



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 07:51 AM EDT

PDB ID : 1YI9
Title : Crystal Structure Analysis of the oxidized form of the M314I mutant of Peptidylglycine alpha-Hydroxylating Monooxygenase
Authors : Siebert, X.; Eipper, B.A.; Mains, R.E.; Prigge, S.T.; Blackburn, N.J.; Amzel, L.M.
Deposited on : 2005-01-11
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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) : 2.35

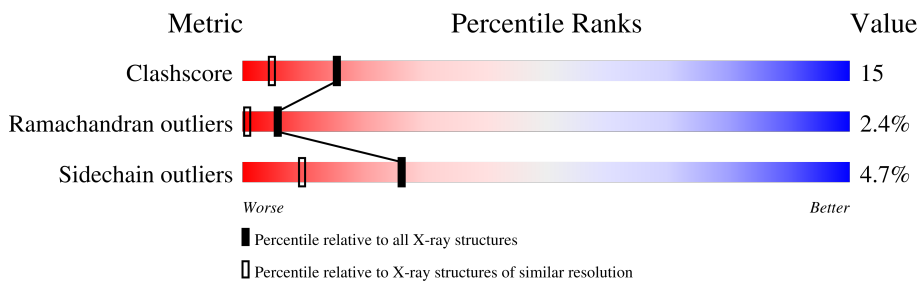
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (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 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	309	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	703	-	-	X	-
3	GOL	A	710	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2461 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 Peptidyl-glycine alpha-amidating monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	295	2313	1482	388	418	25	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	314	ILE	MET	engineered mutation	UNP P14925

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Cu	0	0
			4	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

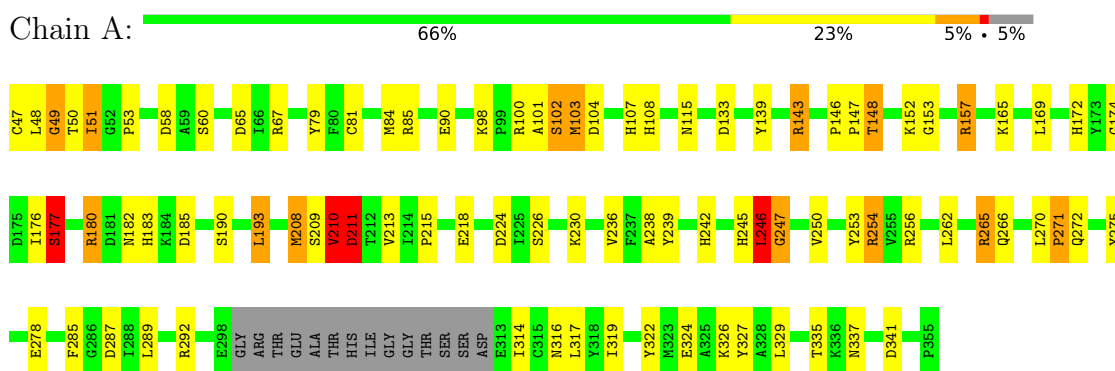
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	132	Total	O	0	0
			132	132		

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 was not executed.

- Molecule 1: Peptidyl-glycine alpha-amidating monooxygenase



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.48Å 66.46Å 70.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.20 – 1.70	Depositor
% Data completeness (in resolution range)	87.0 (48.20-1.70)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.201 , 0.233	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2461	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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: CU, GOL

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	1.25	10/2380 (0.4%)	1.22	16/3237 (0.5%)

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	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	177	SER	CB-OG	20.67	1.69	1.42
1	A	324	GLU	CD-OE2	-6.63	1.18	1.25
1	A	254	ARG	CD-NE	-6.34	1.35	1.46
1	A	322	TYR	CD1-CE1	5.59	1.47	1.39
1	A	285	PHE	CE1-CZ	-5.50	1.26	1.37
1	A	90	GLU	CG-CD	5.28	1.59	1.51
1	A	250	VAL	CB-CG1	-5.28	1.41	1.52
1	A	239	TYR	CB-CG	-5.23	1.43	1.51
1	A	139	TYR	CD1-CE1	-5.19	1.31	1.39
1	A	253	TYR	CD2-CE2	-5.13	1.31	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	ARG	NE-CZ-NH1	14.61	127.60	120.30
1	A	254	ARG	NE-CZ-NH2	-14.27	113.17	120.30
1	A	85	ARG	NE-CZ-NH2	10.28	125.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	ASP	CB-CG-OD2	7.25	124.83	118.30
1	A	211	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	165	LYS	CD-CE-NZ	-6.91	95.81	111.70
1	A	256	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	A	133	ASP	CB-CG-OD2	5.85	123.56	118.30
1	A	185	ASP	CB-CG-OD2	5.85	123.56	118.30
1	A	193	LEU	CA-CB-CG	5.79	128.63	115.30
1	A	341	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	157	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	322	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	A	292	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	329	LEU	CA-CB-CG	5.08	126.98	115.30
1	A	247	GLY	N-CA-C	-5.06	100.44	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	SER	Peptide
1	A	210	VAL	Peptide
1	A	49	GLY	Peptide

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	2313	0	2247	66	0
2	A	4	0	0	0	0
3	A	12	0	15	6	0
4	A	132	0	0	13	0
All	All	2461	0	2262	68	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 15.

All (68) 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:177:SER:CB	1:A:177:SER:OG	1.69	1.40
1:A:262:LEU:HD22	3:A:710:GOL:H2	1.54	0.89
1:A:104:ASP:O	1:A:143:ARG:NH2	2.05	0.88
1:A:213:VAL:O	1:A:215:PRO:HD3	1.78	0.82
1:A:230:LYS:N	3:A:703:GOL:O1	2.13	0.81
1:A:242:HIS:CE1	4:A:842:HOH:O	2.40	0.74
1:A:270:LEU:HB2	1:A:271:PRO:HD2	1.70	0.72
1:A:98:LYS:NZ	1:A:100:ARG:NH2	2.41	0.68
1:A:58:ASP:OD1	4:A:759:HOH:O	2.11	0.68
1:A:245:HIS:O	1:A:247:GLY:N	2.31	0.63
1:A:152:LYS:HD2	1:A:153:GLY:N	2.16	0.60
1:A:242:HIS:ND1	1:A:272:GLN:OE1	2.33	0.60
1:A:314:ILE:HG23	1:A:314:ILE:O	2.01	0.60
1:A:152:LYS:HD2	1:A:153:GLY:H	1.66	0.58
3:A:703:GOL:H31	4:A:789:HOH:O	2.01	0.58
1:A:65:ASP:OD2	1:A:67:ARG:HD2	2.04	0.57
1:A:107:HIS:CD2	1:A:174:GLY:HA3	2.40	0.57
1:A:177:SER:OG	1:A:177:SER:C	2.46	0.54
3:A:703:GOL:C3	4:A:789:HOH:O	2.55	0.54
1:A:100:ARG:HD2	1:A:190:SER:OG	2.08	0.53
1:A:98:LYS:HZ2	1:A:100:ARG:NH2	2.06	0.53
1:A:254:ARG:HD2	1:A:287:ASP:OD2	2.08	0.53
1:A:51:ILE:H	1:A:51:ILE:HD13	1.74	0.53
1:A:143:ARG:HA	4:A:772:HOH:O	2.10	0.52
1:A:270:LEU:HB2	1:A:271:PRO:CD	2.37	0.51
1:A:98:LYS:HE3	1:A:100:ARG:CZ	2.41	0.50
1:A:102:SER:C	1:A:104:ASP:H	2.15	0.50
1:A:208:MET:HG3	1:A:335:THR:HG22	1.94	0.50
1:A:148:THR:HG21	1:A:238:ALA:HB2	1.93	0.50
1:A:47:CYS:SG	1:A:48:LEU:N	2.85	0.50
1:A:265:ARG:HD2	4:A:783:HOH:O	2.12	0.49
1:A:98:LYS:NZ	1:A:100:ARG:HH22	2.08	0.49
1:A:60:SER:OG	4:A:759:HOH:O	2.20	0.49
1:A:101:ALA:O	1:A:103:MET:N	2.46	0.49
1:A:230:LYS:N	3:A:703:GOL:HO1	2.08	0.48
1:A:314:ILE:HD11	1:A:316:ASN:ND2	2.29	0.48
1:A:180:ARG:CZ	1:A:182:ASN:OD1	2.62	0.47
1:A:218:GLU:HA	1:A:218:GLU:OE1	2.14	0.47
1:A:107:HIS:NE2	1:A:174:GLY:HA3	2.30	0.46
1:A:115:ASN:HB3	4:A:804:HOH:O	2.14	0.46
1:A:226:SER:HA	1:A:289:LEU:O	2.16	0.46
1:A:317:LEU:HG	1:A:319:ILE:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:SER:C	1:A:104:ASP:N	2.71	0.45
1:A:102:SER:O	1:A:104:ASP:N	2.50	0.45
1:A:278:GLU:CG	4:A:778:HOH:O	2.64	0.44
1:A:143:ARG:HG3	4:A:772:HOH:O	2.18	0.44
1:A:314:ILE:O	1:A:314:ILE:CG2	2.66	0.44
1:A:79:TYR:CE1	1:A:172:HIS:CD2	3.05	0.44
1:A:326:LYS:HE3	1:A:327:TYR:CZ	2.52	0.44
1:A:146:PRO:HA	1:A:147:PRO:HD3	1.86	0.44
1:A:236:VAL:CG1	1:A:319:ILE:HG23	2.48	0.43
1:A:177:SER:OG	1:A:177:SER:CA	2.54	0.43
1:A:183:HIS:N	4:A:762:HOH:O	2.50	0.43
1:A:157:ARG:HD2	4:A:797:HOH:O	2.17	0.43
1:A:81:CYS:HA	1:A:169:LEU:O	2.19	0.43
1:A:210:VAL:O	1:A:211:ASP:CB	2.66	0.42
1:A:98:LYS:HZ2	1:A:100:ARG:HH22	1.66	0.42
1:A:246:LEU:HD22	1:A:246:LEU:HA	1.69	0.42
1:A:210:VAL:O	1:A:211:ASP:HB2	2.19	0.42
1:A:177:SER:CB	1:A:177:SER:HG	2.12	0.42
1:A:262:LEU:HD13	3:A:710:GOL:H12	2.01	0.42
1:A:266:GLN:NE2	4:A:815:HOH:O	2.20	0.41
1:A:51:ILE:HD13	1:A:51:ILE:N	2.35	0.41
1:A:226:SER:OG	1:A:337:ASN:ND2	2.51	0.41
1:A:53:PRO:HB3	1:A:84:MET:CE	2.51	0.40
1:A:245:HIS:O	1:A:246:LEU:C	2.58	0.40
1:A:242:HIS:HB3	1:A:316:ASN:HB2	2.02	0.40
1:A:270:LEU:CD1	1:A:275:TYR:OH	2.68	0.40

There are no symmetry-related clashes.

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	A	291/309 (94%)	267 (92%)	17 (6%)	7 (2%)	6 1

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	SER
1	A	148	THR
1	A	211	ASP
1	A	49	GLY
1	A	246	LEU
1	A	103	MET
1	A	271	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	A	254/264 (96%)	242 (95%)	12 (5%)	26 10

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	THR
1	A	51	ILE
1	A	108	HIS
1	A	143	ARG
1	A	176	ILE
1	A	177	SER
1	A	180	ARG
1	A	193	LEU
1	A	208	MET
1	A	210	VAL
1	A	246	LEU
1	A	265	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	HIS
1	A	183	HIS
1	A	228	GLN
1	A	337	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
3	GOL	A	703	-	5,5,5	1.14	0	5,5,5	0.47	0
3	GOL	A	710	-	5,5,5	0.50	0	5,5,5	1.42	2 (40%)

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
3	GOL	A	703	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	710	-	-	4/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	710	GOL	C3-C2-C1	2.04	119.65	111.70
3	A	710	GOL	O1-C1-C2	2.04	119.99	110.20

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	703	GOL	O1-C1-C2-C3
3	A	710	GOL	O1-C1-C2-C3
3	A	710	GOL	C1-C2-C3-O3
3	A	710	GOL	O2-C2-C3-O3
3	A	703	GOL	O1-C1-C2-O2
3	A	710	GOL	O1-C1-C2-O2
3	A	703	GOL	C1-C2-C3-O3
3	A	703	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	703	GOL	4	0
3	A	710	GOL	2	0

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.