wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	2YYA
Title	:	Crystal structure of GAR synthetase from Aquifex aeolicus
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Deposited on	:	2007-04-27
Resolution	:	2.40 Å(reported)

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 2.40 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
Rfree		0.277
Clashscore		27
Ramachandran outliers		1.8%
Sidechain outliers		9.9%
RSRZ outliers		8.9%

Worse ← → *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
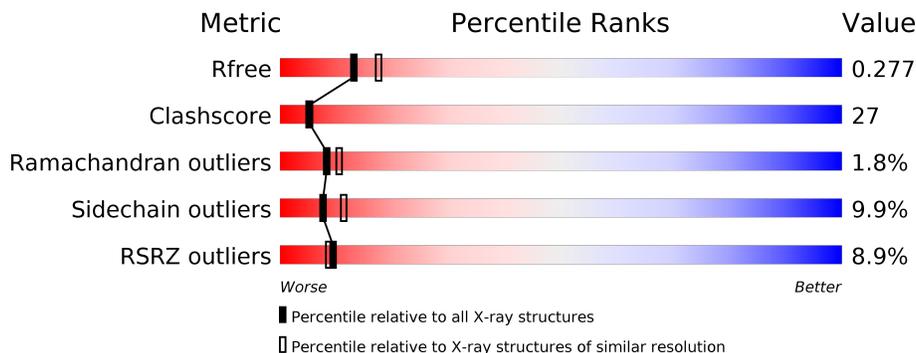
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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% 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.

Mol	Chain	Length	Quality of chain
1	A	424	8%	47% 38% 12% •
1	B	424	10%	47% 38% 10% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6553 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 Phosphoribosylamine--glycine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total 3236	C 2069	N 548	O 608	S 11	0	0	0
1	B	423	Total 3228	C 2065	N 548	O 604	S 11	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	38	Total 38	O 38	0	0
2	B	51	Total 51	O 51	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 the various outlier classes 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.

- Molecule 1: Phosphoribosylamine--glycine ligase
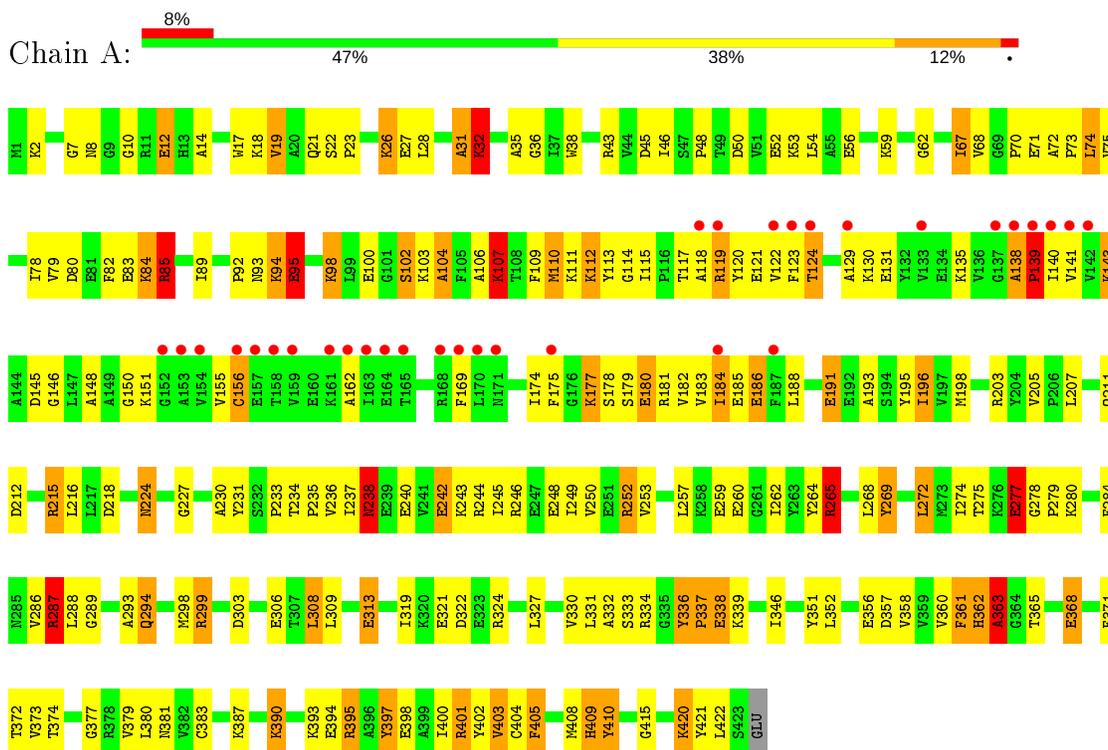
- Molecule 1: Phosphoribosylamine--glycine ligase
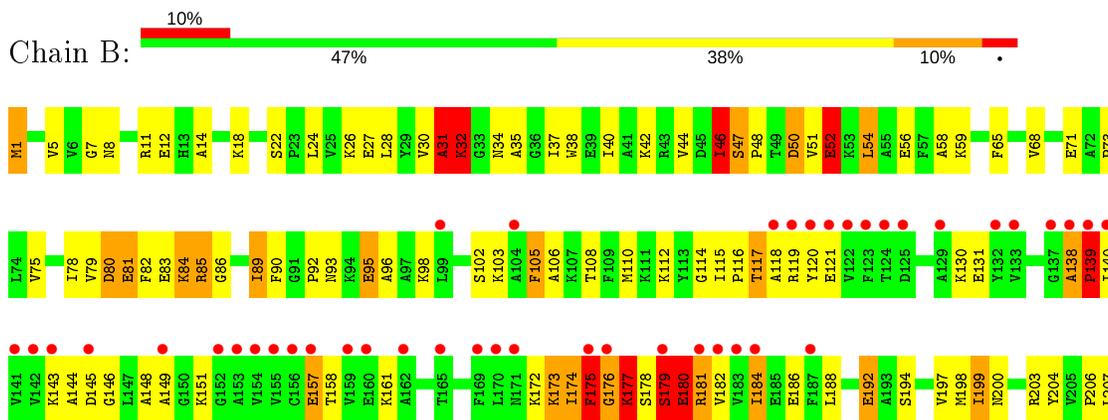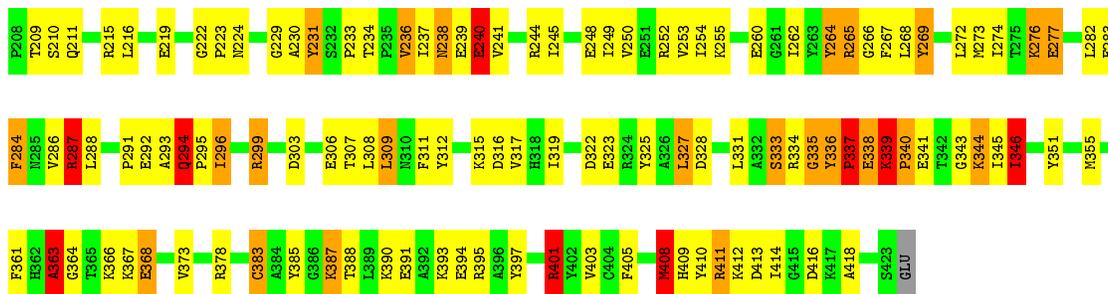
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	97.26Å 45.15Å 103.48Å 90.00° 103.87° 90.00°	Depositor
Resolution (Å)	49.55 – 2.40 49.55 – 2.39	Depositor EDS
% Data completeness (in resolution range)	92.9 (49.55-2.40) 96.2 (49.55-2.39)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.10 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.249 0.228 , 0.277	Depositor DCC
R_{free} test set	1694 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	34.6	Xtriage
Anisotropy	1.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 54.9	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6553	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.32% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	1.78	35/3297 (1.1%)	1.72	76/4447 (1.7%)
1	B	1.74	36/3289 (1.1%)	1.68	64/4436 (1.4%)
All	All	1.76	71/6586 (1.1%)	1.70	140/8883 (1.6%)

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	5
1	B	0	11
All	All	0	16

The worst 5 of 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	175	PHE	C-N	6.58	1.44	1.33
1	B	283	GLU	CD-OE1	5.95	1.32	1.25
1	A	321	GLU	CD-OE2	5.95	1.32	1.25
1	B	401	ARG	CG-CD	5.92	1.66	1.51
1	A	401	ARG	C-O	5.88	1.34	1.23

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	287	ARG	NE-CZ-NH1	14.95	127.77	120.30
1	A	287	ARG	NE-CZ-NH2	-14.23	113.19	120.30
1	B	287	ARG	NE-CZ-NH2	-13.66	113.47	120.30
1	A	395	ARG	NE-CZ-NH2	-12.08	114.26	120.30
1	B	139	PRO	O-C-N	-11.88	103.69	122.70

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	ALA	Peptide
1	A	139	PRO	Peptide
1	A	238	ASN	Peptide
1	A	31	ALA	Peptide
1	A	371	PHE	Peptide

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	3236	0	3194	173	0
1	B	3228	0	3180	171	0
2	A	38	0	0	4	0
2	B	51	0	0	1	0
All	All	6553	0	6374	342	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 27.

The worst 5 of 342 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:B:337:PRO:HD2	1:B:338:GLU:CD	1.49	1.32
1:B:337:PRO:HD2	1:B:338:GLU:OE2	1.38	1.18
1:A:103:LYS:HD2	1:A:143:LYS:HE2	1.27	1.11
1:B:265:ARG:HG2	1:B:265:ARG:HH11	0.94	1.09
1:A:103:LYS:CD	1:A:143:LYS:HE2	1.85	1.05

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	421/424 (99%)	383 (91%)	30 (7%)	8 (2%)	8	10
1	B	421/424 (99%)	366 (87%)	48 (11%)	7 (2%)	9	11
All	All	842/848 (99%)	749 (89%)	78 (9%)	15 (2%)	8	10

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	112	LYS
1	A	139	PRO
1	B	32	LYS
1	B	130	LYS

5.3.2 Protein sidechains (i)

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	324/351 (92%)	299 (92%)	25 (8%)	13	20
1	B	321/351 (92%)	282 (88%)	39 (12%)	5	6
All	All	645/702 (92%)	581 (90%)	64 (10%)	8	11

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	46	ILE

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Mol	Chain	Res	Type
1	B	117	THR
1	B	387	LYS
1	B	52	GLU
1	B	81	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	409	HIS
1	B	224	ASN
1	B	318	HIS
1	A	370	ASN
1	B	310	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)

There are no ligands in this entry.

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)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	423/424 (99%)	0.17	32 (7%)	13	12	21, 43, 103, 125	0
1	B	423/424 (99%)	0.42	43 (10%)	6	6	21, 46, 114, 137	0
All	All	846/848 (99%)	0.30	75 (8%)	9	9	21, 44, 109, 137	0

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	162	ALA	7.8
1	B	179	SER	7.6
1	B	184	ILE	7.2
1	B	142	VAL	6.7
1	B	182	VAL	6.5

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.