wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2023 – 03:53 am GMT

PDB ID	:	1E5E
Title	:	METHIONINE GAMMA-LYASE (MGL) FROM TRICHOMONAS VAGINALIS IN COMPLEX WITH PROPARGYLGLYCINE
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Deposited on	:	2000-07-25
Resolution	:	2.18 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
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)	:	2.36

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 2.18 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly; EDS was not executed - the sequence quality summary graphics cannot be shown.

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
2	PPJ	B	405	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6933 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.

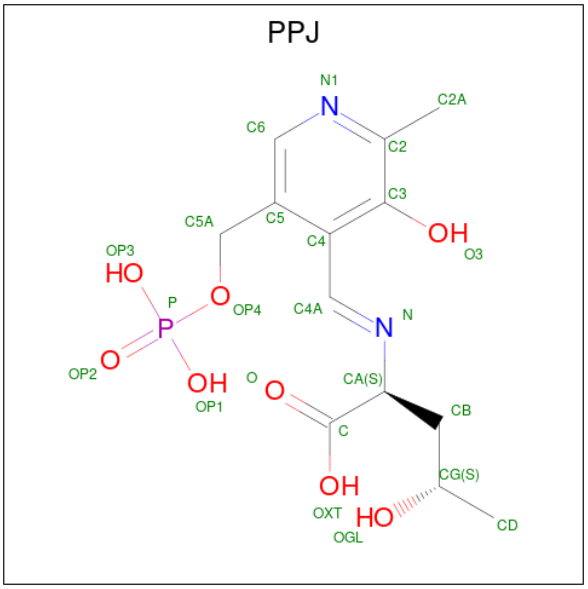
- Molecule 1 is a protein called METHIONINE GAMMA-LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	7	0
			2999	1898	507	569	25			
1	B	393	Total	C	N	O	S	0	12	0
			3004	1897	509	574	24			

There are 4 discrepancies between the modelled and reference sequences:

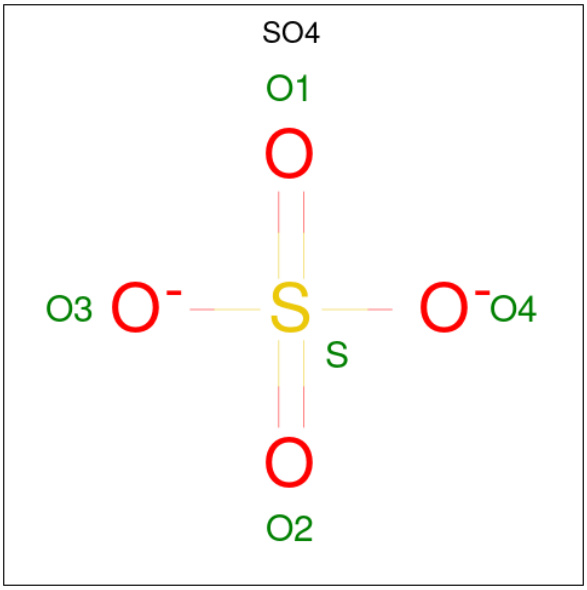
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	cloning artifact	UNP O15564
A	308	TYR	SER	cloning artifact	UNP O15564
B	2	ALA	SER	cloning artifact	UNP O15564
B	308	TYR	SER	cloning artifact	UNP O15564

- Molecule 2 is N-(HYDROXY{3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PYRIDIN-4-YL}METHYL)NORVALINE (three-letter code: PPJ) (formula: $C_{13}H_{19}N_2O_8P$).



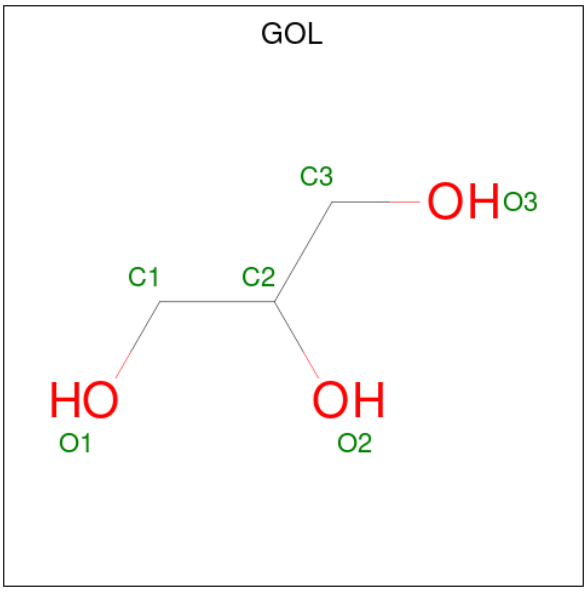
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O P 23 13 2 7 1	0	0
2	B	1	Total C N O P 23 13 2 7 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	428	Total O 428 428	0	0
5	B	419	Total O 419 419	0	0

MolProbity failed to run properly; EDS was not executed - this section is therefore empty.

3 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α, β, γ	88.26Å 88.26Å 217.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.18	Depositor
% Data completeness (in resolution range)	97.6 (25.00-2.18)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.140 , 0.193	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6933	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

9 ligands 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	$\#\|Z\| > 2$
4	GOL	B	412	-	5,5,5	0.84	0	5,5,5	0.88	0
4	GOL	A	411	-	5,5,5	0.72	0	5,5,5	0.51	0
3	SO4	A	409	-	4,4,4	0.58	0	6,6,6	0.32	0
2	PPJ	A	405	1	23,23,24	3.18	9 (39%)	28,32,34	2.21	8 (28%)
3	SO4	A	408	-	4,4,4	0.68	0	6,6,6	0.32	0
3	SO4	B	407	-	4,4,4	0.74	0	6,6,6	0.39	0
3	SO4	B	410	-	4,4,4	0.68	0	6,6,6	0.32	0
3	SO4	B	406	-	4,4,4	0.52	0	6,6,6	0.40	0
2	PPJ	B	405	1	23,23,24	3.41	10 (43%)	28,32,34	2.90	11 (39%)

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
4	GOL	B	412	-	-	4/4/4/4	-
4	GOL	A	411	-	-	4/4/4/4	-
2	PPJ	A	405	1	-	3/18/18/19	0/1/1/1
2	PPJ	B	405	1	1/1/3/5	3/18/18/19	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	405	PPJ	CA-C	-8.22	1.42	1.52
2	A	405	PPJ	CA-C	-7.47	1.43	1.52
2	B	405	PPJ	C4A-N	7.45	1.41	1.27
2	A	405	PPJ	CA-N	-7.34	1.36	1.46
2	B	405	PPJ	CA-N	-6.80	1.37	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	405	PPJ	C4-C4A-N	-7.26	106.89	123.01
2	B	405	PPJ	C4-C3-C2	5.83	123.80	120.19
2	A	405	PPJ	CA-N-C4A	5.19	124.80	117.31
2	A	405	PPJ	C4-C3-C2	4.92	123.23	120.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	405	PPJ	OXT-C-O	-4.92	112.92	124.09

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	405	PPJ	CG

5 of 14 torsion outliers are listed below:

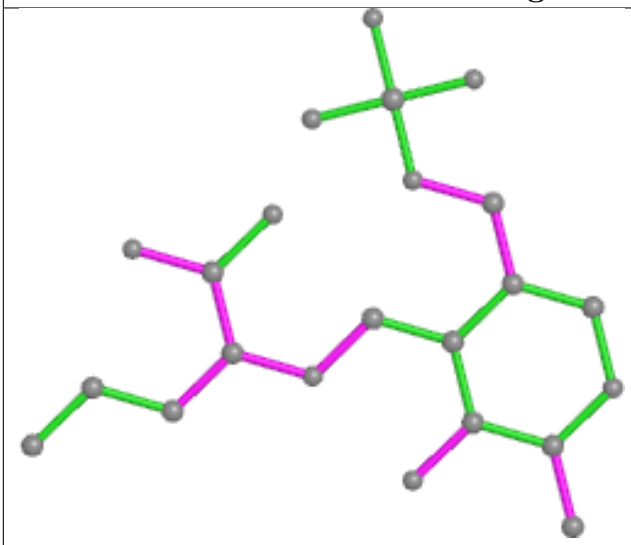
Mol	Chain	Res	Type	Atoms
2	A	405	PPJ	CB-CA-N-C4A
2	A	405	PPJ	C-CA-N-C4A
4	A	411	GOL	O1-C1-C2-C3
4	B	412	GOL	C1-C2-C3-O3
2	B	405	PPJ	CA-CB-CG-CD

There are no ring outliers.

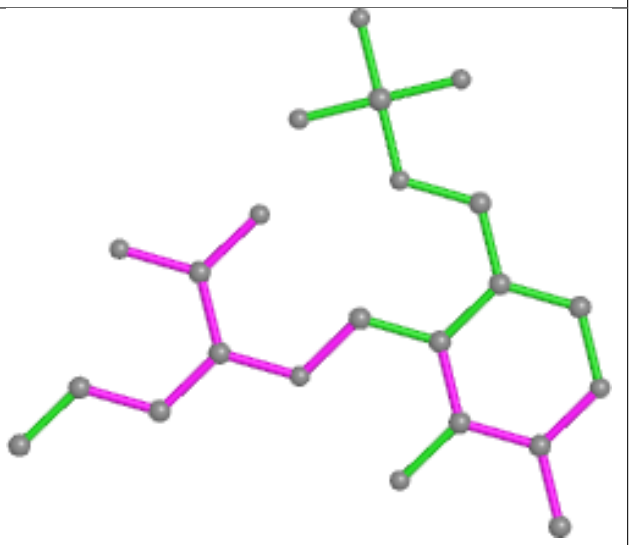
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

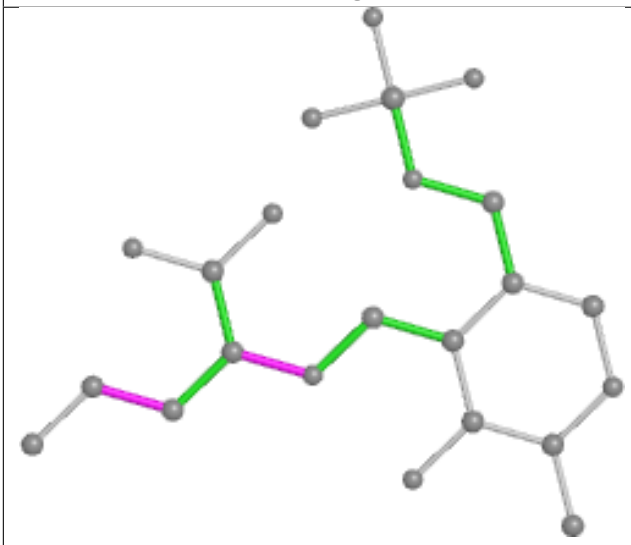
Ligand PPJ A 405



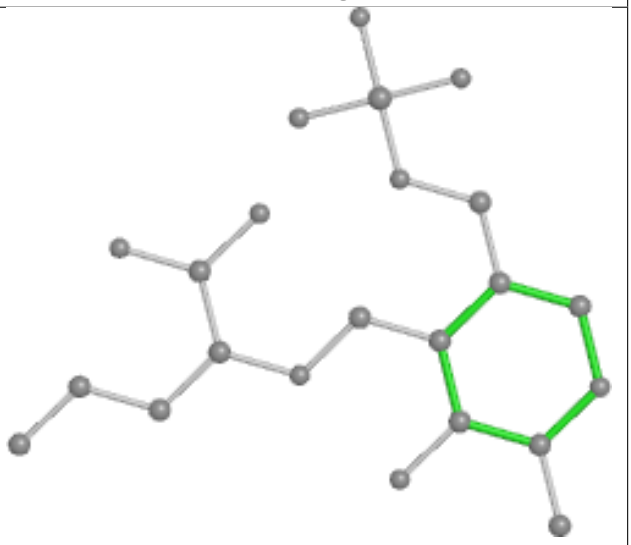
Bond lengths



Bond angles

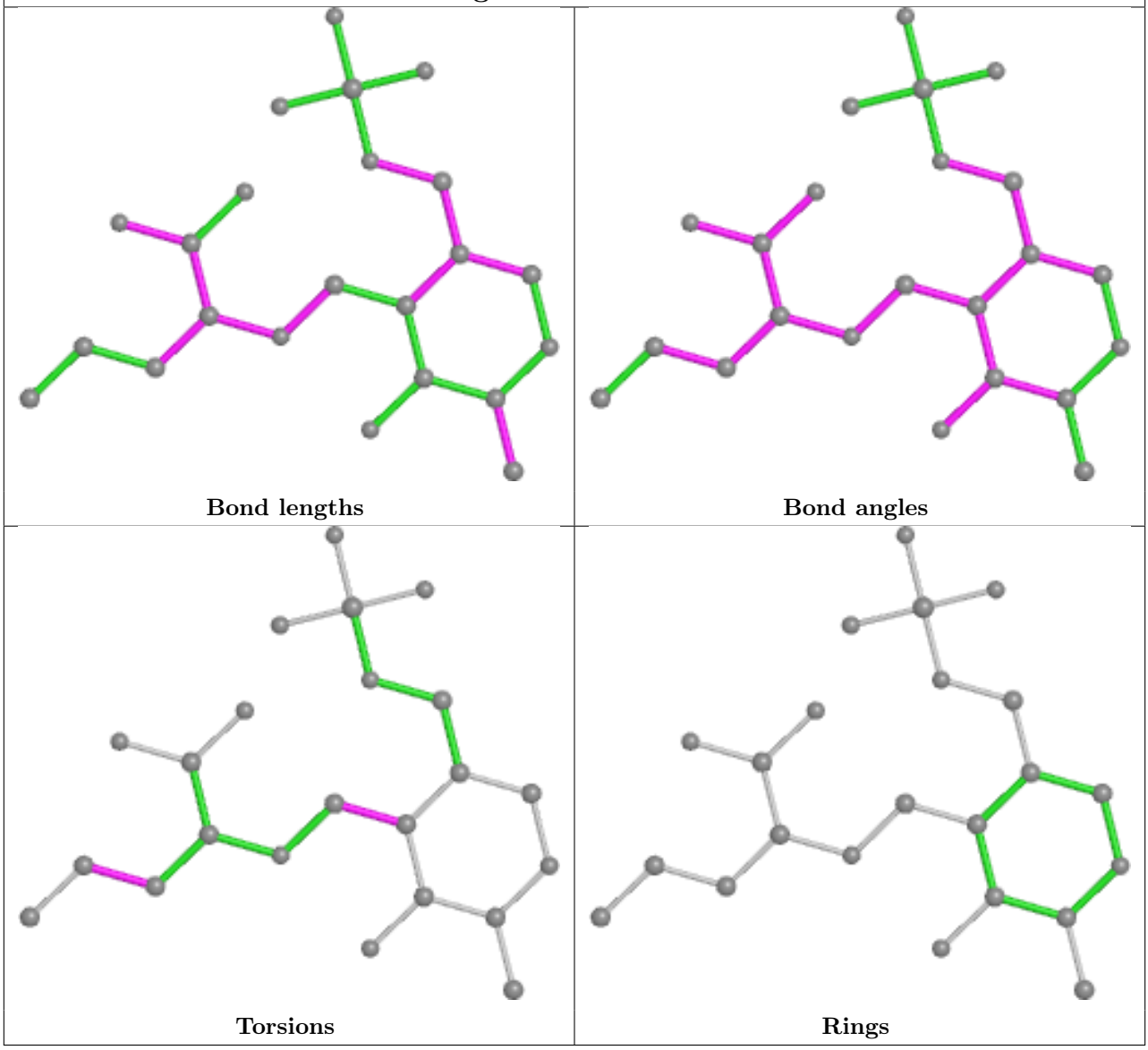


Torsions



Rings

Ligand PPJ B 405



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

5.3 Carbohydrates

EDS was not executed - this section is therefore empty.

5.4 Ligands

EDS was not executed - this section is therefore empty.

5.5 Other polymers

EDS was not executed - this section is therefore empty.