



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 06:46 PM GMT

PDB ID : 1CB7
Title : GLUTAMATE MUTASE FROM CLOSTRIDIUM COCHLEARIIUM RE-
CONSTITUTED WITH METHYL-COBALAMIN
Authors : Gruber, K.; Reitzer, R.; Kratky, C.
Deposited on : 1999-03-02
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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

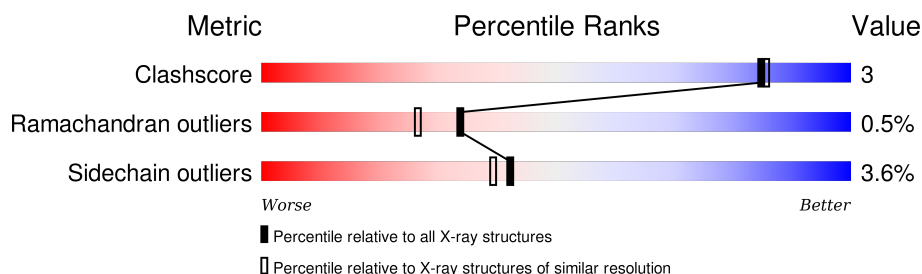
1 Overall quality at a glance

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 $\leq 5\%$. 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	A	137	 91% 6% . .
1	C	137	 88% 12% .
2	B	483	 90% 9% .
2	D	483	 89% 10% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10825 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 PROTEIN (GLUTAMATE MUTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	S	0	0	0
			1041	663	175	198	5			
1	C	137	Total	C	N	O	S	0	0	0
			1041	663	175	198	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	LEU	VAL	CONFLICT	UNP P80078
C	45	LEU	VAL	CONFLICT	UNP P80078
A	60	VAL	LEU	CONFLICT	UNP P80078
C	60	VAL	LEU	CONFLICT	UNP P80078

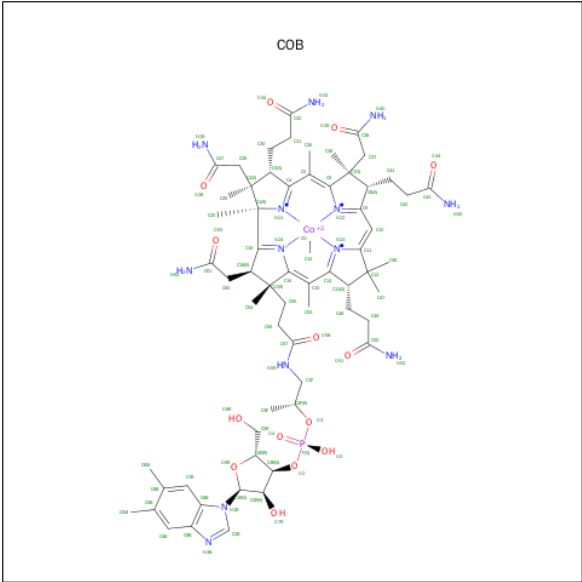
- Molecule 2 is a protein called PROTEIN (GLUTAMATE MUTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	483	Total	C	N	O	S	0	0	0
			3762	2383	643	714	22			
2	D	483	Total	C	N	O	S	0	0	0
			3762	2383	643	714	22			

There are 2 discrepancies between the modelled and reference sequences:

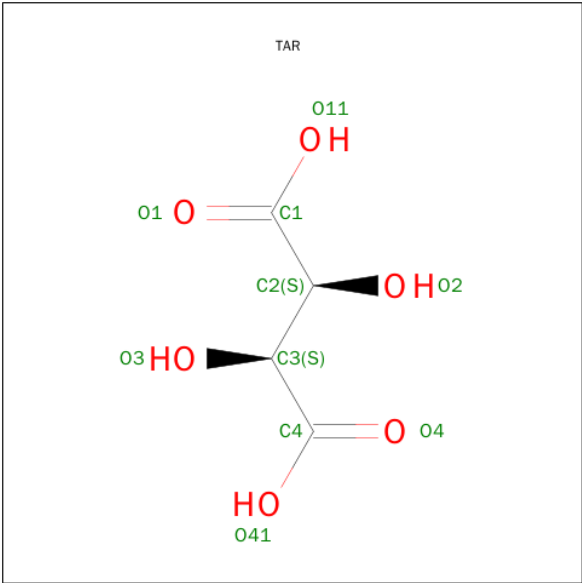
Chain	Residue	Modelled	Actual	Comment	Reference
B	130	PHE	TYR	CONFLICT	UNP P80077
D	130	PHE	TYR	CONFLICT	UNP P80077

- Molecule 3 is CO-METHYLCOBALAMIN (three-letter code: COB) (formula: C₆₃H₉₁CoN₁₃O₁₄P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Co	N	O	P	0	1
			93	64	1	13	14	1		
3	C	1	Total	C	Co	N	O	P	0	1
			93	64	1	13	14	1		

- Molecule 4 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	4	6		
4	D	1	Total	C	O	0	0
			10	4	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	90	Total 90	O 90	0	0
5	B	422	Total 422	O 422	0	0
5	C	81	Total 81	O 81	0	0
5	D	420	Total 420	O 420	0	0

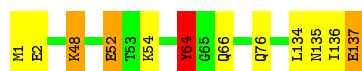
3 Residue-property plots [i](#)

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: PROTEIN (GLUTAMATE MUTASE)

Chain A:  91% 6% ..



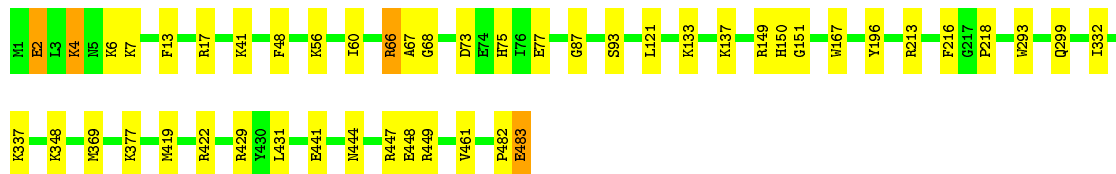
• Molecule 1: PROTEIN (GLUTAMATE MUTASE)

Chain C:  88% 12% .




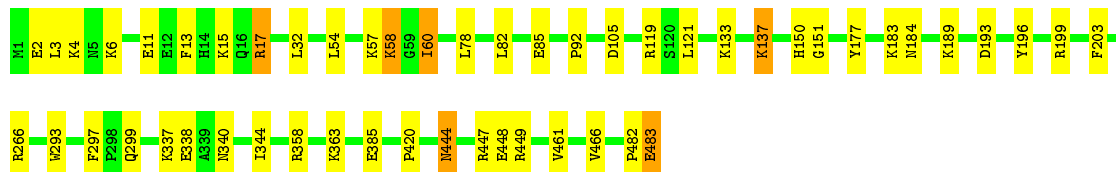
• Molecule 2: PROTEIN (GLUTAMATE MUTASE)

Chain B:  90% 9% .



• Molecule 2: PROTEIN (GLUTAMATE MUTASE)

Chain D:  89% 10% .



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.33 Å 113.14 Å 108.61 Å 90.00° 95.62° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00	Depositor
% Data completeness (in resolution range)	96.1 (25.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.160 , 0.218	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10825	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: COB, TAR

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	0.32	0/1058	0.93	1/1427 (0.1%)
1	C	0.33	0/1058	0.92	1/1427 (0.1%)
2	B	0.33	0/3833	0.98	9/5171 (0.2%)
2	D	0.33	0/3833	0.98	12/5171 (0.2%)
All	All	0.33	0/9782	0.97	23/13196 (0.2%)

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
2	D	0	1

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	196	TYR	CB-CG-CD1	8.80	126.28	121.00
2	B	422	ARG	NE-CZ-NH2	-8.53	116.04	120.30
2	D	447	ARG	NE-CZ-NH1	8.13	124.36	120.30
2	B	447	ARG	NE-CZ-NH1	6.87	123.74	120.30
2	D	358	ARG	NE-CZ-NH2	-6.84	116.88	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	92	PRO	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	1041	0	1057	7	0
1	C	1041	0	1057	8	0
2	B	3762	0	3762	20	0
2	D	3762	0	3762	18	0
3	A	93	0	0	0	0
3	C	93	0	0	0	0
4	B	10	0	4	0	0
4	D	10	0	4	0	0
5	A	90	0	0	1	0
5	B	422	0	0	8	0
5	C	81	0	0	3	0
5	D	420	0	0	4	0
All	All	10825	0	9646	53	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 3.

The worst 5 of 53 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:D:133:LYS:O	2:D:137:LYS:HD2	1.87	0.74
2:D:444:ASN:O	2:D:448:GLU:HG3	1.93	0.68
1:C:82:GLY:HA2	1:C:84:GLU:OE2	1.98	0.64
2:D:189:LYS:HE3	2:D:193:ASP:OD2	2.01	0.61
2:B:137:LYS:HD2	5:B:1298:HOH:O	2.00	0.60

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	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	C	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
2	B	481/483 (100%)	471 (98%)	7 (2%)	3 (1%)	30	22
2	D	481/483 (100%)	470 (98%)	8 (2%)	3 (1%)	30	22
All	All	1232/1240 (99%)	1207 (98%)	19 (2%)	6 (0%)	34	26

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	150	HIS
2	B	151	GLY
2	B	293	TRP
2	D	150	HIS
2	D	151	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	111/111 (100%)	104 (94%)	7 (6%)	22	16
1	C	111/111 (100%)	105 (95%)	6 (5%)	27	21
2	B	396/396 (100%)	387 (98%)	9 (2%)	58	60
2	D	396/396 (100%)	382 (96%)	14 (4%)	43	40
All	All	1014/1014 (100%)	978 (96%)	36 (4%)	42	39

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	3	LYS
1	C	64	TYR
2	D	385	GLU

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Mol	Chain	Res	Type
1	C	48	LYS
1	C	76	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	23	GLN
2	D	23	GLN
2	B	207	GLN
1	A	135	ASN
2	D	5	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
3	COB	A	800[A]	-	74,102,102	0.86	2 (2%)	107,170,170	1.34	15 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	COB	A	800[B]	-	74,102,102	0.86	2 (2%)	107,170,170	1.34	15 (14%)
4	TAR	B	900	-	3,9,9	0.53	0	6,12,12	1.22	1 (16%)
3	COB	C	800[A]	-	74,102,102	0.85	4 (5%)	107,170,170	1.43	19 (17%)
3	COB	C	800[B]	-	74,102,102	0.85	4 (5%)	107,170,170	1.43	19 (17%)
4	TAR	D	900	-	3,9,9	0.62	0	6,12,12	1.53	1 (16%)

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	COB	A	800[A]	-	-	0/51/231/231	0/3/11/11
3	COB	A	800[B]	-	-	0/51/231/231	0/3/11/11
4	TAR	B	900	-	-	0/4/12/12	0/0/0/0
3	COB	C	800[A]	-	-	0/51/231/231	0/3/11/11
3	COB	C	800[B]	-	-	0/51/231/231	0/3/11/11
4	TAR	D	900	-	-	0/4/12/12	0/0/0/0

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	800[A]	COB	C2-C3	-2.57	1.54	1.58
3	C	800[B]	COB	C2-C3	-2.57	1.54	1.58
3	A	800[B]	COB	C2-C3	-2.47	1.54	1.58
3	A	800[A]	COB	C2-C3	-2.47	1.54	1.58
3	C	800[A]	COB	C11-C10	-2.10	1.37	1.41

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	800[A]	COB	C4R-O6R-C1R	-3.47	105.91	109.72
3	C	800[B]	COB	C4R-O6R-C1R	-3.47	105.91	109.72
3	A	800[B]	COB	C4R-O6R-C1R	-3.35	106.04	109.72
3	A	800[A]	COB	C4R-O6R-C1R	-3.35	106.04	109.72
3	C	800[A]	COB	C9-C10-C11	-3.01	124.73	132.28

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.