wwPDB X-ray Structure Validation Summary Report (i)

Apr 20, 2022 – 10:07 am BST

PDB ID	:	7OY9
Title	:	Crystal structure of GMP reductase from mycobacterium smegmatis.
Authors	:	Dolezal, M.; Klima, M.; Pichova, I.
Deposited on	:	2021-06-24
Resolution	:	2.80 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
https://www.wwpdb.org/validation/2017/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:

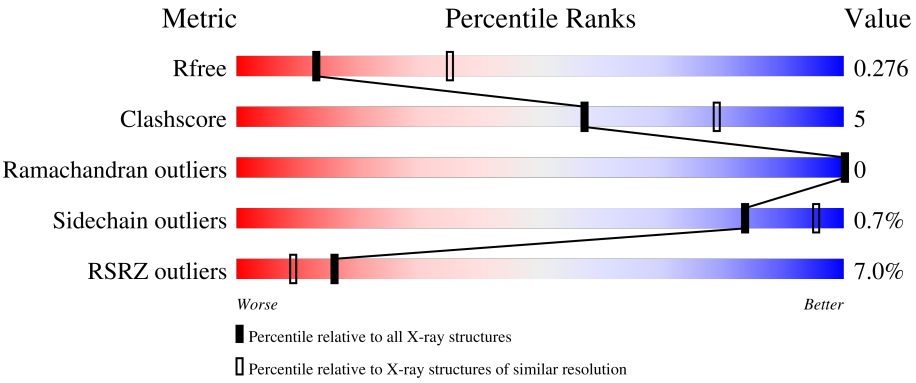
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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% 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	496	5% 80% 12% 8%
1	B	496	5% 83% 8% 8%
1	C	496	5% 83% 9% 8%
1	D	496	7% 82% 10% 8%
1	E	496	8% 79% 12% • 8%

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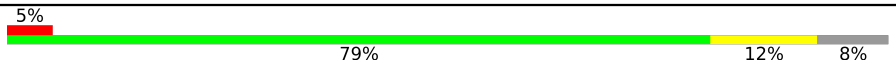
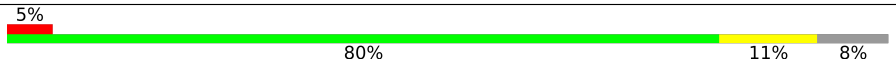
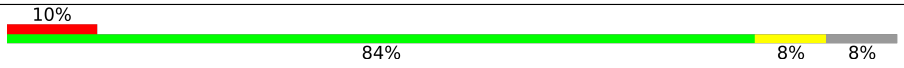
Mol	Chain	Length	Quality of chain
1	F	496	
1	G	496	
1	H	496	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 25837 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 Guanosine 5'-monophosphate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	0	0
			3234	2027	558	636	13			
1	B	456	Total	C	N	O	S	0	0	0
			3243	2031	563	636	13			
1	C	454	Total	C	N	O	S	0	0	0
			3227	2023	558	633	13			
1	D	458	Total	C	N	O	S	0	0	0
			3243	2030	562	638	13			
1	E	454	Total	C	N	O	S	0	0	0
			3227	2024	555	634	14			
1	F	455	Total	C	N	O	S	0	0	0
			3224	2023	556	632	13			
1	G	454	Total	C	N	O	S	0	0	0
			3206	2011	552	630	13			
1	H	458	Total	C	N	O	S	0	0	0
			3233	2026	558	636	13			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	-	insertion	UNP A0A0D6IET0
A	480	THR	-	expression tag	UNP A0A0D6IET0
A	481	ALA	-	expression tag	UNP A0A0D6IET0
A	482	ALA	-	expression tag	UNP A0A0D6IET0
A	483	ALA	-	expression tag	UNP A0A0D6IET0
A	484	LYS	-	expression tag	UNP A0A0D6IET0
A	485	GLU	-	expression tag	UNP A0A0D6IET0
A	486	ASP	-	expression tag	UNP A0A0D6IET0
A	487	LEU	-	expression tag	UNP A0A0D6IET0
A	488	GLU	-	expression tag	UNP A0A0D6IET0
A	489	HIS	-	expression tag	UNP A0A0D6IET0
A	490	HIS	-	expression tag	UNP A0A0D6IET0
A	491	HIS	-	expression tag	UNP A0A0D6IET0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	492	HIS	-	expression tag	UNP A0A0D6IET0
A	493	HIS	-	expression tag	UNP A0A0D6IET0
A	494	HIS	-	expression tag	UNP A0A0D6IET0
A	495	HIS	-	expression tag	UNP A0A0D6IET0
A	496	HIS	-	expression tag	UNP A0A0D6IET0
B	2	VAL	-	insertion	UNP A0A0D6IET0
B	480	THR	-	expression tag	UNP A0A0D6IET0
B	481	ALA	-	expression tag	UNP A0A0D6IET0
B	482	ALA	-	expression tag	UNP A0A0D6IET0
B	483	ALA	-	expression tag	UNP A0A0D6IET0
B	484	LYS	-	expression tag	UNP A0A0D6IET0
B	485	GLU	-	expression tag	UNP A0A0D6IET0
B	486	ASP	-	expression tag	UNP A0A0D6IET0
B	487	LEU	-	expression tag	UNP A0A0D6IET0
B	488	GLU	-	expression tag	UNP A0A0D6IET0
B	489	HIS	-	expression tag	UNP A0A0D6IET0
B	490	HIS	-	expression tag	UNP A0A0D6IET0
B	491	HIS	-	expression tag	UNP A0A0D6IET0
B	492	HIS	-	expression tag	UNP A0A0D6IET0
B	493	HIS	-	expression tag	UNP A0A0D6IET0
B	494	HIS	-	expression tag	UNP A0A0D6IET0
B	495	HIS	-	expression tag	UNP A0A0D6IET0
B	496	HIS	-	expression tag	UNP A0A0D6IET0
C	2	VAL	-	insertion	UNP A0A0D6IET0
C	480	THR	-	expression tag	UNP A0A0D6IET0
C	481	ALA	-	expression tag	UNP A0A0D6IET0
C	482	ALA	-	expression tag	UNP A0A0D6IET0
C	483	ALA	-	expression tag	UNP A0A0D6IET0
C	484	LYS	-	expression tag	UNP A0A0D6IET0
C	485	GLU	-	expression tag	UNP A0A0D6IET0
C	486	ASP	-	expression tag	UNP A0A0D6IET0
C	487	LEU	-	expression tag	UNP A0A0D6IET0
C	488	GLU	-	expression tag	UNP A0A0D6IET0
C	489	HIS	-	expression tag	UNP A0A0D6IET0
C	490	HIS	-	expression tag	UNP A0A0D6IET0
C	491	HIS	-	expression tag	UNP A0A0D6IET0
C	492	HIS	-	expression tag	UNP A0A0D6IET0
C	493	HIS	-	expression tag	UNP A0A0D6IET0
C	494	HIS	-	expression tag	UNP A0A0D6IET0
C	495	HIS	-	expression tag	UNP A0A0D6IET0
C	496	HIS	-	expression tag	UNP A0A0D6IET0
D	2	VAL	-	insertion	UNP A0A0D6IET0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	480	THR	-	expression tag	UNP A0A0D6IET0
D	481	ALA	-	expression tag	UNP A0A0D6IET0
D	482	ALA	-	expression tag	UNP A0A0D6IET0
D	483	ALA	-	expression tag	UNP A0A0D6IET0
D	484	LYS	-	expression tag	UNP A0A0D6IET0
D	485	GLU	-	expression tag	UNP A0A0D6IET0
D	486	ASP	-	expression tag	UNP A0A0D6IET0
D	487	LEU	-	expression tag	UNP A0A0D6IET0
D	488	GLU	-	expression tag	UNP A0A0D6IET0
D	489	HIS	-	expression tag	UNP A0A0D6IET0
D	490	HIS	-	expression tag	UNP A0A0D6IET0
D	491	HIS	-	expression tag	UNP A0A0D6IET0
D	492	HIS	-	expression tag	UNP A0A0D6IET0
D	493	HIS	-	expression tag	UNP A0A0D6IET0
D	494	HIS	-	expression tag	UNP A0A0D6IET0
D	495	HIS	-	expression tag	UNP A0A0D6IET0
D	496	HIS	-	expression tag	UNP A0A0D6IET0
E	2	VAL	-	insertion	UNP A0A0D6IET0
E	480	THR	-	expression tag	UNP A0A0D6IET0
E	481	ALA	-	expression tag	UNP A0A0D6IET0
E	482	ALA	-	expression tag	UNP A0A0D6IET0
E	483	ALA	-	expression tag	UNP A0A0D6IET0
E	484	LYS	-	expression tag	UNP A0A0D6IET0
E	485	GLU	-	expression tag	UNP A0A0D6IET0
E	486	ASP	-	expression tag	UNP A0A0D6IET0
E	487	LEU	-	expression tag	UNP A0A0D6IET0
E	488	GLU	-	expression tag	UNP A0A0D6IET0
E	489	HIS	-	expression tag	UNP A0A0D6IET0
E	490	HIS	-	expression tag	UNP A0A0D6IET0
E	491	HIS	-	expression tag	UNP A0A0D6IET0
E	492	HIS	-	expression tag	UNP A0A0D6IET0
E	493	HIS	-	expression tag	UNP A0A0D6IET0
E	494	HIS	-	expression tag	UNP A0A0D6IET0
E	495	HIS	-	expression tag	UNP A0A0D6IET0
E	496	HIS	-	expression tag	UNP A0A0D6IET0
F	2	VAL	-	insertion	UNP A0A0D6IET0
F	480	THR	-	expression tag	UNP A0A0D6IET0
F	481	ALA	-	expression tag	UNP A0A0D6IET0
F	482	ALA	-	expression tag	UNP A0A0D6IET0
F	483	ALA	-	expression tag	UNP A0A0D6IET0
F	484	LYS	-	expression tag	UNP A0A0D6IET0
F	485	GLU	-	expression tag	UNP A0A0D6IET0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	486	ASP	-	expression tag	UNP A0A0D6IET0
F	487	LEU	-	expression tag	UNP A0A0D6IET0
F	488	GLU	-	expression tag	UNP A0A0D6IET0
F	489	HIS	-	expression tag	UNP A0A0D6IET0
F	490	HIS	-	expression tag	UNP A0A0D6IET0
F	491	HIS	-	expression tag	UNP A0A0D6IET0
F	492	HIS	-	expression tag	UNP A0A0D6IET0
F	493	HIS	-	expression tag	UNP A0A0D6IET0
F	494	HIS	-	expression tag	UNP A0A0D6IET0
F	495	HIS	-	expression tag	UNP A0A0D6IET0
F	496	HIS	-	expression tag	UNP A0A0D6IET0
G	2	VAL	-	insertion	UNP A0A0D6IET0
G	480	THR	-	expression tag	UNP A0A0D6IET0
G	481	ALA	-	expression tag	UNP A0A0D6IET0
G	482	ALA	-	expression tag	UNP A0A0D6IET0
G	483	ALA	-	expression tag	UNP A0A0D6IET0
G	484	LYS	-	expression tag	UNP A0A0D6IET0
G	485	GLU	-	expression tag	UNP A0A0D6IET0
G	486	ASP	-	expression tag	UNP A0A0D6IET0
G	487	LEU	-	expression tag	UNP A0A0D6IET0
G	488	GLU	-	expression tag	UNP A0A0D6IET0
G	489	HIS	-	expression tag	UNP A0A0D6IET0
G	490	HIS	-	expression tag	UNP A0A0D6IET0
G	491	HIS	-	expression tag	UNP A0A0D6IET0
G	492	HIS	-	expression tag	UNP A0A0D6IET0
G	493	HIS	-	expression tag	UNP A0A0D6IET0
G	494	HIS	-	expression tag	UNP A0A0D6IET0
G	495	HIS	-	expression tag	UNP A0A0D6IET0
G	496	HIS	-	expression tag	UNP A0A0D6IET0
H	2	VAL	-	insertion	UNP A0A0D6IET0
H	480	THR	-	expression tag	UNP A0A0D6IET0
H	481	ALA	-	expression tag	UNP A0A0D6IET0
H	482	ALA	-	expression tag	UNP A0A0D6IET0
H	483	ALA	-	expression tag	UNP A0A0D6IET0
H	484	LYS	-	expression tag	UNP A0A0D6IET0
H	485	GLU	-	expression tag	UNP A0A0D6IET0
H	486	ASP	-	expression tag	UNP A0A0D6IET0
H	487	LEU	-	expression tag	UNP A0A0D6IET0
H	488	GLU	-	expression tag	UNP A0A0D6IET0
H	489	HIS	-	expression tag	UNP A0A0D6IET0
H	490	HIS	-	expression tag	UNP A0A0D6IET0
H	491	HIS	-	expression tag	UNP A0A0D6IET0

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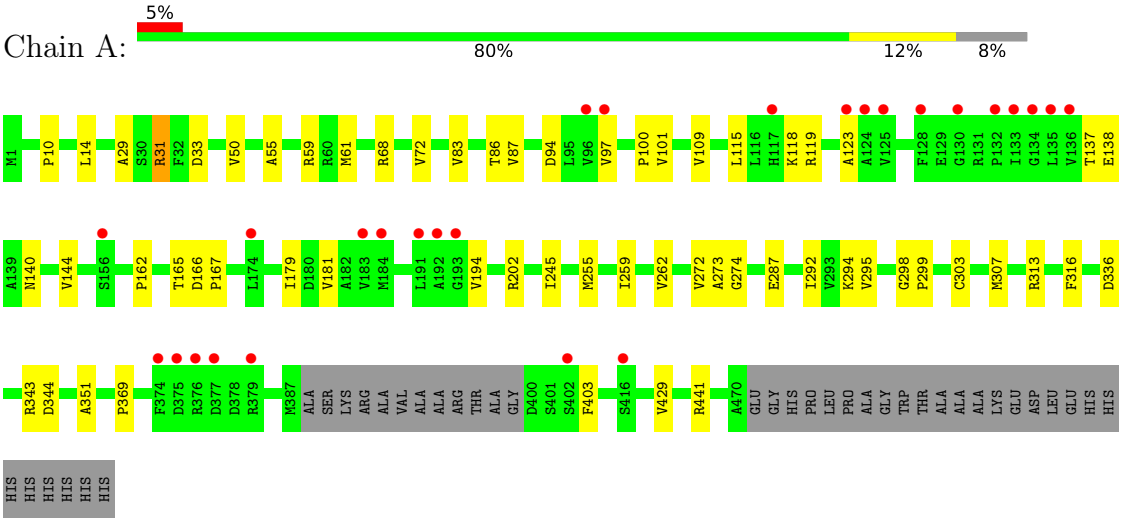
Chain	Residue	Modelled	Actual	Comment	Reference
H	492	HIS	-	expression tag	UNP A0A0D6IET0
H	493	HIS	-	expression tag	UNP A0A0D6IET0
H	494	HIS	-	expression tag	UNP A0A0D6IET0
H	495	HIS	-	expression tag	UNP A0A0D6IET0
H	496	HIS	-	expression tag	UNP A0A0D6IET0

3 Residue-property plots (i)

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 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.

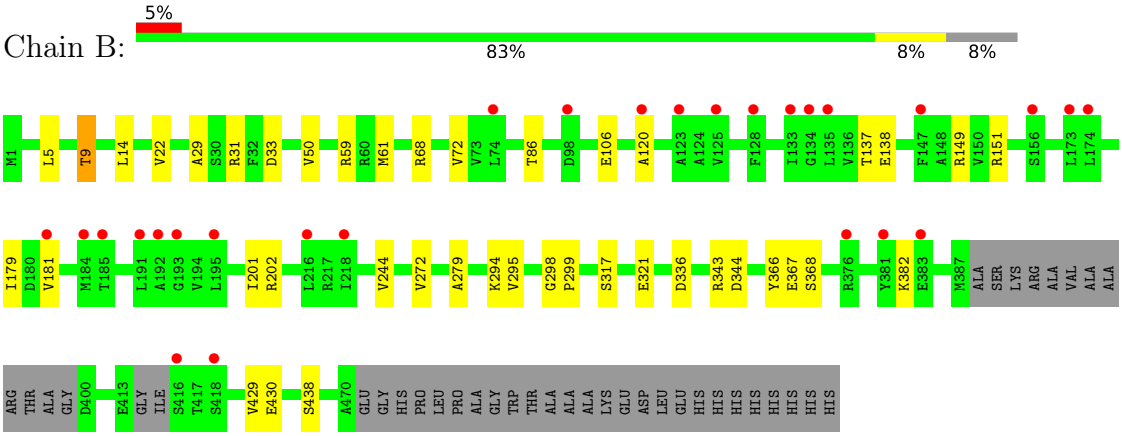
• Molecule 1: Guanosine 5'-monophosphate reductase

Chain A:



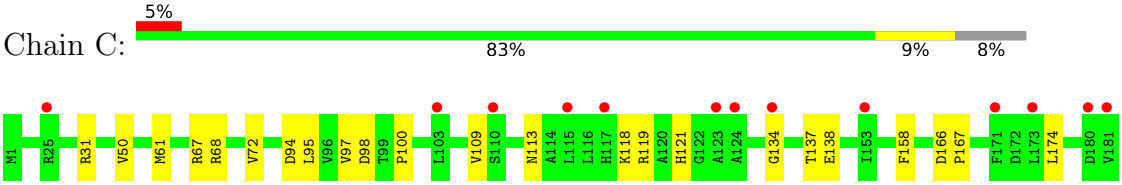
• Molecule 1: Guanosine 5'-monophosphate reductase

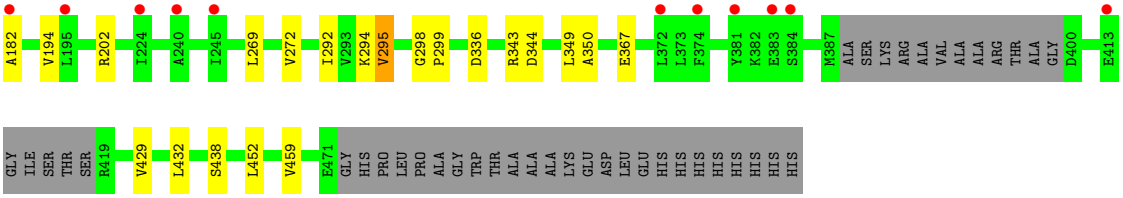
Chain B:



• Molecule 1: Guanosine 5'-monophosphate reductase

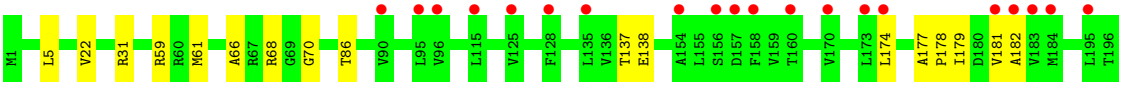
Chain C:

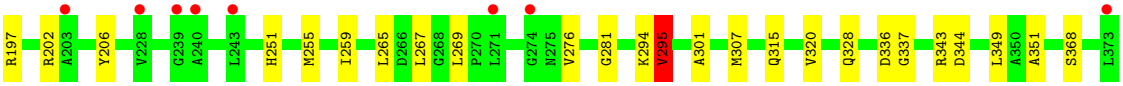


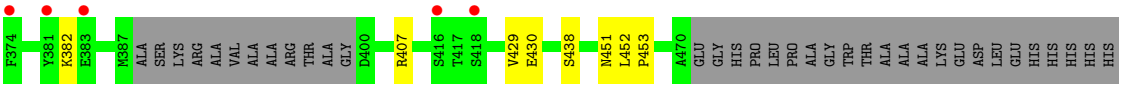


• Molecule 1: Guanosine 5'-monophosphate reductase

Chain D:

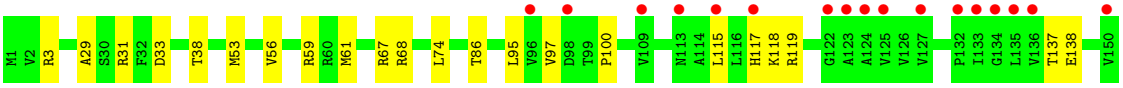


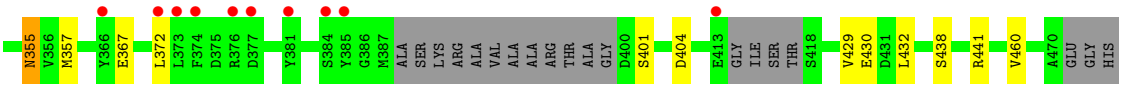




• Molecule 1: Guanosine 5'-monophosphate reductase

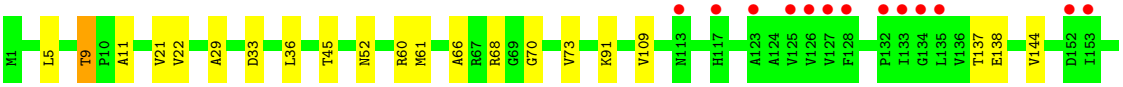
Chain E:

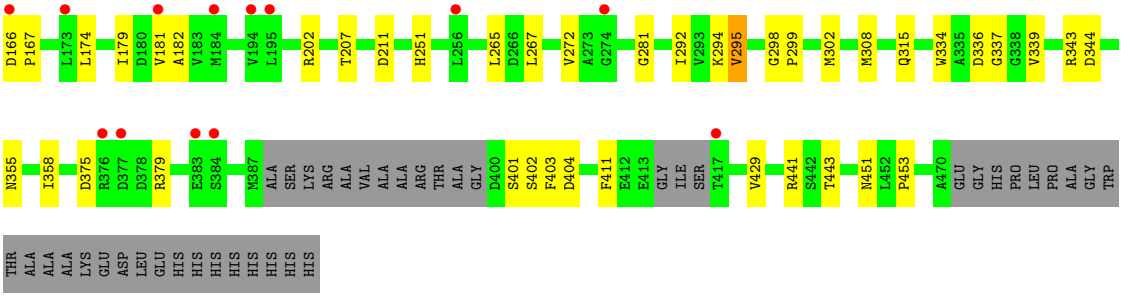




• Molecule 1: Guanosine 5'-monophosphate reductase

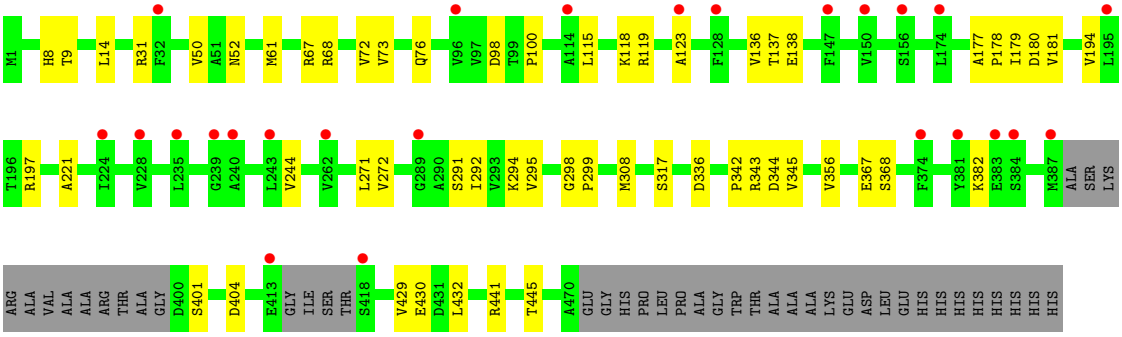
Chain F:





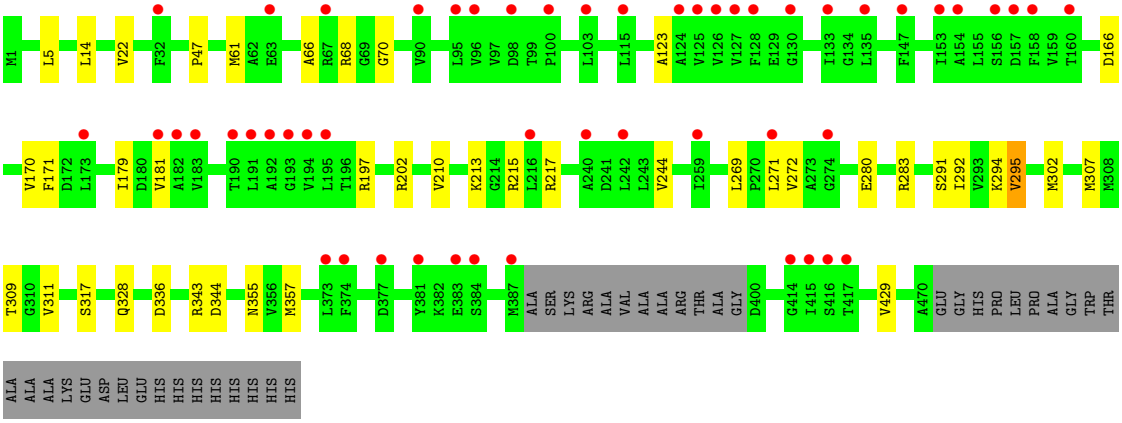
• Molecule 1: Guanosine 5'-monophosphate reductase

Chain G:



• Molecule 1: Guanosine 5'-monophosphate reductase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	253.06Å 109.83Å 200.82Å 90.00° 119.43° 90.00°	Depositor
Resolution (Å)	43.73 – 2.80 49.15 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.73-2.80) 100.0 (49.15-2.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.234 , 0.275 0.237 , 0.276	Depositor DCC
R_{free} test set	5908 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	99.5	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	25837	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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

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	0.52	1/3288 (0.0%)	0.65	3/4497 (0.1%)
1	B	0.44	0/3296	0.60	0/4502
1	C	0.45	0/3280	0.60	0/4481
1	D	0.47	0/3296	0.64	0/4505
1	E	0.55	1/3280 (0.0%)	0.70	0/4480
1	F	0.52	0/3277	0.69	0/4478
1	G	0.47	0/3259	0.60	0/4456
1	H	0.44	0/3287	0.60	0/4496
All	All	0.48	2/26263 (0.0%)	0.63	3/35895 (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	2
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	2
1	F	0	1
1	H	0	1
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	303	CYS	CB-SG	5.74	1.92	1.82
1	E	303	CYS	CB-SG	5.16	1.91	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	274	GLY	N-CA-C	5.65	127.23	113.10
1	A	31	ARG	NE-CZ-NH2	5.61	123.10	120.30
1	A	313	ARG	NE-CZ-NH1	-5.29	117.66	120.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	273	ALA	Peptide
1	A	295	VAL	Peptide
1	B	295	VAL	Peptide
1	C	295	VAL	Peptide
1	D	295	VAL	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	3234	0	3141	35	0
1	B	3243	0	3162	29	0
1	C	3227	0	3140	24	0
1	D	3243	0	3159	33	0
1	E	3227	0	3143	38	0
1	F	3224	0	3140	48	0
1	G	3206	0	3109	38	0
1	H	3233	0	3136	27	0
All	All	25837	0	25130	251	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 251 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:343:ARG:NH1	1:A:344:ASP:OD1	2.06	0.87
1:C:343:ARG:NH1	1:C:344:ASP:OD1	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:343:ARG:NH1	1:H:344:ASP:OD1	2.10	0.83
1:E:61:MET:HE1	1:E:429:VAL:HG21	1.60	0.82
1:D:343:ARG:NH1	1:D:344:ASP:OD1	2.15	0.79

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	454/496 (92%)	448 (99%)	6 (1%)	0	100	100
1	B	450/496 (91%)	443 (98%)	7 (2%)	0	100	100
1	C	448/496 (90%)	441 (98%)	7 (2%)	0	100	100
1	D	454/496 (92%)	447 (98%)	7 (2%)	0	100	100
1	E	448/496 (90%)	441 (98%)	7 (2%)	0	100	100
1	F	449/496 (90%)	441 (98%)	8 (2%)	0	100	100
1	G	448/496 (90%)	441 (98%)	7 (2%)	0	100	100
1	H	454/496 (92%)	446 (98%)	8 (2%)	0	100	100
All	All	3605/3968 (91%)	3548 (98%)	57 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	323/372 (87%)	323 (100%)	0	100	100
1	B	325/372 (87%)	324 (100%)	1 (0%)	92	98
1	C	322/372 (87%)	320 (99%)	2 (1%)	86	96
1	D	324/372 (87%)	322 (99%)	2 (1%)	86	96
1	E	323/372 (87%)	318 (98%)	5 (2%)	65	89
1	F	322/372 (87%)	319 (99%)	3 (1%)	78	94
1	G	319/372 (86%)	318 (100%)	1 (0%)	92	98
1	H	322/372 (87%)	319 (99%)	3 (1%)	78	94
All	All	2580/2976 (87%)	2563 (99%)	17 (1%)	84	95

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	269	LEU
1	H	302	MET
1	E	333	VAL
1	E	343	ARG
1	E	355	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	315	GLN
1	F	315	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 monosaccharides 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

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	458/496 (92%)	0.27	27 (5%) 22 14	66, 104, 160, 176	0
1	B	456/496 (91%)	0.30	27 (5%) 22 14	73, 119, 156, 178	0
1	C	454/496 (91%)	0.40	24 (5%) 26 17	68, 118, 158, 170	0
1	D	458/496 (92%)	0.34	33 (7%) 15 8	66, 108, 168, 188	0
1	E	454/496 (91%)	0.40	42 (9%) 8 4	61, 98, 162, 185	0
1	F	455/496 (91%)	0.39	26 (5%) 23 15	65, 100, 162, 188	0
1	G	454/496 (91%)	0.34	25 (5%) 25 16	63, 118, 155, 174	0
1	H	458/496 (92%)	0.55	52 (11%) 5 3	66, 123, 174, 190	0
All	All	3647/3968 (91%)	0.37	256 (7%) 16 9	61, 112, 163, 190	0

The worst 5 of 256 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	383	GLU	9.1
1	F	133	ILE	7.1
1	C	384	SER	7.0
1	F	195	LEU	6.7
1	E	133	ILE	6.6

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.