	0	0

- Molecule 1: Methane monooxygenase component A alpha chain

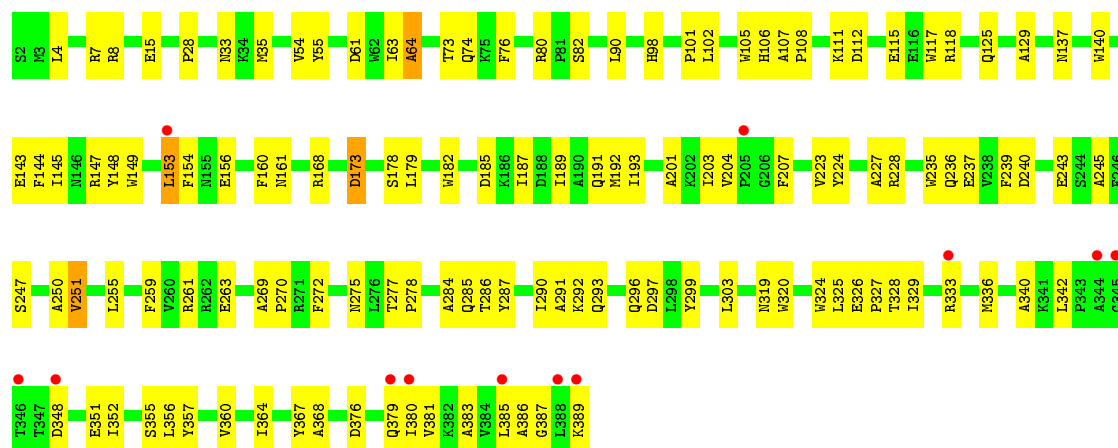




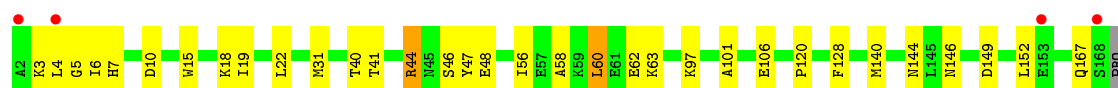
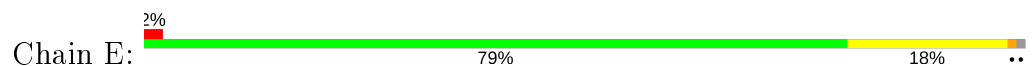
- Molecule 2: Methane monooxygenase component A beta chain



- Molecule 2: Methane monooxygenase component A beta chain



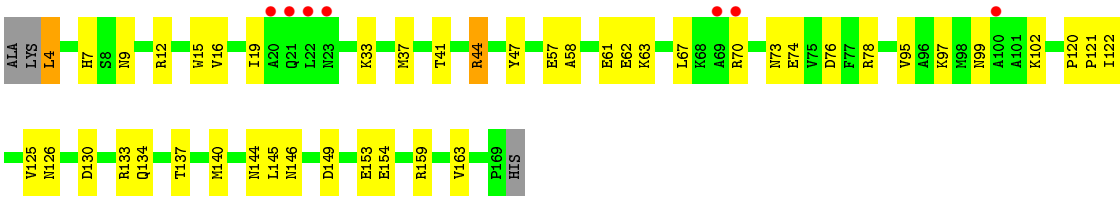
- Molecule 3: Methane monooxygenase component A gamma chain



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- Molecule 3: Methane monooxygenase component A gamma chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.44Å 171.84Å 220.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.55 – 2.32 29.55 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.5 (29.55-2.32) 90.9 (29.55-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.194 , 0.225 0.194 , 0.226	Depositor DCC
R_{free} test set	3972 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18154	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CO

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	0.33	0/4263	0.56	0/5797
1	B	0.36	1/4266 (0.0%)	0.61	3/5801 (0.1%)
2	C	0.37	0/3263	0.58	0/4435
2	D	0.33	0/3247	0.54	0/4417
3	E	0.35	0/1396	0.60	0/1881
3	F	0.29	0/1387	0.53	0/1873
All	All	0.35	1/17822 (0.0%)	0.57	3/24204 (0.0%)

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	42	ASN	C-N	6.34	1.48	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	ASN	O-C-N	-10.78	105.46	122.70
1	B	41	ASN	CA-C-N	5.72	129.78	117.20
1	B	41	ASN	OD1-CG-ND2	-5.40	109.48	121.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	41	ASN	Sidechain

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	4138	0	3897	123	0
1	B	4141	0	3889	154	0
2	C	3167	0	2987	63	0
2	D	3151	0	2957	113	0
3	E	1368	0	1353	24	0
3	F	1358	0	1335	38	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	187	0	0	8	0
5	B	189	0	0	6	0
5	C	225	0	0	1	0
5	D	97	0	0	2	0
5	E	90	0	0	1	0
5	F	39	0	0	3	0
All	All	18154	0	16418	439	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 439 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:352:ALA:HA	1:A:404:PRO:HB2	1.39	1.00
1:A:435:THR:CG2	1:A:437:ARG:HE	1.80	0.94
1:B:155:ASN:HD22	1:B:168:HIS:HD2	1.12	0.94
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.08	0.92
2:C:3:MET:HE3	2:D:28:PRO:HG3	1.55	0.89

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	508/527 (96%)	484 (95%)	21 (4%)	3 (1%)	25	30
1	B	509/527 (97%)	476 (94%)	31 (6%)	2 (0%)	34	41
2	C	386/388 (100%)	376 (97%)	9 (2%)	1 (0%)	41	50
2	D	386/388 (100%)	365 (95%)	18 (5%)	3 (1%)	19	23
3	E	165/169 (98%)	163 (99%)	2 (1%)	0	100	100
3	F	164/169 (97%)	158 (96%)	6 (4%)	0	100	100
All	All	2118/2168 (98%)	2022 (96%)	87 (4%)	9 (0%)	34	41

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	LYS
2	D	64	ALA
2	D	386	ALA
2	C	64	ALA
1	A	94	ARG

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	423/442 (96%)	411 (97%)	12 (3%)	43	59
1	B	422/442 (96%)	409 (97%)	13 (3%)	40	55
2	C	316/323 (98%)	309 (98%)	7 (2%)	52	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	312/323 (97%)	306 (98%)	6 (2%)	57	73
3	E	143/146 (98%)	140 (98%)	3 (2%)	53	70
3	F	142/146 (97%)	140 (99%)	2 (1%)	67	80
All	All	1758/1822 (96%)	1715 (98%)	43 (2%)	49	65

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	279	GLN
1	B	440	GLU
3	E	60	LEU
1	B	302	VAL
1	B	311	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	227	ASN
1	B	344	HIS
3	F	7	HIS
1	B	249	ASN
1	B	278	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 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 [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	510/527 (96%)	-0.32	8 (1%) 72 78	22, 34, 56, 69	0
1	B	511/527 (96%)	-0.42	10 (1%) 65 72	15, 35, 53, 66	0
2	C	388/388 (100%)	-0.65	2 (0%) 91 94	18, 25, 41, 53	0
2	D	388/388 (100%)	-0.08	12 (3%) 49 56	25, 42, 58, 86	0
3	E	167/169 (98%)	-0.59	4 (2%) 59 66	19, 29, 42, 65	0
3	F	166/169 (98%)	0.31	7 (4%) 36 43	36, 51, 64, 70	0
All	All	2130/2168 (98%)	-0.33	43 (2%) 65 72	15, 35, 57, 86	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	2	ALA	6.7
2	D	389	LYS	6.3
3	F	100	ALA	4.4
1	B	40	LYS	4.2
3	E	168	SER	3.9

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 carbohydrates in this entry.

6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
4	CO	B	5173	1/1	0.98	0.04	50,50,50,50	0
4	CO	A	5170	1/1	0.99	0.02	42,42,42,42	0
4	CO	A	5171	1/1	0.99	0.04	30,30,30,30	0
4	CO	B	5172	1/1	1.00	0.06	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.