WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jun 11, 2024 – 11:15 PM EDT

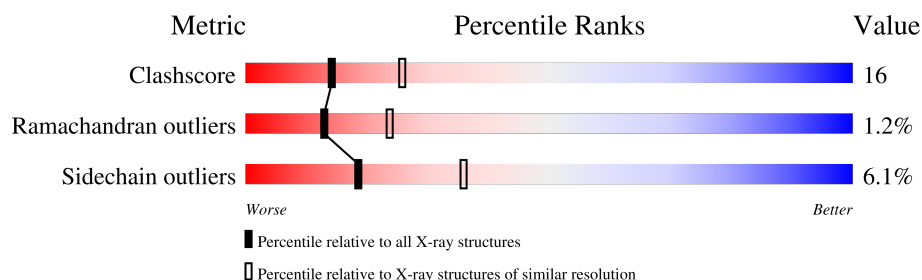|		
PDB ID	:	1CLI
Title	:	X-RAY CRYSTAL STRUCTURE OF AMINOIMIDAZOLE RIBONU-CLEOTIDE SYNTHETASE (PURM), FROM THE E. COLI PURINE BIOSYNTHETIC PATHWAY, AT 2.5 A RESOLUTION
Authors	:	Li, C.; Kappock, T.J.; Stubbe, J.; Weaver, T.M.; Ealick, S.E.
Deposited on	:	1999-04-28
Resolution	:	2.50 Å(reported)

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 2.50 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		16
Ramachandran outliers		1.2%
Sidechain outliers		6.1%

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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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	345	63% 32% • •
1	B	345	66% 26% • 6%
1	C	345	62% 34% • •
1	D	345	71% 21% • 6%

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	B	1350	-	-	X	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 10513 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 (PHOSPHORIBOSYL-AMINOIMIDAZOLE SYNTHETASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2554	1612	431	497	14			
1	B	325	Total	C	N	O	S	0	0	0
			2441	1544	413	470	14			
1	C	341	Total	C	N	O	S	0	0	0
			2554	1612	431	497	14			
1	D	325	Total	C	N	O	S	0	0	0
			2441	1544	413	470	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	MET	conflict	UNP P08178
B	1001	VAL	MET	conflict	UNP P08178
C	2001	VAL	MET	conflict	UNP P08178
D	3001	VAL	MET	conflict	UNP P08178

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

• Molecule 3 is water.

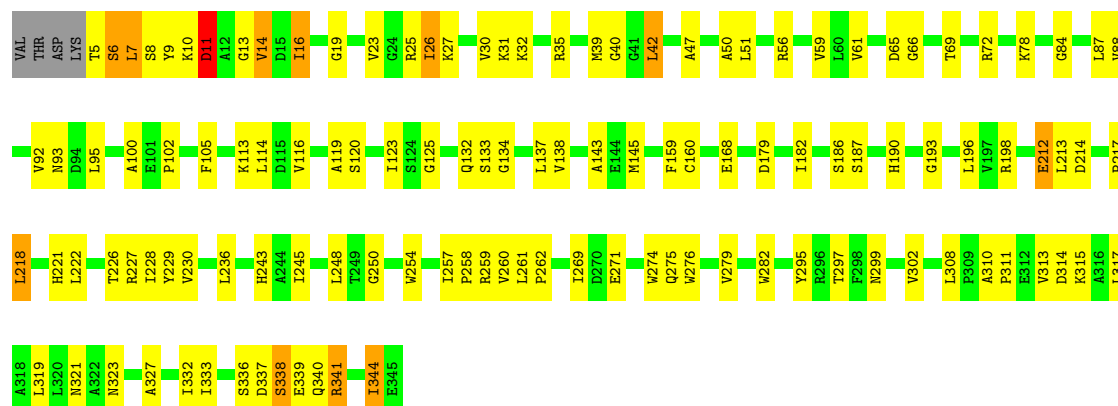| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	118	Total 118	O 118	0	0
3	B	126	Total 126	O 126	0	0
3	C	133	Total 133	O 133	0	0
3	D	126	Total 126	O 126	0	0

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.
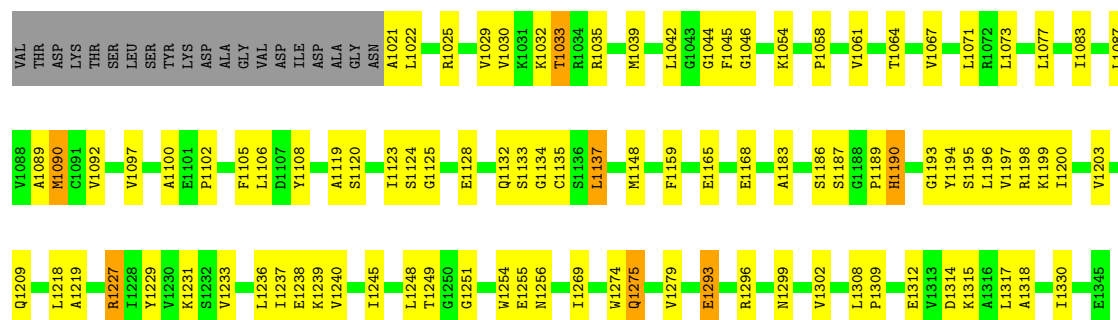
• Molecule 1: PROTEIN (PHOSPHORIBOSYL-AMINOIMIDAZOLE SYNTHETASE)

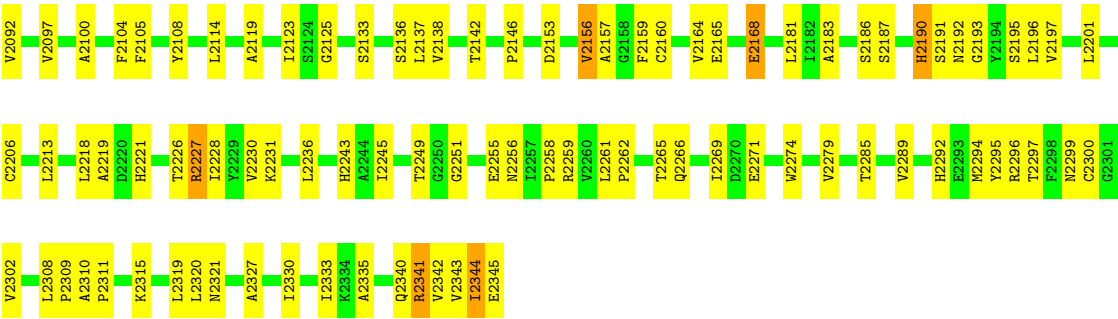• Molecule 1: PROTEIN (PHOSPHORIBOSYL-AMINOIMIDAZOLE SYNTHETASE)

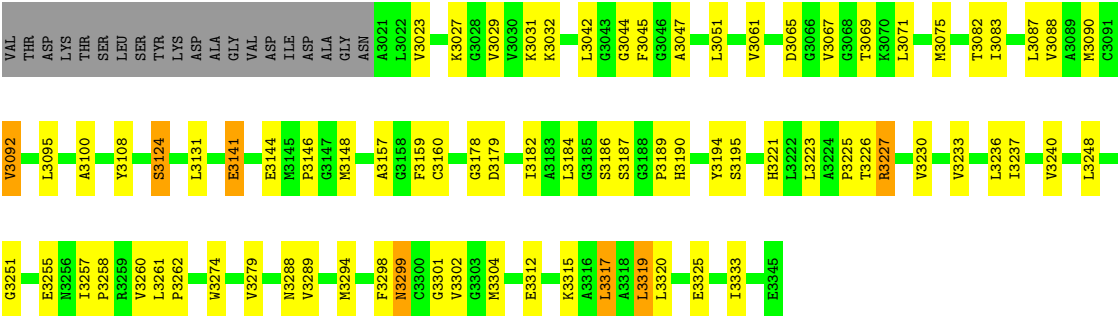• Molecule 1: PROTEIN (PHOSPHORIBOSYL-AMINOIMIDAZOLE SYNTHETASE)

• Molecule 1: PROTEIN (PHOSPHORIBOSYL-AMINOIMIDAZOLE SYNTHETASE)

Chain D:

4 Data and refinement statistics ⓘ

Xtriage (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	71.17Å 211.68Å 94.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	86.6 (20.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	4.70	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.192 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10513	wwPDB-VP
Average B, all atoms (Å²)	13.0	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: 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	0.33	0/2601	0.63	0/3531
1	B	0.32	0/2487	0.61	0/3376
1	C	0.33	0/2601	0.61	0/3531
1	D	0.32	0/2487	0.62	1/3376 (0.0%)
All	All	0.33	0/10176	0.62	1/13814 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	3319	LEU	CA-CB-CG	5.21	127.27	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts (i)

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	2554	0	2538	102	0
1	B	2441	0	2434	72	0
1	C	2554	0	2538	98	0
1	D	2441	0	2434	63	0
2	A	5	0	0	1	0
2	B	5	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	1	0
2	D	5	0	0	0	0
3	A	118	0	0	21	0
3	B	126	0	0	14	0
3	C	133	0	0	16	0
3	D	126	0	0	18	0
All	All	10513	0	9944	311	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 16.

The worst 5 of 311 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:259:ARG:HH21	1:B:1044:GLY:HA2	1.40	0.85
1:D:3299:ASN:HD22	1:D:3301:GLY:H	1.25	0.84
1:A:92:VAL:HG12	1:A:230:VAL:HG21	1.61	0.83
1:C:2051:LEU:HD11	1:D:3051:LEU:HD11	1.61	0.82
1:A:16:ILE:HD13	1:A:16:ILE:H	1.45	0.82

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	339/345 (98%)	316 (93%)	12 (4%)	11 (3%)	4	5
1	B	323/345 (94%)	309 (96%)	13 (4%)	1 (0%)	41	61
1	C	339/345 (98%)	318 (94%)	18 (5%)	3 (1%)	17	31
1	D	323/345 (94%)	303 (94%)	19 (6%)	1 (0%)	41	61
All	All	1324/1380 (96%)	1246 (94%)	62 (5%)	16 (1%)	13	24

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	7	LEU
1	A	13	GLY
1	A	40	GLY
1	A	42	LEU

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	274/278 (99%)	257 (94%)	17 (6%)	18	35
1	B	262/278 (94%)	246 (94%)	16 (6%)	18	36
1	C	274/278 (99%)	254 (93%)	20 (7%)	14	27
1	D	262/278 (94%)	250 (95%)	12 (5%)	27	50
All	All	1072/1112 (96%)	1007 (94%)	65 (6%)	18	36

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3141	GLU
1	D	3227	ARG
1	B	1218	LEU
1	B	1209	GLN
1	D	3236	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2256	ASN
1	D	3190	HIS
1	D	3323	ASN
1	D	3299	ASN
1	A	323	ASN

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 ⓘ

4 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	B	1350	-	4,4,4	1.43	0	6,6,6	0.82	0
2	SO4	C	2350	-	4,4,4	2.38	2 (50%)	6,6,6	1.06	0
2	SO4	A	4350	-	4,4,4	1.68	1 (25%)	6,6,6	0.73	0
2	SO4	D	3350	-	4,4,4	1.48	0	6,6,6	0.98	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2350	SO4	O2-S	3.24	1.64	1.44
2	C	2350	SO4	O1-S	2.58	1.60	1.44
2	A	4350	SO4	O1-S	2.24	1.58	1.44

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1350	SO4	2	0
2	C	2350	SO4	1	0
2	A	4350	SO4	1	0

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.