wwPDB X-ray Structure Validation Summary Report (i)

Jan 24, 2017 – 09:27 PM EST

PDB ID	:	3D54
Title	:	Structure of PurLQS from Thermotoga maritima
Authors	:	Ealick, S.E.; Morar, M.
Deposited on	:	2008-05-15
Resolution	:	3.50 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

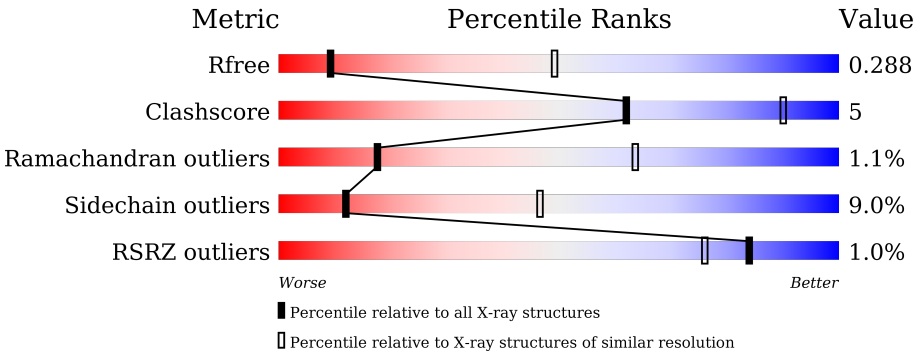
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 3.50 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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. 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	629	78% 14% • 7%
1	E	629	81% 12% 7%
1	I	629	4% 80% 12% 7%
2	B	82	73% 22% 5%
2	C	82	78% 18% •
2	F	82	78% 17% • •

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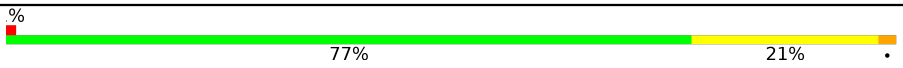
Mol	Chain	Length	Quality of chain
2	G	82	
2	J	82	
2	K	82	
3	D	213	
3	H	213	
3	L	213	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22584 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 Phosphoribosylformylglycinamidine synthase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	0	0	0
			4493	2859	769	846	19			
1	E	583	Total	C	N	O	S	0	0	0
			4493	2859	769	846	19			
1	I	583	Total	C	N	O	S	0	0	0
			4493	2859	769	846	19			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	Expression Tag	UNP Q9X0X3
A	-24	GLY	-	Expression Tag	UNP Q9X0X3
A	-23	SER	-	Expression Tag	UNP Q9X0X3
A	-22	HIS	-	Expression Tag	UNP Q9X0X3
A	-21	HIS	-	Expression Tag	UNP Q9X0X3
A	-20	HIS	-	Expression Tag	UNP Q9X0X3
A	-19	HIS	-	Expression Tag	UNP Q9X0X3
A	-18	HIS	-	Expression Tag	UNP Q9X0X3
A	-17	HIS	-	Expression Tag	UNP Q9X0X3
A	-16	ASP	-	Expression Tag	UNP Q9X0X3
A	-15	ILE	-	Expression Tag	UNP Q9X0X3
A	-14	THR	-	Expression Tag	UNP Q9X0X3
A	-13	SER	-	Expression Tag	UNP Q9X0X3
A	-12	LEU	-	Expression Tag	UNP Q9X0X3
A	-11	TYR	-	Expression Tag	UNP Q9X0X3
A	-10	LYS	-	Expression Tag	UNP Q9X0X3
A	-9	LYS	-	Expression Tag	UNP Q9X0X3
A	-8	ALA	-	Expression Tag	UNP Q9X0X3
A	-7	GLY	-	Expression Tag	UNP Q9X0X3
A	-6	SER	-	Expression Tag	UNP Q9X0X3
A	-5	GLU	-	Expression Tag	UNP Q9X0X3
A	-4	ASN	-	Expression Tag	UNP Q9X0X3
A	-3	LEU	-	Expression Tag	UNP Q9X0X3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	TYR	-	Expression Tag	UNP Q9X0X3
A	-1	PHE	-	Expression Tag	UNP Q9X0X3
A	0	GLN	-	Expression Tag	UNP Q9X0X3
E	-25	MET	-	Expression Tag	UNP Q9X0X3
E	-24	GLY	-	Expression Tag	UNP Q9X0X3
E	-23	SER	-	Expression Tag	UNP Q9X0X3
E	-22	HIS	-	Expression Tag	UNP Q9X0X3
E	-21	HIS	-	Expression Tag	UNP Q9X0X3
E	-20	HIS	-	Expression Tag	UNP Q9X0X3
E	-19	HIS	-	Expression Tag	UNP Q9X0X3
E	-18	HIS	-	Expression Tag	UNP Q9X0X3
E	-17	HIS	-	Expression Tag	UNP Q9X0X3
E	-16	ASP	-	Expression Tag	UNP Q9X0X3
E	-15	ILE	-	Expression Tag	UNP Q9X0X3
E	-14	THR	-	Expression Tag	UNP Q9X0X3
E	-13	SER	-	Expression Tag	UNP Q9X0X3
E	-12	LEU	-	Expression Tag	UNP Q9X0X3
E	-11	TYR	-	Expression Tag	UNP Q9X0X3
E	-10	LYS	-	Expression Tag	UNP Q9X0X3
E	-9	LYS	-	Expression Tag	UNP Q9X0X3
E	-8	ALA	-	Expression Tag	UNP Q9X0X3
E	-7	GLY	-	Expression Tag	UNP Q9X0X3
E	-6	SER	-	Expression Tag	UNP Q9X0X3
E	-5	GLU	-	Expression Tag	UNP Q9X0X3
E	-4	ASN	-	Expression Tag	UNP Q9X0X3
E	-3	LEU	-	Expression Tag	UNP Q9X0X3
E	-2	TYR	-	Expression Tag	UNP Q9X0X3
E	-1	PHE	-	Expression Tag	UNP Q9X0X3
E	0	GLN	-	Expression Tag	UNP Q9X0X3
I	-25	MET	-	Expression Tag	UNP Q9X0X3
I	-24	GLY	-	Expression Tag	UNP Q9X0X3
I	-23	SER	-	Expression Tag	UNP Q9X0X3
I	-22	HIS	-	Expression Tag	UNP Q9X0X3
I	-21	HIS	-	Expression Tag	UNP Q9X0X3
I	-20	HIS	-	Expression Tag	UNP Q9X0X3
I	-19	HIS	-	Expression Tag	UNP Q9X0X3
I	-18	HIS	-	Expression Tag	UNP Q9X0X3
I	-17	HIS	-	Expression Tag	UNP Q9X0X3
I	-16	ASP	-	Expression Tag	UNP Q9X0X3
I	-15	ILE	-	Expression Tag	UNP Q9X0X3
I	-14	THR	-	Expression Tag	UNP Q9X0X3
I	-13	SER	-	Expression Tag	UNP Q9X0X3

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-12	LEU	-	Expression Tag	UNP Q9X0X3
I	-11	TYR	-	Expression Tag	UNP Q9X0X3
I	-10	LYS	-	Expression Tag	UNP Q9X0X3
I	-9	LYS	-	Expression Tag	UNP Q9X0X3
I	-8	ALA	-	Expression Tag	UNP Q9X0X3
I	-7	GLY	-	Expression Tag	UNP Q9X0X3
I	-6	SER	-	Expression Tag	UNP Q9X0X3
I	-5	GLU	-	Expression Tag	UNP Q9X0X3
I	-4	ASN	-	Expression Tag	UNP Q9X0X3
I	-3	LEU	-	Expression Tag	UNP Q9X0X3
I	-2	TYR	-	Expression Tag	UNP Q9X0X3
I	-1	PHE	-	Expression Tag	UNP Q9X0X3
I	0	GLN	-	Expression Tag	UNP Q9X0X3

- Molecule 2 is a protein called Formylglycinamide ribonucleotide amidotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	82	Total	C	N	O	S	0	0	0
			678	431	118	127	2			
2	C	82	Total	C	N	O	S	0	0	0
			678	431	118	127	2			
2	F	82	Total	C	N	O	S	0	0	0
			678	431	118	127	2			
2	G	82	Total	C	N	O	S	0	0	0
			678	431	118	127	2			
2	J	82	Total	C	N	O	S	0	0	0
			678	431	118	127	2			
2	K	82	Total	C	N	O	S	0	0	0
			678	431	118	127	2			

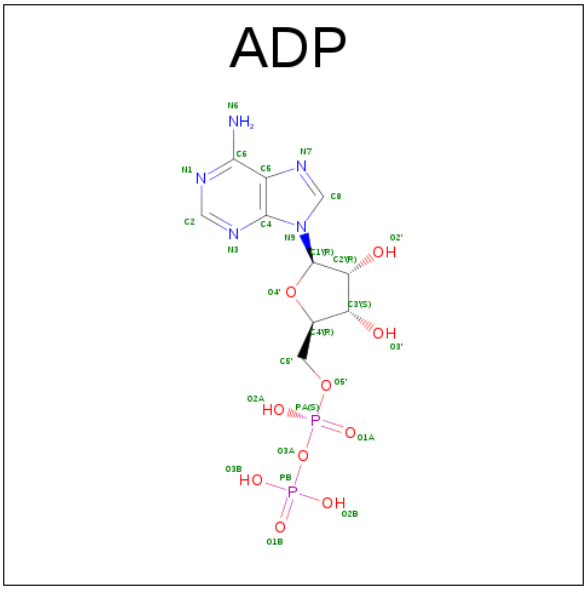
- Molecule 3 is a protein called Phosphoribosylformylglycinamidine synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	212	Total	C	N	O	S	0	0	0
			1651	1056	279	309	7			
3	H	212	Total	C	N	O	S	0	0	0
			1651	1056	279	309	7			
3	L	212	Total	C	N	O	S	0	0	0
			1651	1056	279	309	7			

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	1	Total Na 1 1	0	0
4	A	1	Total Na 1 1	0	0
4	E	1	Total Na 1 1	0	0

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



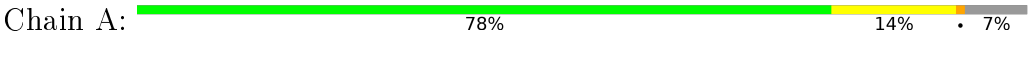
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 27 10 5 10 2	0	0
5	E	1	Total C N O P 27 10 5 10 2	0	0
5	I	1	Total C N O P 27 10 5 10 2	0	0

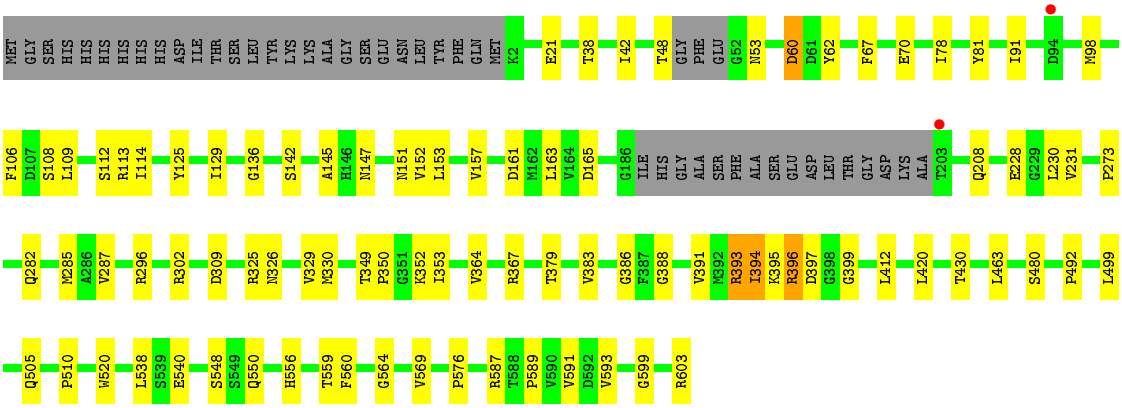
3 Residue-property plots (i)

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.

- Molecule 1: Phosphoribosylformylglycinamidine synthase II

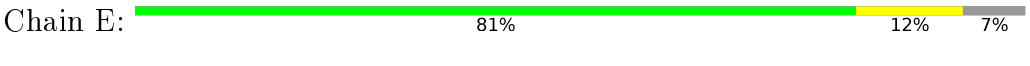
Chain A:

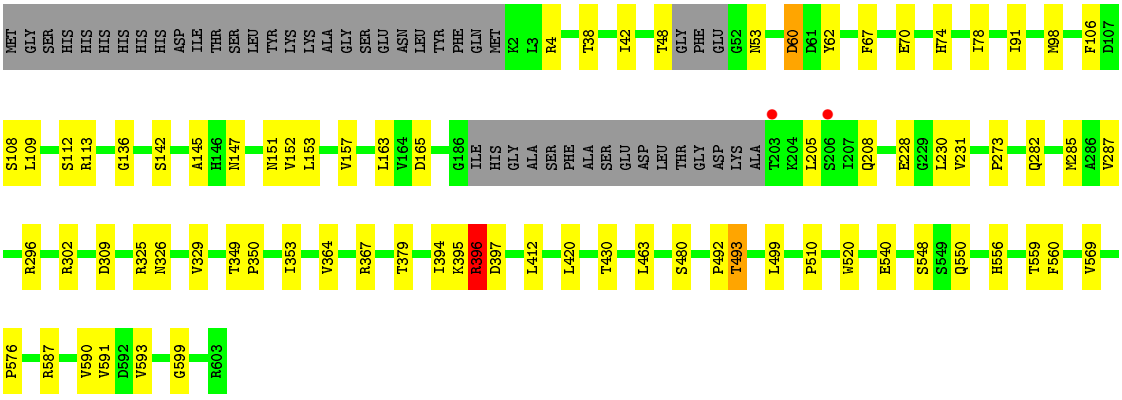




- Molecule 1: Phosphoribosylformylglycinamidine synthase II

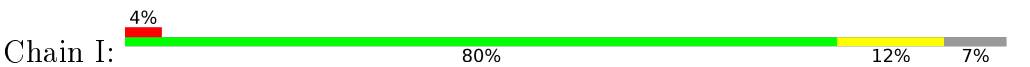
Chain E:

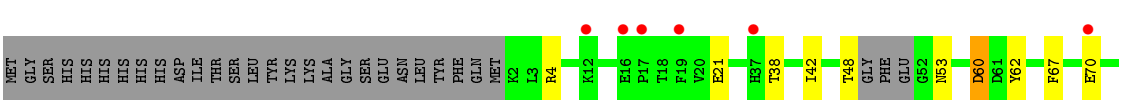


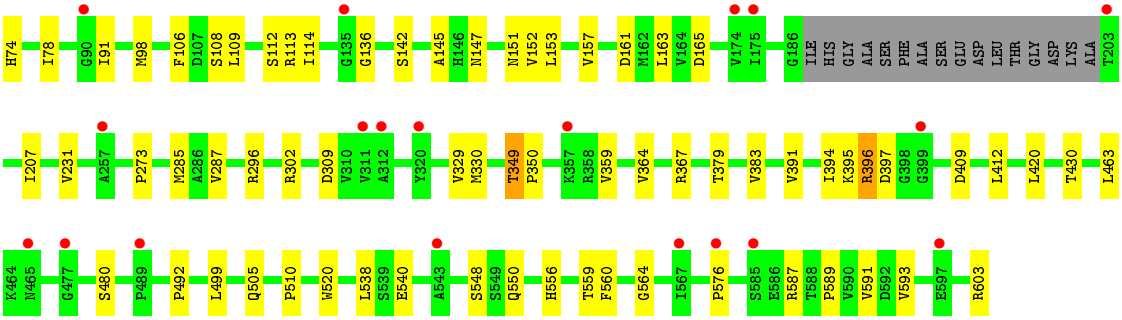


- Molecule 1: Phosphoribosylformylglycinamidine synthase II

Chain I:

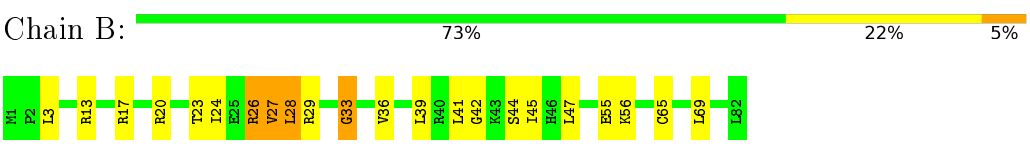






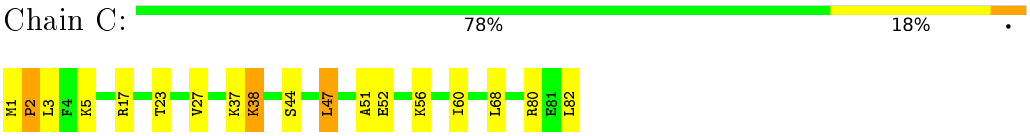
• Molecule 2: Formylglycinamide ribonucleotide amidotransferase

Chain B:



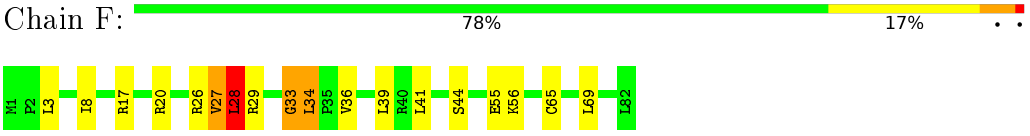
• Molecule 2: Formylglycinamide ribonucleotide amidotransferase

Chain C:



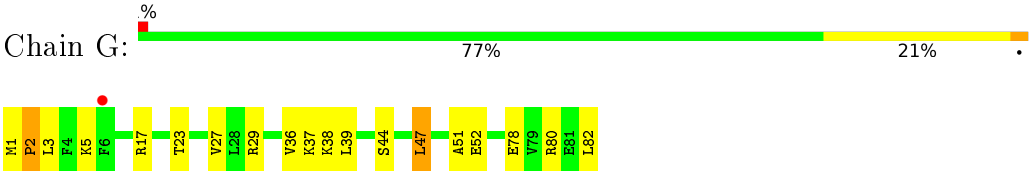
• Molecule 2: Formylglycinamide ribonucleotide amidotransferase

Chain F:



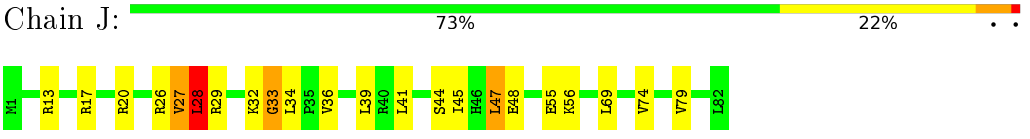
• Molecule 2: Formylglycinamide ribonucleotide amidotransferase

Chain G:



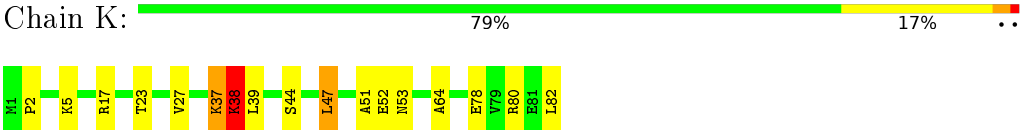
• Molecule 2: Formylglycinamide ribonucleotide amidotransferase

Chain J:



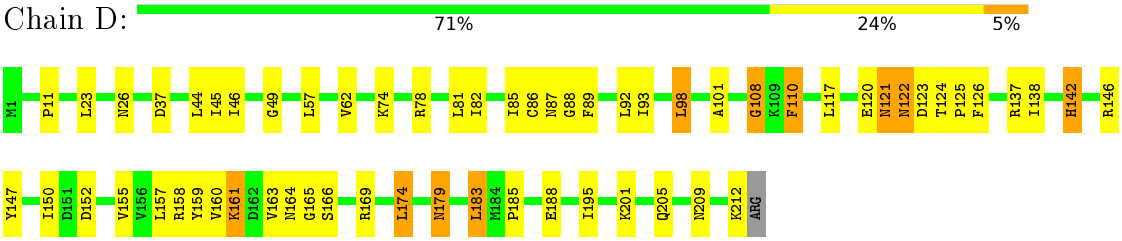
• Molecule 2: Formylglycinamide ribonucleotide amidotransferase

Chain K:



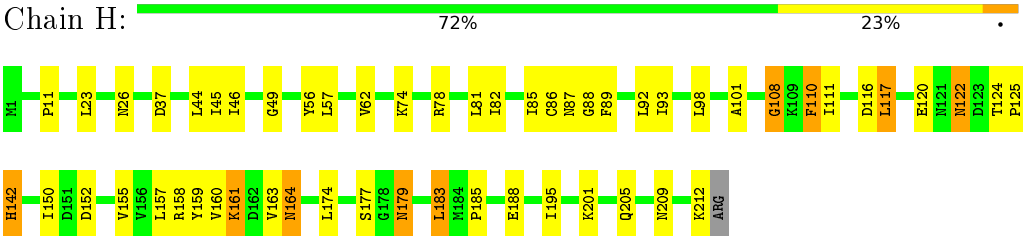
• Molecule 3: Phosphoribosylformylglycinamidine synthase 1

Chain D:



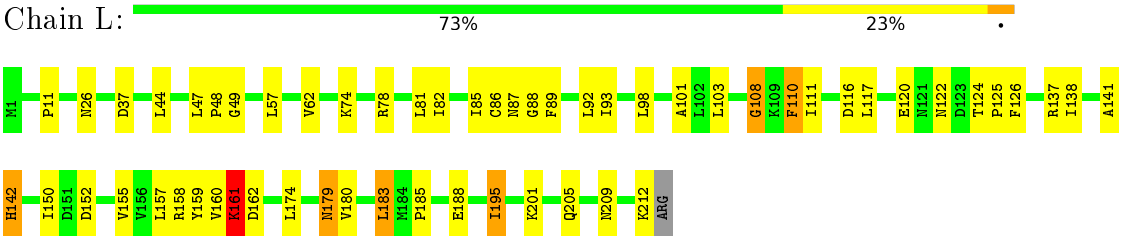
• Molecule 3: Phosphoribosylformylglycinamidine synthase 1

Chain H:



• Molecule 3: Phosphoribosylformylglycinamidine synthase 1

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	256.85Å 187.34Å 159.18Å 90.00° 99.12° 90.00°	Depositor
Resolution (Å)	45.70 – 3.50 48.10 – 3.50	Depositor EDS
% Data completeness (in resolution range)	83.8 (45.70-3.50) 83.8 (48.10-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 3.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.252 , 0.282 0.265 , 0.288	Depositor DCC
R_{free} test set	7909 reflections (10.08%)	DCC
Wilson B-factor (Å^2)	88.4	Xtriage
Anisotropy	0.766	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 70.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	22584	wwPDB-VP
Average B, all atoms (Å^2)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CYG, ADP

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	0.67	0/4582	0.77	0/6217
1	E	0.67	0/4582	0.77	1/6217 (0.0%)
1	I	0.70	0/4582	0.76	0/6217
2	B	0.66	0/687	0.73	1/920 (0.1%)
2	C	0.64	0/687	0.75	0/920
2	F	0.66	0/687	0.79	2/920 (0.2%)
2	G	0.61	0/687	0.77	0/920
2	J	0.65	0/687	0.76	2/920 (0.2%)
2	K	0.68	0/687	0.80	0/920
3	D	0.71	0/1667	0.84	1/2249 (0.0%)
3	H	0.70	0/1667	0.85	2/2249 (0.1%)
3	L	0.72	0/1667	0.88	2/2249 (0.1%)
All	All	0.68	0/22869	0.79	11/30918 (0.0%)

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	3
1	E	0	2
1	I	0	2
2	C	0	1
2	K	0	1
3	D	0	3
3	H	0	2
3	L	0	2
All	All	0	16

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	161	LYS	CB-CA-C	5.99	122.38	110.40
1	E	205	LEU	CA-CB-CG	5.93	128.94	115.30
2	F	33	GLY	N-CA-C	5.72	127.41	113.10
2	J	33	GLY	N-CA-C	5.62	127.14	113.10
2	B	33	GLY	N-CA-C	5.36	126.50	113.10

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	394	ILE	Peptide
1	A	396	ARG	Peptide
1	A	397	ASP	Peptide
2	C	68	LEU	Peptide
3	D	121	ASN	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	4493	0	4532	27	0
1	E	4493	0	4532	17	0
1	I	4493	0	4532	16	0
2	B	678	0	707	22	0
2	C	678	0	707	12	0
2	F	678	0	707	16	0
2	G	678	0	707	10	0
2	J	678	0	707	19	0
2	K	678	0	707	13	0
3	D	1651	0	1642	41	0
3	H	1651	0	1642	32	0
3	L	1651	0	1642	34	0
4	A	1	0	0	0	0
4	E	1	0	0	0	0
4	I	1	0	0	0	0
5	A	27	0	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	27	0	12	2	0
5	I	27	0	12	2	0
All	All	22584	0	22800	243	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 5.

The worst 5 of 243 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:395:LYS:O	1:A:396:ARG:HD2	1.43	1.19
2:B:26:ARG:HH11	2:B:26:ARG:HG2	1.06	1.14
2:J:28:LEU:O	2:J:28:LEU:HG	1.42	1.08
2:F:28:LEU:HD12	2:F:34:LEU:HD13	1.44	0.99
2:B:41:LEU:HD22	2:B:42:GLY:H	1.29	0.96

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	577/629 (92%)	520 (90%)	53 (9%)	4 (1%)	26 72
1	E	577/629 (92%)	519 (90%)	56 (10%)	2 (0%)	46 84
1	I	577/629 (92%)	519 (90%)	55 (10%)	3 (0%)	34 78
2	B	80/82 (98%)	69 (86%)	10 (12%)	1 (1%)	15 60
2	C	80/82 (98%)	75 (94%)	4 (5%)	1 (1%)	15 60
2	F	80/82 (98%)	69 (86%)	9 (11%)	2 (2%)	7 46
2	G	80/82 (98%)	74 (92%)	5 (6%)	1 (1%)	15 60
2	J	80/82 (98%)	68 (85%)	10 (12%)	2 (2%)	7 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	K	80/82 (98%)	73 (91%)	6 (8%)	1 (1%)	15 60
3	D	209/213 (98%)	184 (88%)	21 (10%)	4 (2%)	10 51
3	H	209/213 (98%)	186 (89%)	18 (9%)	5 (2%)	7 47
3	L	209/213 (98%)	186 (89%)	18 (9%)	5 (2%)	7 47
All	All	2838/3018 (94%)	2542 (90%)	265 (9%)	31 (1%)	17 63

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	108	GLY
3	H	108	GLY
2	J	27	VAL
2	K	38	LYS
3	L	108	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	487/525 (93%)	445 (91%)	42 (9%)	13 49
1	E	487/525 (93%)	442 (91%)	45 (9%)	11 45
1	I	487/525 (93%)	441 (91%)	46 (9%)	11 44
2	B	75/75 (100%)	68 (91%)	7 (9%)	11 45
2	C	75/75 (100%)	70 (93%)	5 (7%)	20 61
2	F	75/75 (100%)	68 (91%)	7 (9%)	11 45
2	G	75/75 (100%)	67 (89%)	8 (11%)	8 37
2	J	75/75 (100%)	67 (89%)	8 (11%)	8 37
2	K	75/75 (100%)	70 (93%)	5 (7%)	20 61
3	D	171/174 (98%)	156 (91%)	15 (9%)	12 48
3	H	171/174 (98%)	155 (91%)	16 (9%)	11 44
3	L	171/174 (98%)	156 (91%)	15 (9%)	12 48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2424/2547 (95%)	2205 (91%)	219 (9%)	12 46

5 of 219 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	463	LEU
2	G	17	ARG
2	K	78	GLU
1	E	493	THR
1	E	590	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	11	GLN
3	H	164	ASN
3	L	164	ASN
3	H	26	ASN
3	H	175	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)

3 non-standard protein/DNA/RNA residues 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	CYG	D	86	3	9,14,15	1.33	1 (11%)	7,17,19	4.08	3 (42%)
3	CYG	H	86	3	9,14,15	1.34	1 (11%)	7,17,19	4.05	3 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	CYG	L	86	3	9,14,15	1.35	1 (11%)	7,17,19	4.16	4 (57%)

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	CYG	D	86	3	-	0/10/16/18	0/0/0/0
3	CYG	H	86	3	-	0/10/16/18	0/0/0/0
3	CYG	L	86	3	-	0/10/16/18	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	86	CYG	CG1-CD1	3.16	1.53	1.50
3	H	86	CYG	CG1-CD1	3.17	1.53	1.50
3	L	86	CYG	CG1-CD1	3.20	1.53	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	86	CYG	OE2-CD1-CG1	-5.32	120.28	123.94
3	D	86	CYG	OE2-CD1-CG1	-5.22	120.35	123.94
3	H	86	CYG	OE2-CD1-CG1	-5.18	120.38	123.94
3	L	86	CYG	OE2-CD1-SG	-4.61	119.17	122.83
3	H	86	CYG	OE2-CD1-SG	-4.52	119.25	122.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	86	CYG	2	0
3	H	86	CYG	1	0
3	L	86	CYG	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
5	ADP	A	2004	-	24,29,29	1.16	2 (8%)	23,45,45	2.18	2 (8%)
5	ADP	E	2006	-	24,29,29	1.16	2 (8%)	23,45,45	2.21	2 (8%)
5	ADP	I	2005	-	24,29,29	1.16	2 (8%)	23,45,45	2.18	3 (13%)

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
5	ADP	A	2004	-	-	0/12/32/32	0/3/3/3
5	ADP	E	2006	-	-	0/12/32/32	0/3/3/3
5	ADP	I	2005	-	-	0/12/32/32	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	2006	ADP	O4'-C1'	2.02	1.44	1.41
5	A	2004	ADP	O4'-C1'	2.03	1.44	1.41
5	I	2005	ADP	O4'-C1'	2.13	1.44	1.41
5	A	2004	ADP	PB-O1B	3.32	1.61	1.50
5	E	2006	ADP	PB-O1B	3.33	1.61	1.50

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	2006	ADP	N3-C2-N1	-9.00	121.80	128.87
5	I	2005	ADP	N3-C2-N1	-8.92	121.87	128.87
5	A	2004	ADP	N3-C2-N1	-8.87	121.91	128.87
5	A	2004	ADP	C2'-C3'-C4'	-2.13	98.28	102.64
5	E	2006	ADP	C2'-C3'-C4'	-2.13	98.28	102.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2004	ADP	4	0
5	E	2006	ADP	2	0
5	I	2005	ADP	2	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

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, 95^{th} 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	583/629 (92%)	-0.25	2 (0%) 94 91	71, 126, 177, 203	0
1	E	583/629 (92%)	-0.19	2 (0%) 94 91	83, 139, 183, 205	0
1	I	583/629 (92%)	0.41	25 (4%) 39 30	111, 185, 205, 205	0
2	B	82/82 (100%)	-0.43	0 100 100	72, 114, 152, 160	0
2	C	82/82 (100%)	-0.38	0 100 100	77, 128, 163, 183	0
2	F	82/82 (100%)	0.10	0 100 100	93, 151, 193, 202	0
2	G	82/82 (100%)	0.09	1 (1%) 81 72	114, 165, 197, 204	0
2	J	82/82 (100%)	-0.26	0 100 100	83, 126, 169, 192	0
2	K	82/82 (100%)	-0.20	0 100 100	95, 141, 172, 187	0
3	D	211/213 (99%)	-0.39	0 100 100	72, 117, 162, 203	0
3	H	211/213 (99%)	-0.22	0 100 100	90, 141, 182, 205	0
3	L	211/213 (99%)	-0.23	0 100 100	95, 141, 177, 205	0
All	All	2874/3018 (95%)	-0.10	30 (1%) 84 76	71, 143, 201, 205	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	203	THR	4.3
1	I	17	PRO	3.7
1	I	312	ALA	3.4
1	I	19	PHE	3.3
1	A	203	THR	3.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CYG	D	86	15/16	0.93	0.36	-	165,167,168,170	0
3	CYG	H	86	15/16	0.89	0.33	-	165,167,168,170	0
3	CYG	L	86	15/16	0.87	0.35	-	165,167,168,170	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	ADP	A	2004	27/27	0.89	0.32	0.57	161,167,186,306	0
5	ADP	E	2006	27/27	0.84	0.29	0.25	161,167,186,306	0
5	ADP	I	2005	27/27	0.82	0.24	-0.91	161,167,186,306	0
4	NA	A	3003	1/1	0.77	1.94	-	145,145,145,145	0
4	NA	E	3002	1/1	0.87	1.61	-	145,145,145,145	0
4	NA	I	3001	1/1	0.51	0.93	-	145,145,145,145	0

6.5 Other polymers (i)

There are no such residues in this entry.