



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 06:45 PM GMT

PDB ID : 1CBU
Title : ADENOSYLCOBINAMIDE KINASE/ADENOSYLCOBINAMIDE PHOSPHATE GUANYLYLTRANSFERASE (COBU) FROM SALMONELLA TYPHIMURIUM
Authors : Thompson, T.B.; Thomas, M.G.; Escalante-Semerena, J.C.; Rayment, I.
Deposited on : 1998-03-12
Resolution : 2.30 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

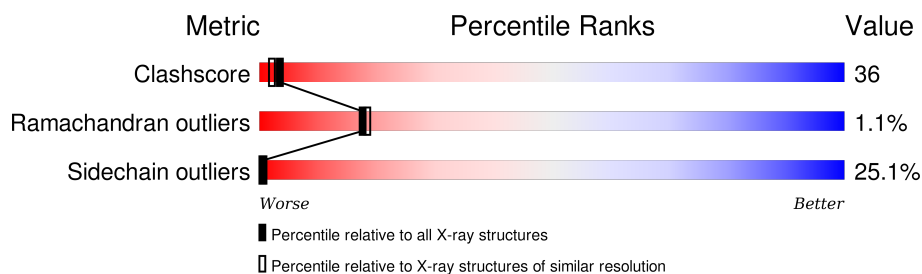
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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	180	
1	B	180	
1	C	180	

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	SO4	A	801	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	802	-	-	X	-

2 Entry composition [i](#)

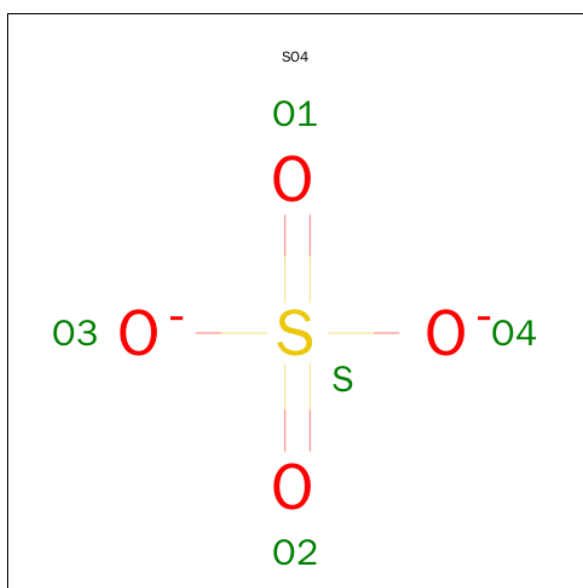
There are 3 unique types of molecules in this entry. The entry contains 4334 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ADENOSYLCOBINAMIDE KINASE/ADENOSYLCOBINAMIDE PHOSPHATE GUANYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1376	862	248	257	9			
1	B	180	Total	C	N	O	S	0	0	0
			1380	864	249	258	9			
1	C	179	Total	C	N	O	S	0	0	0
			1361	853	243	256	9			

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	72	Total 72	O 72	0	0
3	B	80	Total 80	O 80	0	0
3	C	50	Total 50	O 50	0	0

Y532	Y533	Y534	E535	Y536		L540	Y541	P542	E543	Y544	R545	L546	R547	R548		D552	L553		Y557		R560	L561		A565	D566	E567	Y568	R569	L570	Y571	Y572		L575	R576	Y577	R578	L579	R580
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4 Data and refinement statistics

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	96.40 Å 114.40 Å 106.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	88.5 (20.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	TNT V. 4-C	Depositor
R, R_{free}	0.198 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4334	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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: SO4

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	1.12	11/1399 (0.8%)	1.47	31/1901 (1.6%)
1	B	1.10	11/1403 (0.8%)	1.51	34/1906 (1.8%)
1	C	1.14	11/1383 (0.8%)	1.50	36/1880 (1.9%)
All	All	1.12	33/4185 (0.8%)	1.49	101/5687 (1.8%)

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	335	GLU	CD-OE1	8.70	1.35	1.25
1	C	458	GLU	CD-OE2	8.57	1.35	1.25
1	C	496	GLU	CD-OE2	8.05	1.34	1.25
1	A	100	GLU	CD-OE1	7.70	1.34	1.25
1	A	96	GLU	CD-OE1	7.64	1.34	1.25

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	250	ARG	C-N-CD	-17.39	82.33	120.60
1	C	422	ASP	CB-CG-OD1	10.66	127.90	118.30
1	C	422	ASP	CB-CG-OD2	-9.99	109.31	118.30
1	C	512	ASP	CB-CG-OD2	9.40	126.76	118.30
1	C	512	ASP	CB-CG-OD1	-9.28	109.95	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1376	0	1376	103	1
1	B	1380	0	1379	85	1
1	C	1361	0	1348	123	0
2	A	5	0	0	2	0
2	B	5	0	0	3	0
2	C	5	0	0	0	0
3	A	72	0	0	6	0
3	B	80	0	0	6	0
3	C	50	0	0	6	0
All	All	4334	0	4103	299	1

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 36.

The worst 5 of 299 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:C:402:ILE:HG12	1:C:567:GLU:HG3	1.14	1.07
1:A:14:ARG:HH11	1:A:14:ARG:HG2	1.26	1.01
1:B:234:ILE:HD12	1:B:234:ILE:H	1.30	0.95
1:A:145:ARG:H	1:A:145:ARG:HD3	1.34	0.92
1:B:379:ILE:HG13	1:C:575:ILE:HG21	1.51	0.91

All (1) 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)
1:A:145:ARG:NH2	1:B:343:GLU:OE1[3_656]	2.11	0.09

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	178/180 (99%)	171 (96%)	7 (4%)	0	100	100
1	B	178/180 (99%)	169 (95%)	6 (3%)	3 (2%)	11	10
1	C	175/180 (97%)	157 (90%)	15 (9%)	3 (2%)	11	10
All	All	531/540 (98%)	497 (94%)	28 (5%)	6 (1%)	17	18

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	251	PRO
1	C	420	ILE
1	C	424	PRO
1	C	467	ILE
1	B	299	PRO

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	141/143 (99%)	107 (76%)	34 (24%)	1	0
1	B	142/143 (99%)	108 (76%)	34 (24%)	1	0
1	C	139/143 (97%)	101 (73%)	38 (27%)	0	0
All	All	422/429 (98%)	316 (75%)	106 (25%)	1	0

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	266	LEU
1	B	328	LYS
1	C	533	THR
1	B	278	LEU
1	B	297	ASN

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

Mol	Chain	Res	Type
1	B	225	GLN
1	C	534	ASN
1	C	501	GLN
1	A	123	GLN
1	C	516	GLN

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](#)

3 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
2	SO4	A	801	-	4,4,4	0.45	0	6,6,6	0.16	0
2	SO4	B	802	-	4,4,4	0.53	0	6,6,6	0.08	0
2	SO4	C	803	-	4,4,4	0.45	0	6,6,6	0.09	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	SO4	A	801	-	-	0/0/0/0	0/0/0/0
2	SO4	B	802	-	-	0/0/0/0	0/0/0/0
2	SO4	C	803	-	-	0/0/0/0	0/0/0/0

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.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	SO4	2	0
2	B	802	SO4	3	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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