wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:57 PM GMT

PDB ID	:	1MTY
Title	:	METHANE MONOOXYGENASE HYDROXYLASE FROM METHYLOCOCCUS CAPSULATUS (BATH)
Authors	:	Rosenzweig, A.C.; Nordlund, P.; Lippard, S.J.; Frederick, C.A.
Deposited on	:	1996-07-10
Resolution	:	1.70 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

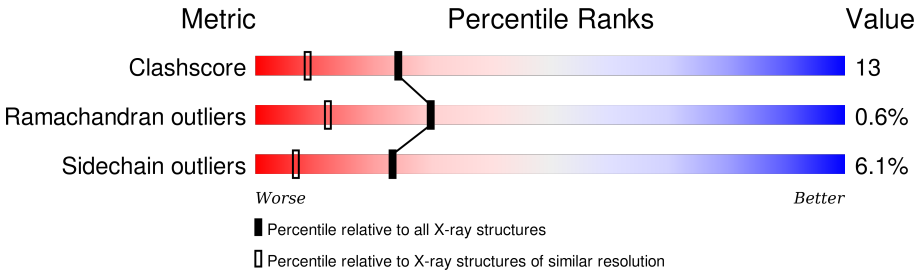
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.70 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	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	D	512	75% 23%
1	E	512	73% 23%
2	B	384	79% 18%
2	C	384	77% 20%
3	G	162	78% 20%
3	H	162	78% 19%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25065 atoms, of which 6193 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 HYDROXYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	D	512	Total	C	H	N	O	S	0	0	0
			5120	2680	934	721	767	18			
1	E	512	Total	C	H	N	O	S	0	0	0
			5120	2680	934	721	767	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	306	ASP	ASN	CONFLICT	UNP P22869
D	444	GLU	GLN	CONFLICT	UNP P22869
E	306	ASP	ASN	CONFLICT	UNP P22869
E	444	GLU	GLN	CONFLICT	UNP P22869

- Molecule 2 is a protein called METHANE MONOOXYGENASE HYDROXYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	384	Total	C	N	O	S		0	0	0
			3167	2038	547	575	7				
2	C	384	Total	C	H	N	O	S	0	0	0
			3874	2038	707	547	575	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	142	ASP	THR	CONFLICT	UNP P18798
B	143	GLU	SER	CONFLICT	UNP P18798
B	144	PHE	SER	CONFLICT	UNP P18798
B	145	ILE	CYS	CONFLICT	UNP P18798
C	142	ASP	THR	CONFLICT	UNP P18798
C	143	GLU	SER	CONFLICT	UNP P18798
C	144	PHE	SER	CONFLICT	UNP P18798
C	145	ILE	CYS	CONFLICT	UNP P18798

- Molecule 3 is a protein called METHANE MONOOXYGENASE HYDROXYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	G	162	Total	C	H	N	O	S	0	0	0
			1658	847	321	241	244	5			
3	H	162	Total	C	H	N	O	S	0	0	0
			1658	847	321	241	244	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	38	ASP	HIS	CONFLICT	UNP P11987
G	80	LYS	ASN	CONFLICT	UNP P11987
H	38	ASP	HIS	CONFLICT	UNP P11987
H	80	LYS	ASN	CONFLICT	UNP P11987

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Fe	0	0
			2	2		
4	E	2	Total	Fe	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	263	Total	H	O	0	0
			789	526	263		
5	C	269	Total	H	O	0	0
			807	538	269		
5	D	292	Total	H	O	0	0
			876	584	292		
5	E	308	Total	H	O	0	0
			924	616	308		
5	G	157	Total	H	O	0	0
			471	314	157		
5	H	199	Total	H	O	0	0
			597	398	199		

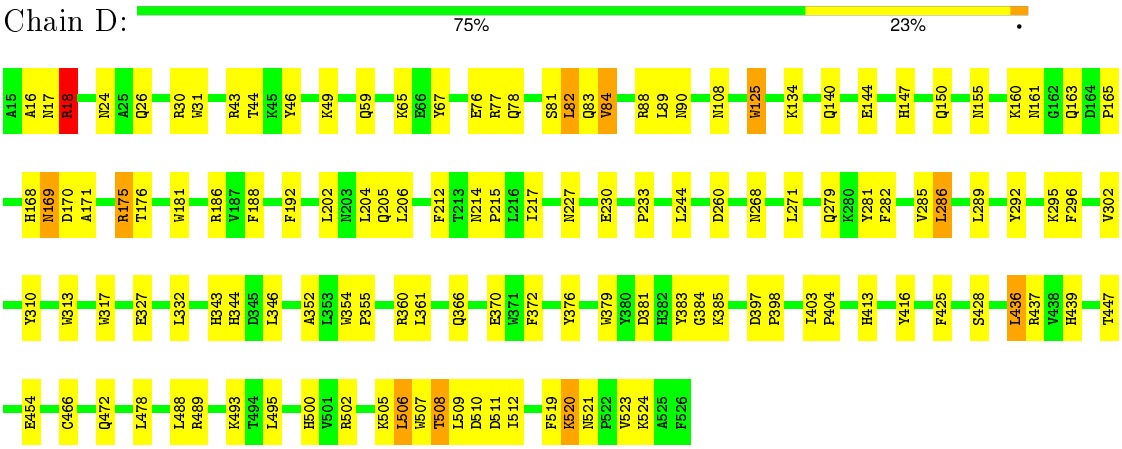
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

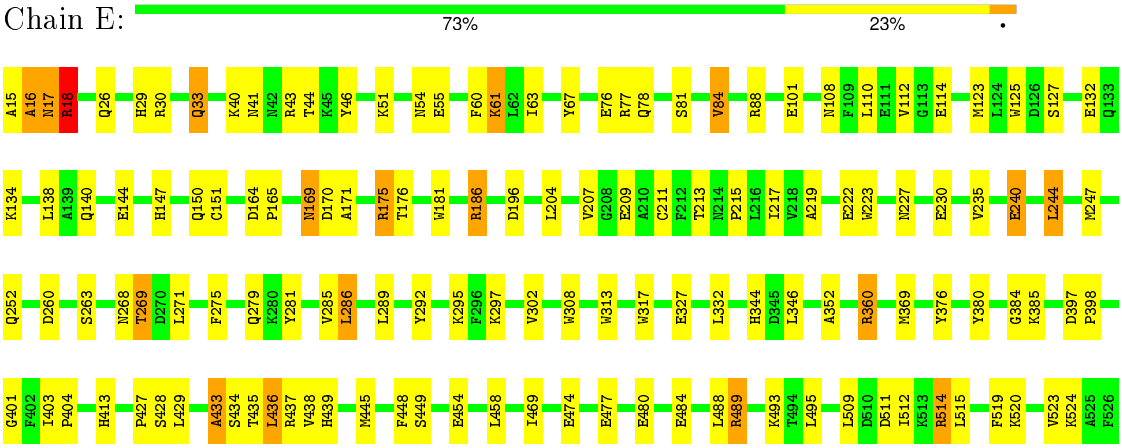
• Molecule 1: METHANE MONOOXYGENASE HYDROXYLASE

Chain D:



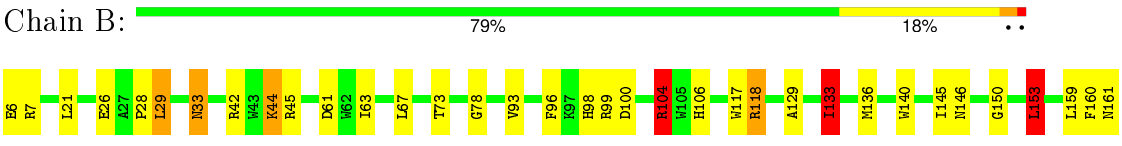
• Molecule 1: METHANE MONOOXYGENASE HYDROXYLASE

Chain E:



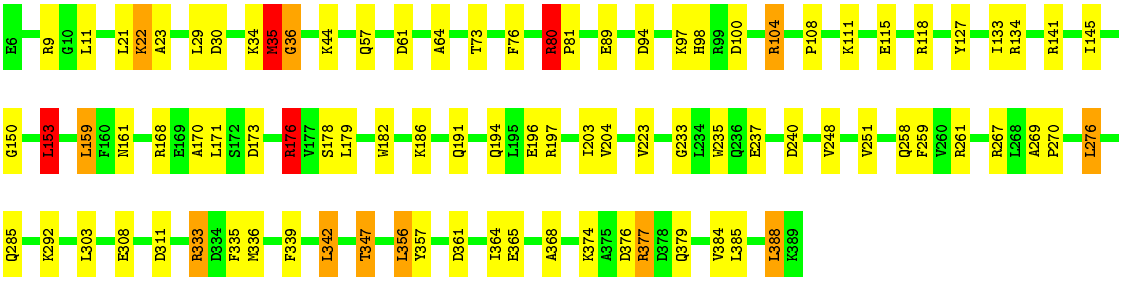
• Molecule 2: METHANE MONOOXYGENASE HYDROXYLASE

Chain B:



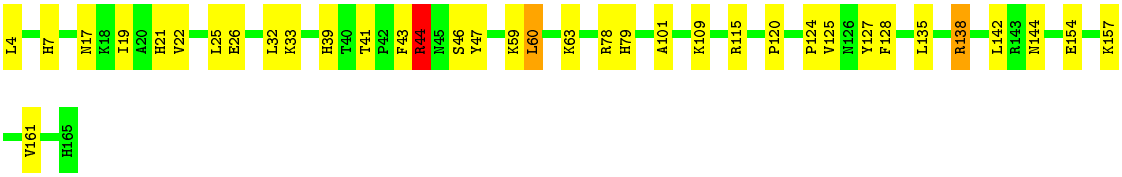
- Molecule 2: METHANE MONOOXYGENASE HYDROXYLASE

Chain C:



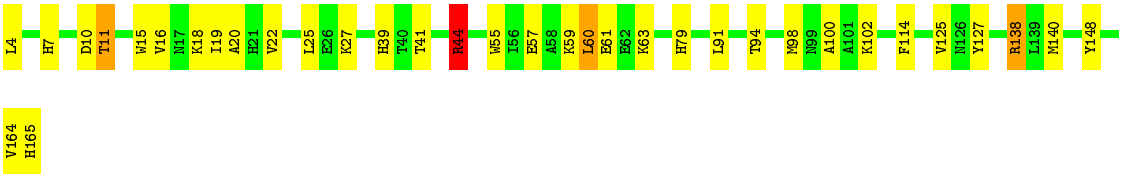
- Molecule 3: METHANE MONOOXYGENASE HYDROXYLASE

Chain G:



- Molecule 3: METHANE MONOOXYGENASE HYDROXYLASE

Chain H:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	61.70Å 109.60Å 330.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 1.70	Depositor
% Data completeness (in resolution range)	77.0 (5.00-1.70)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.183 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	25065	wwPDB-VP
Average B, all atoms (Å^2)	9.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	D	0.48	0/4311	0.70	0/5855
1	E	0.49	0/4311	0.76	8/5855 (0.1%)
2	B	0.51	0/3263	0.78	10/4430 (0.2%)
2	C	0.50	0/3263	0.77	8/4430 (0.2%)
3	G	0.49	0/1366	0.72	2/1840 (0.1%)
3	H	0.50	0/1366	0.78	3/1840 (0.2%)
All	All	0.49	0/17880	0.75	31/24250 (0.1%)

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	D	0	1
1	E	0	1
2	B	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	360	ARG	NE-CZ-NH2	-10.30	115.15	120.30
2	B	168	ARG	NE-CZ-NH2	-10.24	115.18	120.30
2	B	118	ARG	NE-CZ-NH2	-10.10	115.25	120.30
2	B	168	ARG	NE-CZ-NH1	9.01	124.80	120.30
2	C	118	ARG	NE-CZ-NH2	-8.81	115.89	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	299	TYR	Sidechain
1	D	67	TYR	Sidechain
1	E	67	TYR	Sidechain

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	D	4186	934	3990	127	1
1	E	4186	934	3990	137	0
2	B	3167	0	3014	89	0
2	C	3167	707	3014	90	0
3	G	1337	321	1323	31	0
3	H	1337	321	1323	35	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
5	B	263	526	0	14	0
5	C	269	538	0	11	0
5	D	292	584	0	23	7
5	E	308	616	0	22	2
5	G	157	314	0	8	2
5	H	199	398	0	11	5
All	All	18872	6193	16654	442	11

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 442 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)
2:C:133:ILE:HG21	2:C:203:ILE:HD12	1.45	0.97
3:G:41:THR:O	3:G:44:ARG:HD2	1.70	0.91
1:E:78:GLN:HE22	1:E:150:GLN:HE21	1.19	0.88
2:C:336:MET:SD	5:C:627:HOH:O	2.32	0.87
1:D:84:VAL:HG21	1:E:77:ARG:HB3	1.55	0.87

The worst 5 of 11 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)
1:D:502:ARG:HE	5:D:760:HOH:H2[3_755]	1.26	0.34
5:H:2509:HOH:O	5:H:2644:HOH:H2[4_565]	1.48	0.12
5:D:720:HOH:O	5:E:813:HOH:H2[3_645]	1.48	0.12
5:H:2506:HOH:O	5:H:2640:HOH:H1[4_565]	1.51	0.09
5:H:2509:HOH:H2	5:H:2638:HOH:O[4_565]	1.53	0.07

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	D	510/512 (100%)	491 (96%)	17 (3%)	2 (0%)	39 20
1	E	510/512 (100%)	489 (96%)	16 (3%)	5 (1%)	19 4
2	B	382/384 (100%)	369 (97%)	12 (3%)	1 (0%)	46 26
2	C	382/384 (100%)	369 (97%)	9 (2%)	4 (1%)	19 4
3	G	160/162 (99%)	158 (99%)	2 (1%)	0	100 100
3	H	160/162 (99%)	158 (99%)	2 (1%)	0	100 100
All	All	2104/2116 (99%)	2034 (97%)	58 (3%)	12 (1%)	30 12

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	18	ARG
1	E	16	ALA
1	E	18	ARG
2	C	35	MET
1	E	433	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	D	432/432 (100%)	405 (94%)	27 (6%)	22 6
1	E	432/432 (100%)	402 (93%)	30 (7%)	19 5
2	B	319/319 (100%)	299 (94%)	20 (6%)	22 6
2	C	319/319 (100%)	301 (94%)	18 (6%)	26 9
3	G	140/140 (100%)	133 (95%)	7 (5%)	30 11
3	H	140/140 (100%)	134 (96%)	6 (4%)	35 14
All	All	1782/1782 (100%)	1674 (94%)	108 (6%)	23 7

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	289	LEU
2	B	44	LYS
3	G	135	LEU
1	E	346	LEU
1	E	469	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	259	ASN
1	E	413	HIS
3	G	79	HIS
1	E	268	ASN
1	E	279	GLN

5.3.3 RNA (i)

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.