wwPDB X-ray Structure Validation Summary Report (i)

Dec 10, 2023 – 12:12 am GMT

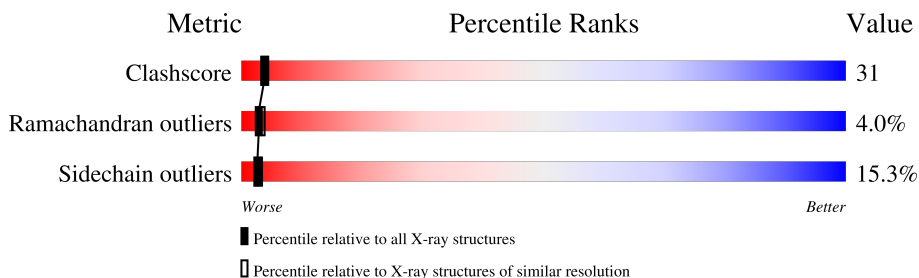|		
PDB ID	:	1QM4
Title	:	Methionine Adenosyltransferase Complexed with a L-Methionine Analogue
Authors	:	Gonzalez, B.; Pajares, M.A.; Hermoso, J.A.; Sanz-Aparicio, J.
Deposited on	:	1999-09-20
Resolution	:	2.66 Å(reported)

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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 2.66 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	Percentile Ranks	Value
Clashscore		31
Ramachandran outliers		4.0%
Sidechain outliers		15.3%

Worse ⬛ *Better*

⬛ Percentile relative to all X-ray structures

⬛ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	396	48% 33% 10% · 7%
1	B	396	46% 35% 10% · 7%

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	SO4	B	401	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5918 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 ADENOSYLTRANSFERASE, ALPHA FORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2846	1803	491	536	16			
1	B	368	Total	C	N	O	S	0	0	0
			2846	1803	491	536	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP P13444
B	?	-	ASP	deletion	UNP P13444

- Molecule 2 is L-2-AMINO-4-METHOXY-CIS-BUT-3-ENOIC ACID (three-letter code: AMB) (formula: $C_5H_9NO_3$).
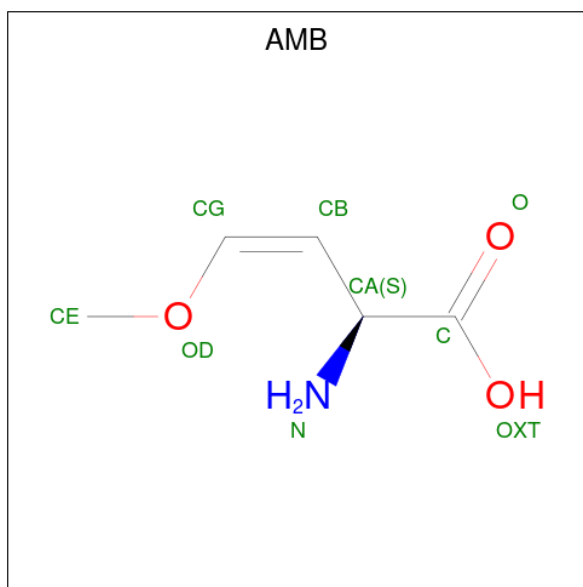
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	5	1	3		

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

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	K 2	0	0
5	B	1	Total 1	K 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	104	Total 104	O 104	0	0
6	B	93	Total 93	O 93	0	0

3 Residue-property plots ⓘ

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: METHIONINE ADENOSYLTRANSFERASE, ALPHA FORM

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L329 S330 I331 S332 I333 F334 T335 T338 S339 K340 K341 T342 E343 R344 E345 L346 L347 E348 V349 K352 N353 F354 D355 L356 R357 P358 G359 V360 R363 K368 K369 P370 I371 K374 T375 H380 F381 G382 R383 S384 E385 F386 E389 K393 L394 V395 F396
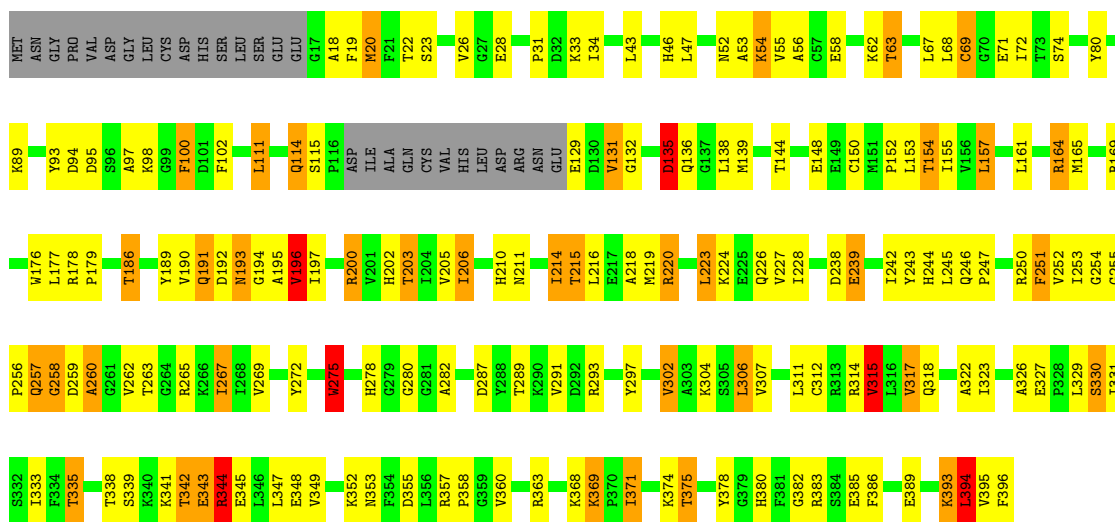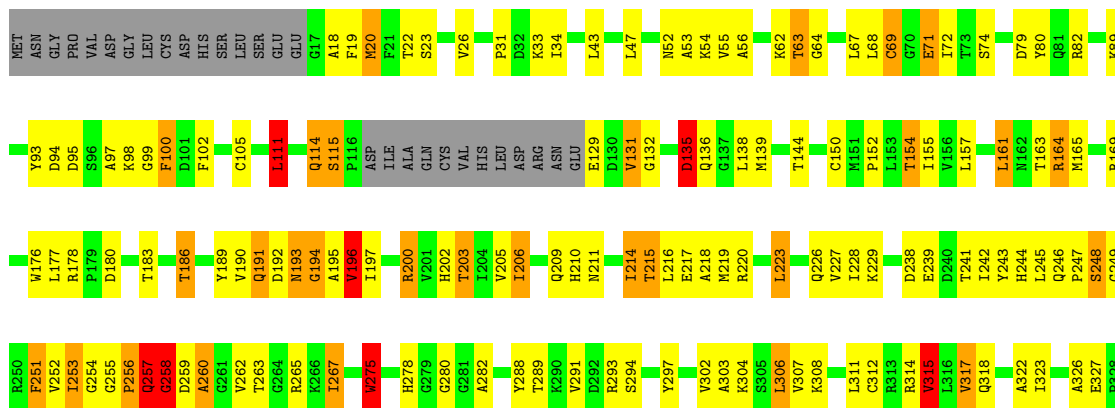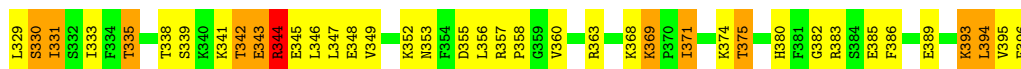
4 Data and refinement statistics ⓘ

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

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	115.20Å 115.20Å 159.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.66	Depositor
% Data completeness (in resolution range)	84.3 (10.00-2.66)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.230 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5918	wwPDB-VP
Average B, all atoms (Å^2)	31.0	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: K, SO4, MG, AMB

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	0.79	1/2901 (0.0%)	1.02	14/3926 (0.4%)
1	B	0.78	2/2901 (0.1%)	1.04	14/3926 (0.4%)
All	All	0.79	3/5802 (0.1%)	1.03	28/7852 (0.4%)

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	1
1	B	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	CYS	CB-SG	-5.98	1.72	1.81
1	B	69	CYS	CB-SG	-5.21	1.73	1.81
1	B	258	GLY	CA-C	5.01	1.59	1.51

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	196	VAL	N-CA-C	8.15	133.00	111.00
1	A	344	ARG	NE-CZ-NH2	8.12	124.36	120.30
1	B	344	ARG	NE-CZ-NH2	8.08	124.34	120.30
1	B	196	VAL	N-CA-C	7.87	132.26	111.00
1	B	257	GLN	N-CA-C	-7.79	89.96	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	272	TYR	Sidechain
1	B	257	GLN	Mainchain
1	B	258	GLY	Mainchain

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	2846	0	2852	179	0
1	B	2846	0	2852	183	0
2	A	9	0	8	0	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
4	A	2	0	0	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
6	A	104	0	0	4	0
6	B	93	0	0	7	0
All	All	5918	0	5712	356	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 31.

The worst 5 of 356 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:341:LYS:O	1:A:342:THR:HG22	1.56	1.04
1:B:341:LYS:O	1:B:342:THR:HG22	1.58	1.03
1:A:344:ARG:NE	1:A:347:LEU:HD23	1.71	1.03
1:B:344:ARG:NE	1:B:347:LEU:HD23	1.75	1.01
1:A:262:VAL:HG11	1:B:262:VAL:HG11	1.43	1.00

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	364/396 (92%)	314 (86%)	36 (10%)	14 (4%)	3	3
1	B	364/396 (92%)	310 (85%)	39 (11%)	15 (4%)	3	3
All	All	728/792 (92%)	624 (86%)	75 (10%)	29 (4%)	3	3

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ALA
1	A	193	ASN
1	B	18	ALA
1	B	193	ASN
1	B	258	GLY

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	307/332 (92%)	261 (85%)	46 (15%)	3	3
1	B	307/332 (92%)	259 (84%)	48 (16%)	2	2
All	All	614/664 (92%)	520 (85%)	94 (15%)	2	3

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	139	MET

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Mol	Chain	Res	Type
1	B	239	GLU
1	B	157	LEU
1	B	200	ARG
1	B	265	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	114	GLN
1	B	162	ASN
1	B	159	HIS
1	B	191	GLN
1	A	191	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 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	SO4	B	401	5	4,4,4	1.03	0	6,6,6	1.87	4 (66%)
3	SO4	A	402	4	4,4,4	1.35	1 (25%)	6,6,6	2.28	2 (33%)
3	SO4	A	403	5	4,4,4	2.14	1 (25%)	6,6,6	1.78	2 (33%)
2	AMB	A	401	4	7,8,8	1.48	1 (14%)	4,9,9	1.72	0

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
2	AMB	A	401	4	-	3/7/8/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	SO4	O1-S	3.75	1.66	1.46
2	A	401	AMB	CG-CB	2.51	1.43	1.30
3	A	402	SO4	O1-S	2.06	1.57	1.46

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	SO4	O4-S-O2	3.86	129.48	109.31
3	A	403	SO4	O3-S-O1	-3.26	92.29	109.31
3	A	402	SO4	O3-S-O1	-2.87	94.32	109.31
3	B	401	SO4	O3-S-O1	-2.46	96.45	109.31
3	A	403	SO4	O2-S-O1	2.39	127.07	109.43

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	AMB	OXT-C-CA-CB
2	A	401	AMB	OXT-C-CA-N
2	A	401	AMB	O-C-CA-CB

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3   Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4   Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5   Other polymers ⓘ

EDS was not executed - this section is therefore empty.