wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:52 PM GMT

PDB ID	:	1MHY
Title	:	METHANE MONOOXYGENASE HYDROXYLASE
Authors	:	Elango, N.; Radhakrishnan, R.; Froland, W.A.; Waller, B.J.; Earhart, C.A.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on	:	1996-10-21
Resolution	:	2.00 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:

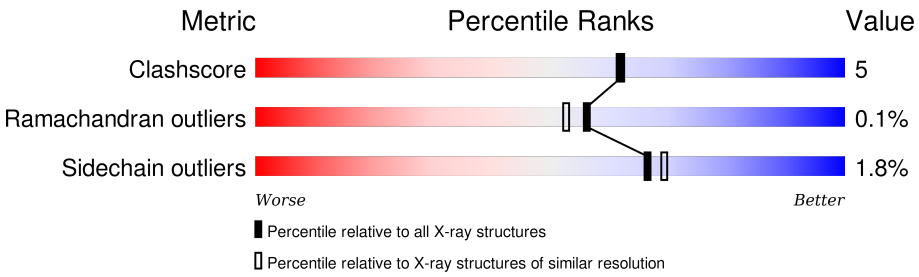
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (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 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	B	395	87% 9% • •
2	D	521	84% 14% •
3	G	169	89% 9% ••

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12729 atoms, of which 3397 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
			Total	C	H	N	O	S			
1	B	383	3808	1989	700	537	577	5	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	255	TYR	MET	CONFLICT	UNP P27354
B	256	ASP	ILE	CONFLICT	UNP P27354
B	348	VAL	-	INSERTION	UNP P27354
B	349	ALA	SER	CONFLICT	UNP P27354
B	350	GLY	ARG	CONFLICT	UNP P27354
B	352	THR	ASP	CONFLICT	UNP P27354
B	353	ASP	ARG	CONFLICT	UNP P27354
B	?	-	ARG	DELETION	UNP P27354
B	?	-	ARG	DELETION	UNP P27354
B	?	-	ARG	DELETION	UNP P27354
B	?	-	LEU	DELETION	UNP P27354
B	?	-	ARG	DELETION	UNP P27354
B	?	-	GLY	DELETION	UNP P27354
B	356	GLY	ALA	CONFLICT	UNP P27354
B	357	VAL	ALA	CONFLICT	UNP P27354
B	359	GLU	SER	CONFLICT	UNP P27354
B	361	LEU	ILE	CONFLICT	UNP P27354
B	362	GLN	GLY	CONFLICT	UNP P27354
B	364	VAL	-	INSERTION	UNP P27354
B	365	PHE	-	INSERTION	UNP P27354
B	366	GLY	-	INSERTION	UNP P27354
B	367	ASP	-	INSERTION	UNP P27354
B	368	TRP	-	INSERTION	UNP P27354
B	369	LYS	SER	CONFLICT	UNP P27354
B	371	ASP	-	INSERTION	UNP P27354
B	372	TYR	THR	CONFLICT	UNP P27354
B	373	ALA	PRO	ENGINEERED INSERTION	UNP P27354

- Molecule 2 is a protein called METHANE MONOOXYGENASE HYDROXYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	D	510	5058	2649	920	720	757	12	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ASP	DELETION	UNP P27353
D	?	-	ALA	DELETION	UNP P27353
D	?	-	LEU	DELETION	UNP P27353
D	?	-	LYS	DELETION	UNP P27353
D	?	-	VAL	DELETION	UNP P27353
D	37	TRP	ARG	CONFLICT	UNP P27353
D	195	GLY	ARG	CONFLICT	UNP P27353
D	209	GLU	ASP	CONFLICT	UNP P27353
D	210	ALA	THR	CONFLICT	UNP P27353
D	225	SER	ILE	CONFLICT	UNP P27353
D	226	ALA	GLY	CONFLICT	UNP P27353
D	329	PRO	-	INSERTION	UNP P27353
D	331	SER	VAL	CONFLICT	UNP P27353
D	357	GLY	ALA	CONFLICT	UNP P27353

- Molecule 3 is a protein called METHANE MONOOXYGENASE HYDROXYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	G	167	1662	868	311	230	252	1	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	88	ALA	ARG	CONFLICT	UNP P27355
G	109	GLU	ASP	CONFLICT	UNP P27355
G	110	ALA	GLY	CONFLICT	UNP P27355
G	160	ARG	PRO	CONFLICT	UNP P27355

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
5	B	283	849	566	283	0	0
5	D	331	993	662	331	0	0
5	G	119	357	238	119	0	0

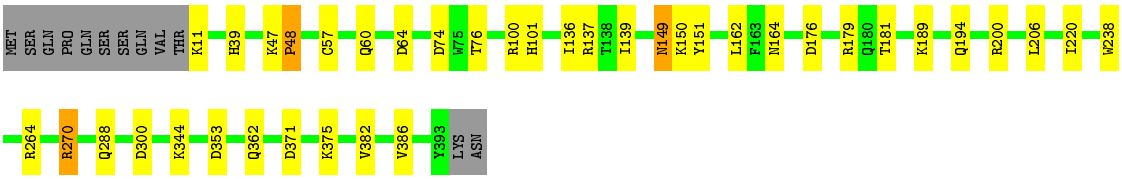
3 Residue-property plots (i)

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.

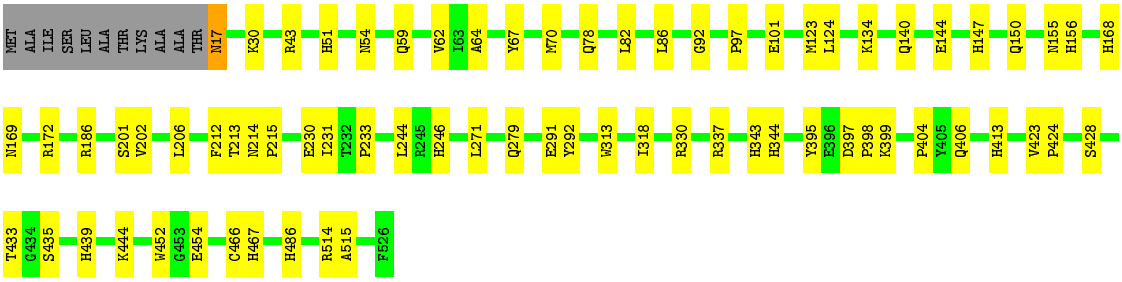
- Molecule 1: METHANE MONOOXYGENASE HYDROXYLASE

Chain B:



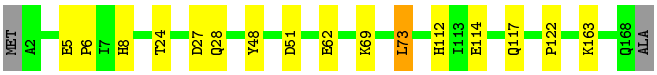
- Molecule 2: METHANE MONOOXYGENASE HYDROXYLASE

Chain D:



- Molecule 3: METHANE MONOOXYGENASE HYDROXYLASE

Chain G:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	264.49Å 71.19Å 139.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.00	Depositor
% Data completeness (in resolution range)	96.8 (5.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.137 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12729	wwPDB-VP
Average B, all atoms ($Å^2$)	14.0	wwPDB-VP

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: 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	B	0.80	0/3201	0.81	3/4356 (0.1%)
2	D	0.75	0/4267	0.79	0/5797
3	G	0.69	0/1377	0.79	0/1863
All	All	0.76	0/8845	0.80	3/12016 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	100	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	B	100	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	B	353	ASP	CB-CG-OD1	5.31	123.08	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	B	3108	700	2942	35	1
2	D	4138	920	3934	56	0
3	G	1351	311	1387	12	0
4	D	2	0	0	0	0
5	B	283	566	0	4	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	331	662	0	8	0
5	G	119	238	0	0	0
All	All	9332	3397	8263	91	2

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 5.

The worst 5 of 91 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:47:LYS:HB2	1:B:48:PRO:HD3	1.48	0.96
2:D:78:GLN:HE22	2:D:150:GLN:HE21	1.13	0.90
1:B:194:GLN:HE22	2:D:64:ALA:H	1.26	0.82
2:D:155:ASN:HD22	2:D:168:HIS:HD2	1.31	0.79
2:D:202:VAL:HG11	2:D:271:LEU:HA	1.65	0.78

All (2) 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)
5:B:678:HOH:H1	5:B:678:HOH:H2[4_575]	0.96	0.64
1:B:137:ARG:HH21	5:B:520:HOH:H2[4_575]	1.17	0.43

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	B	381/395 (96%)	368 (97%)	12 (3%)	1 (0%)	46 41
2	D	508/521 (98%)	490 (96%)	18 (4%)	0	100 100
3	G	165/169 (98%)	161 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1054/1085 (97%)	1019 (97%)	34 (3%)	1 (0%)	56 53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	48	PRO

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	B	315/327 (96%)	311 (99%)	4 (1%)	76 79
2	D	423/430 (98%)	414 (98%)	9 (2%)	61 63
3	G	144/145 (99%)	141 (98%)	3 (2%)	61 63
All	All	882/902 (98%)	866 (98%)	16 (2%)	66 69

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	169	ASN
2	D	186	ARG
2	D	435	SER
2	D	62	VAL
3	G	27	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	168	HIS
2	D	279	GLN
3	G	28	GLN
2	D	169	ASN
2	D	343	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates 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 was not executed - this section will therefore be empty.

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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