



# Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

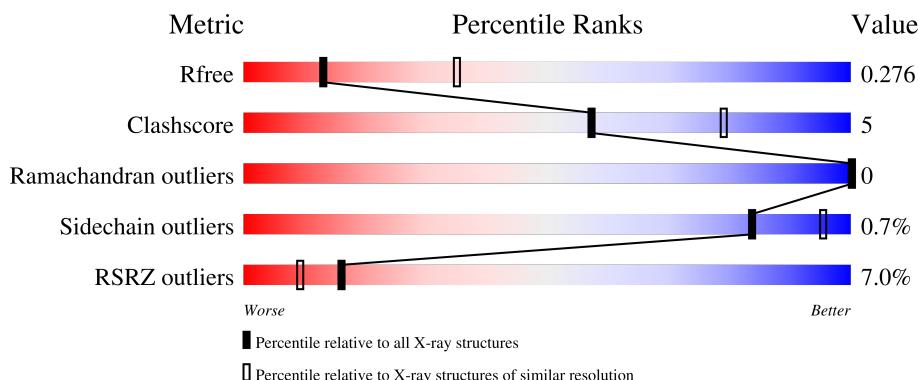
# 1 Overall quality at a glance

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  $\geq 3$ , 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  $\leq 5\%$ . 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.



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Mol	Chain	Length	Quality of chain			
1	F	496	5%	79%	12%	8%
1	G	496	5%	80%	11%	8%
1	H	496	10%	84%	8%	8%

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

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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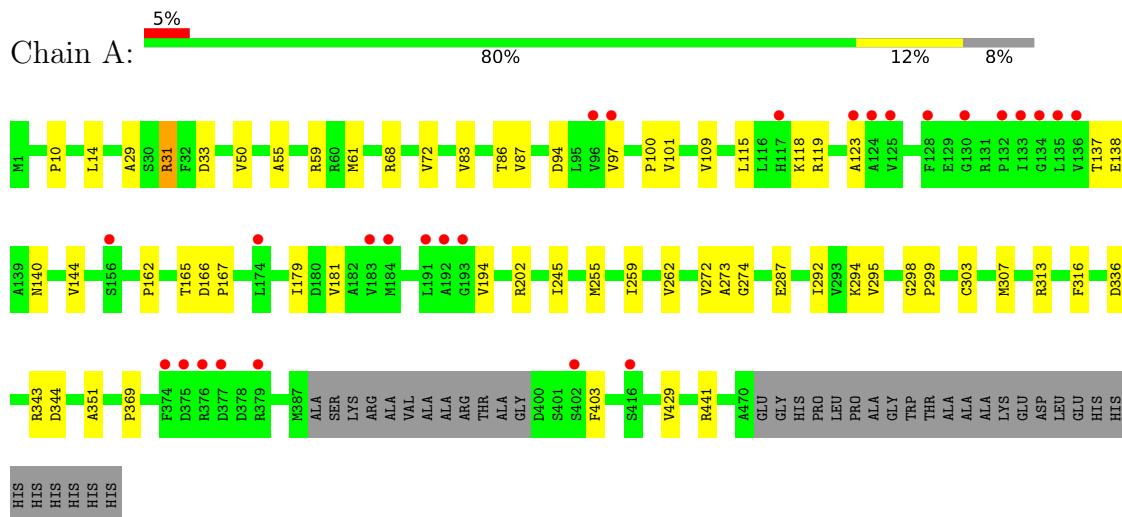
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Chain	Residue	Modelled	Actual	Comment	Reference
H	492	HIS	-	expression tag	UNP A0A0D6IET0
H	493	HIS	-	expression tag	UNP A0A0D6IET0
H	494	HIS	-	expression tag	UNP A0A0D6IET0
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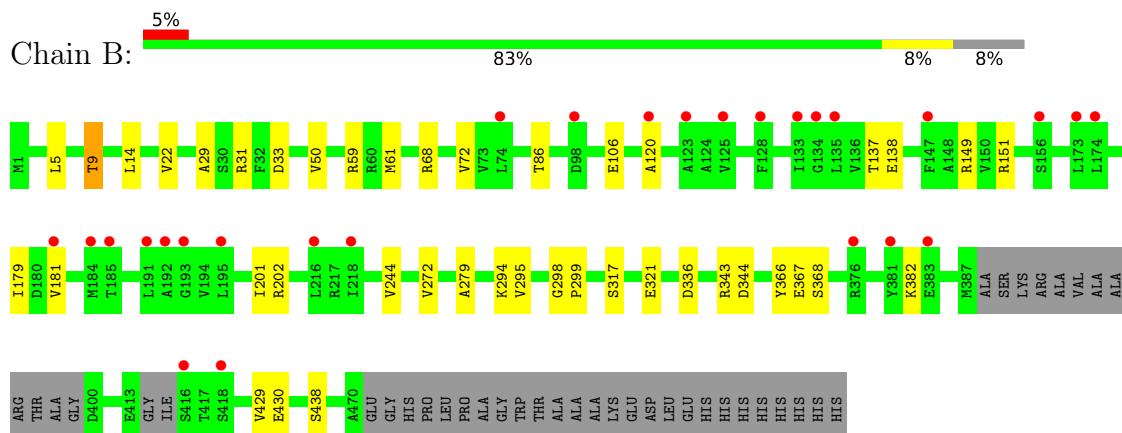
### 3 Residue-property plots

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 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.

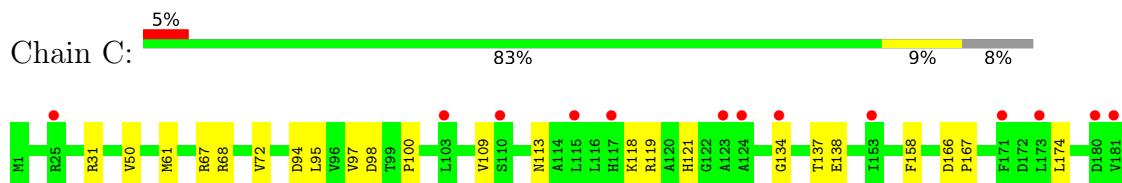
- Molecule 1: Guanosine 5'-monophosphate reductase

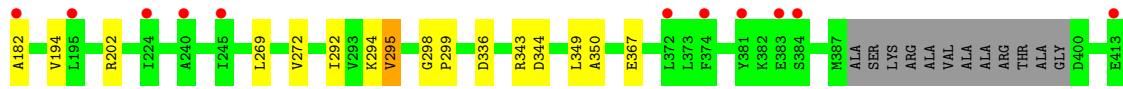


- Molecule 1: Guanosine 5'-monophosphate reductase

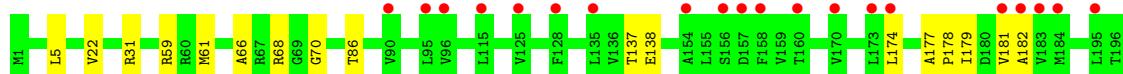
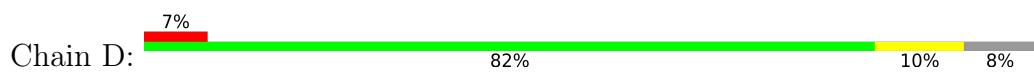


- Molecule 1: Guanosine 5'-monophosphate reductase

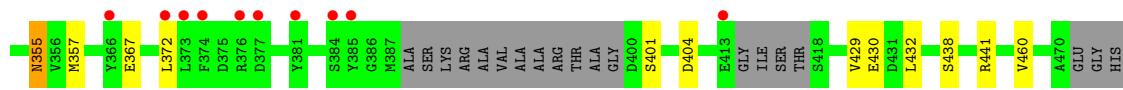
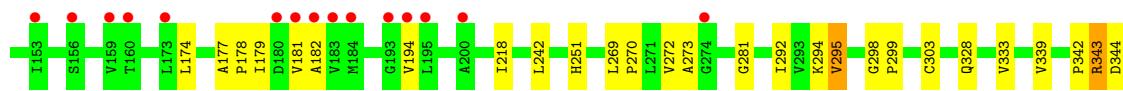
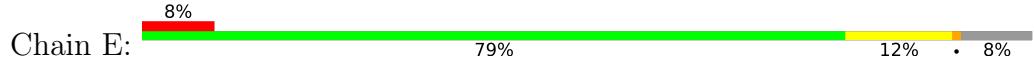




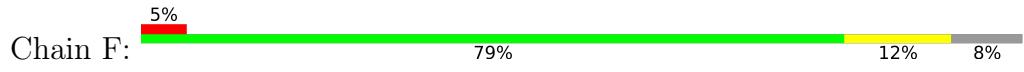
- Molecule 1: Guanosine 5'-monophosphate reductase

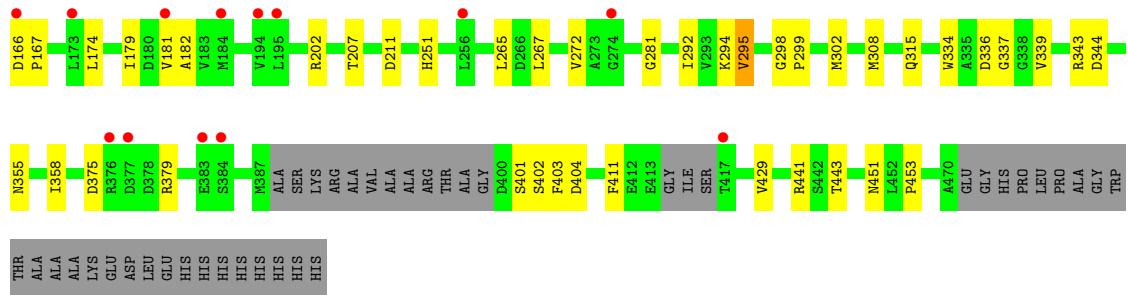


- Molecule 1: Guanosine 5'-monophosphate reductase

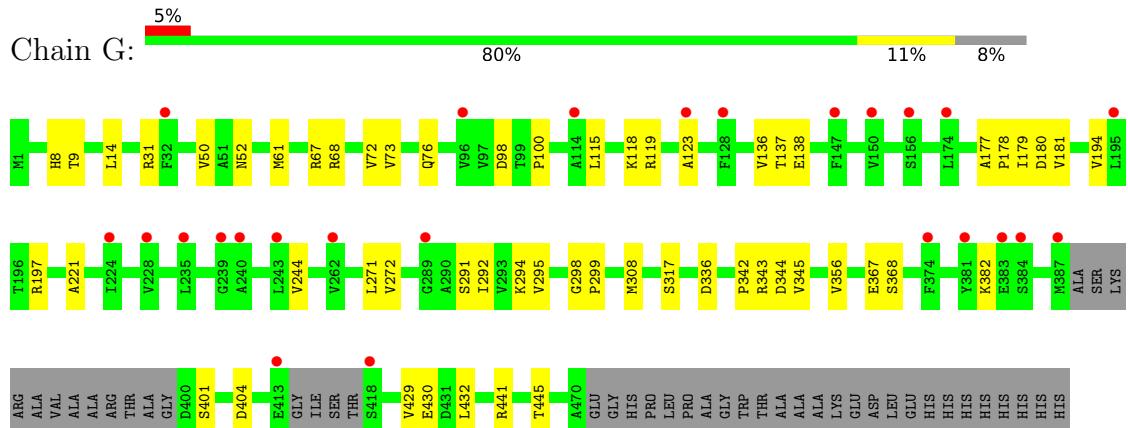


- Molecule 1: Guanosine 5'-monophosphate reductase

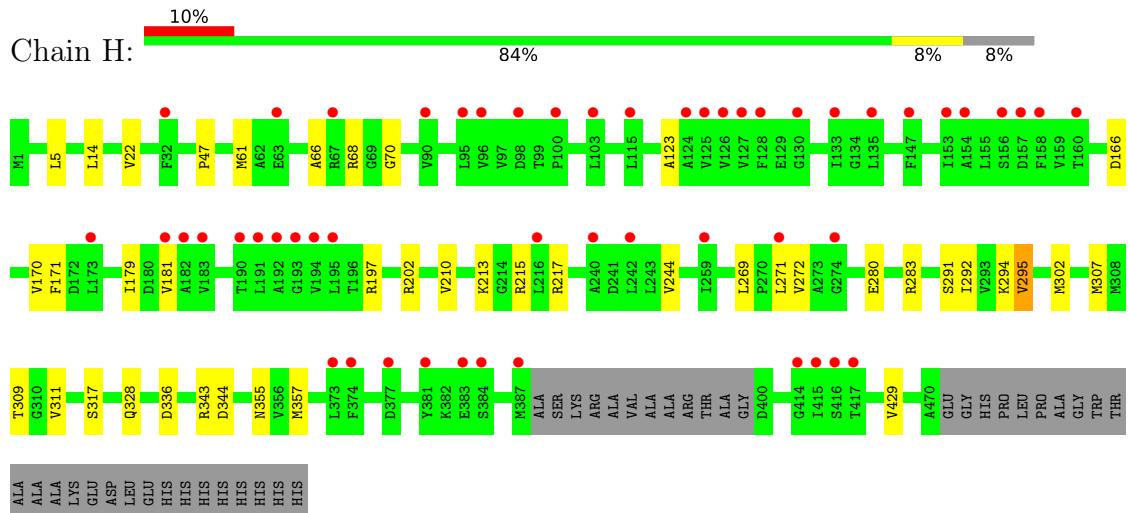




- Molecule 1: Guanosine 5'-monophosphate reductase



- Molecule 1: Guanosine 5'-monophosphate reductase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$< I/\sigma(I) >$ <sup>1</sup>	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 <sup>2</sup> )	99.5	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.51$ , $< L^2 > = 0.34$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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	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(°)	Ideal(°)
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.

All (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
1	E	273	ALA	Peptide
1	E	295	VAL	Peptide
1	F	295	VAL	Peptide
1	H	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.

All (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
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
1:G:61:MET:HE1	1:G:429:VAL:HG21	1.66	0.78
1:B:31:ARG:NH1	1:B:438:SER:OG	2.18	0.76
1:E:343:ARG:NH1	1:E:344:ASP:OD1	2.19	0.75
1:B:343:ARG:NH1	1:B:344:ASP:OD1	2.21	0.73
1:E:31:ARG:HB3	1:E:441:ARG:HB3	1.71	0.71
1:D:61:MET:HE1	1:D:429:VAL:HG21	1.71	0.71
1:C:61:MET:HE1	1:C:429:VAL:HG21	1.73	0.71
1:B:9:THR:HG23	1:H:328:GLN:HG3	1.72	0.70
1:D:294:LYS:HG2	1:D:336:ASP:HB2	1.72	0.70
1:D:68:ARG:NH1	1:D:430:GLU:OE2	2.24	0.69
1:G:244:VAL:HG22	1:G:272:VAL:HB	1.76	0.67
1:G:294:LYS:HG2	1:G:336:ASP:HB2	1.76	0.67
1:G:343:ARG:NH1	1:G:344:ASP:OD1	2.27	0.67
1:A:59:ARG:HG2	1:A:86:THR:HG23	1.76	0.67
1:E:68:ARG:NH1	1:E:430:GLU:OE2	2.28	0.65
1:B:68:ARG:NH1	1:B:430:GLU:OE2	2.28	0.65
1:B:59:ARG:HG2	1:B:86:THR:HG23	1.79	0.65
1:B:294:LYS:HG2	1:B:336:ASP:HB2	1.79	0.65
1:B:61:MET:HE1	1:B:429:VAL:HG21	1.80	0.63
1:B:368:SER:O	1:B:382:LYS:NZ	2.30	0.62
1:G:67:ARG:NH1	1:G:98:ASP:HA	2.13	0.62
1:F:343:ARG:NH1	1:F:344:ASP:OD1	2.31	0.62
1:C:367:GLU:N	1:C:367:GLU:OE1	2.32	0.62
1:D:368:SER:O	1:D:382:LYS:NZ	2.32	0.62
1:H:294:LYS:HG2	1:H:336:ASP:HB2	1.80	0.62
1:G:401:SER:HB2	1:G:404:ASP:HB2	1.81	0.61
1:B:9:THR:CG2	1:H:328:GLN:HG3	2.31	0.60
1:A:294:LYS:HG2	1:A:336:ASP:HB2	1.83	0.60
1:D:328:GLN:HG3	1:F:9:THR:HG23	1.82	0.60
1:C:31:ARG:NH1	1:C:438:SER:OG	2.35	0.60
1:C:119:ARG:HB3	1:C:121:HIS:CD2	2.37	0.59
1:E:429:VAL:HA	1:E:432:LEU:HD23	1.86	0.58
1:G:14:LEU:H	1:G:317:SER:HB2	1.69	0.58
1:B:5:LEU:HD11	1:B:22:VAL:HG21	1.85	0.58
1:E:31:ARG:NH1	1:E:438:SER:OG	2.36	0.58
1:D:61:MET:CE	1:D:429:VAL:HG21	2.34	0.58
1:H:14:LEU:H	1:H:317:SER:HB2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:272:VAL:HG22	1:F:292:ILE:HB	1.85	0.57
1:F:91:LYS:NZ	1:F:211:ASP:OD2	2.36	0.57
1:F:61:MET:HE1	1:F:429:VAL:HG11	1.85	0.57
1:F:68:ARG:HH11	1:F:202:ARG:CB	2.18	0.56
1:E:74:LEU:HD11	1:E:218:ILE:HD11	1.87	0.56
1:F:411:PHE:CE2	1:G:441:ARG:HD2	2.41	0.56
1:A:61:MET:HE1	1:A:429:VAL:HG21	1.85	0.56
1:C:100:PRO:HG3	1:C:194:VAL:HG13	1.88	0.55
1:E:272:VAL:HG22	1:E:292:ILE:HB	1.89	0.55
1:F:60:ARG:HG3	1:F:60:ARG:HH11	1.73	0.54
1:A:50:VAL:HB	1:A:72:VAL:HG22	1.90	0.54
1:B:14:LEU:H	1:B:317:SER:HB2	1.72	0.54
1:A:94:ASP:OD2	1:A:97:VAL:N	2.40	0.53
1:F:315:GLN:NE2	1:F:337:GLY:H	2.07	0.53
1:D:5:LEU:HD11	1:D:22:VAL:HG21	1.91	0.53
1:F:68:ARG:HH11	1:F:202:ARG:CG	2.22	0.53
1:E:100:PRO:HG3	1:E:194:VAL:HG13	1.90	0.53
1:E:174:LEU:HD11	1:E:182:ALA:HB2	1.91	0.53
1:F:36:LEU:HD22	1:F:441:ARG:NH1	2.24	0.53
1:E:115:LEU:HD23	1:E:118:LYS:HD2	1.90	0.52
1:H:294:LYS:HD2	1:H:357:MET:SD	2.49	0.52
1:A:100:PRO:HG3	1:A:194:VAL:HG13	1.91	0.52
1:H:5:LEU:HD11	1:H:22:VAL:HG21	1.92	0.52
1:A:10:PRO:HG2	1:A:14:LEU:HD21	1.92	0.52
1:B:9:THR:HG21	1:H:328:GLN:HA	1.90	0.52
1:G:179:ILE:HG22	1:G:181:VAL:H	1.74	0.52
1:C:118:LYS:O	1:C:119:ARG:HG2	2.10	0.52
1:B:179:ILE:HG22	1:B:181:VAL:H	1.75	0.52
1:F:294:LYS:HG2	1:F:336:ASP:HB2	1.91	0.51
1:F:343:ARG:HB3	1:H:307:MET:O	2.10	0.51
1:G:271:LEU:H	1:G:291:SER:HB3	1.74	0.51
1:B:106:GLU:OE2	1:B:151:ARG:NH2	2.43	0.51
1:F:66:ALA:HA	1:F:70:GLY:O	2.10	0.51
1:C:294:LYS:HG2	1:C:336:ASP:HB2	1.92	0.51
1:E:100:PRO:HD3	1:E:194:VAL:HG22	1.93	0.51
1:E:401:SER:HB2	1:E:404:ASP:HB2	1.93	0.51
1:F:251:HIS:CD2	1:F:281:GLY:HA2	2.46	0.51
1:G:31:ARG:HB3	1:G:441:ARG:HB3	1.93	0.51
1:F:179:ILE:HG22	1:F:181:VAL:H	1.76	0.51
1:A:31:ARG:HB3	1:A:441:ARG:HB3	1.92	0.51
1:E:59:ARG:HG2	1:E:86:THR:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:ARG:HG2	1:D:86:THR:HG23	1.94	0.50
1:G:61:MET:HE1	1:G:429:VAL:CG2	2.41	0.50
1:A:179:ILE:HG22	1:A:181:VAL:H	1.76	0.50
1:D:251:HIS:CD2	1:D:281:GLY:HA2	2.46	0.50
1:G:441:ARG:O	1:G:445:THR:HG23	2.11	0.50
1:G:118:LYS:O	1:G:119:ARG:HG2	2.12	0.50
1:A:83:VAL:O	1:A:87:VAL:HG23	2.12	0.49
1:E:61:MET:CE	1:E:429:VAL:HG21	2.37	0.49
1:E:367:GLU:OE1	1:E:367:GLU:N	2.42	0.49
1:G:68:ARG:NH1	1:G:430:GLU:OE2	2.46	0.49
1:A:101:VAL:HG11	1:A:115:LEU:HB3	1.94	0.49
1:A:272:VAL:HG22	1:A:292:ILE:HB	1.93	0.49
1:F:265:LEU:HB2	1:F:267:LEU:HD11	1.95	0.49
1:H:179:ILE:HG22	1:H:181:VAL:H	1.76	0.49
1:A:118:LYS:O	1:A:119:ARG:HG2	2.13	0.49
1:C:137:THR:HG22	1:C:138:GLU:N	2.28	0.49
1:G:298:GLY:N	1:G:299:PRO:HD3	2.28	0.48
1:E:29:ALA:HB3	1:E:33:ASP:OD2	2.12	0.48
1:E:343:ARG:HG3	1:E:343:ARG:HH11	1.78	0.48
1:F:68:ARG:HH11	1:F:202:ARG:HG2	1.77	0.48
1:F:315:GLN:HE22	1:F:337:GLY:H	1.61	0.48
1:A:403:PHE:HE2	1:D:197:ARG:HH21	1.59	0.48
1:B:29:ALA:HB3	1:B:33:ASP:OD2	2.14	0.48
1:D:265:LEU:HB2	1:D:267:LEU:HD11	1.95	0.48
1:C:272:VAL:HG22	1:C:292:ILE:HB	1.95	0.48
1:C:174:LEU:HD11	1:C:182:ALA:HB2	1.95	0.48
1:G:345:VAL:HG13	1:G:356:VAL:HG21	1.95	0.48
1:F:5:LEU:HD11	1:F:22:VAL:HG21	1.95	0.48
1:G:61:MET:CE	1:G:429:VAL:HG21	2.40	0.48
1:A:68:ARG:HH11	1:A:202:ARG:HG2	1.79	0.47
1:E:118:LYS:O	1:E:119:ARG:HG2	2.14	0.47
1:F:21:VAL:HB	1:H:311:VAL:HG22	1.96	0.47
1:H:280:GLU:HA	1:H:283:ARG:NH1	2.29	0.47
1:A:137:THR:HG22	1:A:138:GLU:N	2.29	0.47
1:D:328:GLN:HG3	1:F:9:THR:CG2	2.44	0.47
1:A:140:ASN:N	1:A:140:ASN:OD1	2.47	0.47
1:D:315:GLN:NE2	1:D:337:GLY:H	2.12	0.47
1:F:137:THR:HG22	1:F:138:GLU:H	1.80	0.47
1:C:109:VAL:O	1:C:113:ASN:N	2.41	0.47
1:B:137:THR:HG22	1:B:138:GLU:H	1.79	0.47
1:F:61:MET:HE2	1:F:429:VAL:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:ARG:HG3	1:C:95:LEU:O	2.15	0.47
1:D:179:ILE:HG22	1:D:181:VAL:H	1.80	0.47
1:G:52:ASN:HB3	1:G:73:VAL:CG1	2.45	0.47
1:H:213:LYS:HD2	1:H:215:ARG:CZ	2.45	0.47
1:F:375:ASP:OD1	1:F:379:ARG:N	2.39	0.46
1:C:50:VAL:HB	1:C:72:VAL:HG22	1.96	0.46
1:C:137:THR:HG22	1:C:138:GLU:H	1.80	0.46
1:H:210:VAL:O	1:H:217:ARG:NE	2.48	0.46
1:A:137:THR:HG22	1:A:138:GLU:H	1.80	0.46
1:E:251:HIS:CD2	1:E:281:GLY:HA2	2.50	0.46
1:D:301:ALA:O	1:D:307:MET:HE2	2.16	0.46
1:A:123:ALA:HB3	1:A:181:VAL:HG21	1.98	0.46
1:C:68:ARG:NH1	1:C:202:ARG:HG2	2.31	0.46
1:F:109:VAL:HG11	1:F:144:VAL:HG13	1.98	0.46
1:F:251:HIS:NE2	1:F:281:GLY:HA2	2.31	0.45
1:H:271:LEU:H	1:H:291:SER:HB3	1.80	0.45
1:F:137:THR:HG22	1:F:138:GLU:N	2.32	0.45
1:G:180:ASP:OD1	1:G:197:ARG:HG3	2.16	0.45
1:C:67:ARG:NH1	1:C:98:ASP:HA	2.32	0.45
1:C:350:ALA:HB1	1:C:459:VAL:HG21	1.99	0.45
1:B:137:THR:HG22	1:B:138:GLU:N	2.32	0.45
1:G:123:ALA:HA	1:G:136:VAL:O	2.16	0.45
1:D:320:VAL:HG23	1:D:351:ALA:HB1	1.98	0.45
1:E:242:LEU:HG	1:E:270:PRO:HB2	1.97	0.45
1:F:174:LEU:HD11	1:F:182:ALA:HB2	1.99	0.45
1:G:115:LEU:HD23	1:G:118:LYS:HD2	1.99	0.45
1:D:202:ARG:O	1:D:206:TYR:N	2.42	0.44
1:F:334:TRP:NE1	1:F:355:ASN:HB2	2.33	0.44
1:G:100:PRO:HG3	1:G:194:VAL:HG13	1.99	0.44
1:B:367:GLU:OE1	1:B:367:GLU:N	2.49	0.44
1:F:343:ARG:HE	1:H:307:MET:CE	2.31	0.44
1:A:61:MET:CE	1:A:429:VAL:HG21	2.47	0.44
1:E:61:MET:HE1	1:E:429:VAL:CG2	2.40	0.44
1:G:244:VAL:HG22	1:G:272:VAL:CB	2.46	0.44
1:E:137:THR:HG22	1:E:138:GLU:N	2.33	0.44
1:E:401:SER:CB	1:E:404:ASP:HB2	2.47	0.44
1:F:61:MET:CE	1:F:429:VAL:HG11	2.48	0.44
1:G:367:GLU:OE1	1:G:367:GLU:N	2.47	0.44
1:B:298:GLY:N	1:B:299:PRO:HD3	2.31	0.44
1:G:52:ASN:HB3	1:G:73:VAL:HG12	1.99	0.44
1:A:316:PHE:CE1	1:A:351:ALA:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:HIS:HB3	1:E:372:LEU:HD23	1.99	0.44
1:F:11:ALA:HB1	1:G:9:THR:H	1.83	0.44
1:A:162:PRO:O	1:A:165:THR:OG1	2.27	0.44
1:A:255:MET:O	1:A:259:ILE:HG13	2.17	0.44
1:D:177:ALA:HA	1:D:178:PRO:HD3	1.81	0.44
1:F:52:ASN:HB3	1:F:73:VAL:CG1	2.48	0.43
1:D:328:GLN:HA	1:F:9:THR:HG21	2.00	0.43
1:F:52:ASN:HB3	1:F:73:VAL:HG12	2.00	0.43
1:B:149:ARG:HA	1:B:149:ARG:HD3	1.70	0.43
1:B:149:ARG:HA	1:B:149:ARG:HH11	1.83	0.43
1:D:137:THR:HG22	1:D:138:GLU:H	1.83	0.43
1:A:55:ALA:O	1:A:369:PRO:HD2	2.18	0.43
1:D:174:LEU:HD11	1:D:182:ALA:HB2	2.01	0.43
1:B:343:ARG:HB3	1:D:307:MET:O	2.19	0.43
1:F:11:ALA:O	1:G:8:HIS:HA	2.19	0.43
1:F:343:ARG:HH21	1:H:307:MET:HE1	1.84	0.43
1:B:68:ARG:NH1	1:B:202:ARG:HG2	2.34	0.43
1:B:279:ALA:HB2	1:B:321:GLU:HG2	2.01	0.43
1:F:29:ALA:HB3	1:F:33:ASP:OD2	2.18	0.43
1:E:298:GLY:N	1:E:299:PRO:HD3	2.34	0.42
1:F:45:THR:HG21	1:F:207:THR:HG22	2.01	0.42
1:D:451:ASN:OD1	1:D:453:PRO:HD2	2.19	0.42
1:E:3:ARG:HE	1:E:460:VAL:HG22	1.85	0.42
1:E:177:ALA:HA	1:E:178:PRO:HD3	1.85	0.42
1:F:451:ASN:OD1	1:F:453:PRO:HD2	2.20	0.42
1:E:339:VAL:O	1:E:339:VAL:HG23	2.20	0.42
1:F:298:GLY:N	1:F:299:PRO:HD3	2.34	0.42
1:F:401:SER:HB3	1:F:404:ASP:HB2	2.01	0.42
1:G:76:GLN:HA	1:G:221:ALA:O	2.18	0.42
1:G:50:VAL:HB	1:G:72:VAL:HG22	2.00	0.42
1:H:47:PRO:HA	1:H:355:ASN:OD1	2.20	0.42
1:C:94:ASP:OD2	1:C:97:VAL:N	2.52	0.42
1:F:402:SER:OG	1:F:403:PHE:N	2.51	0.42
1:G:272:VAL:HG22	1:G:292:ILE:HB	2.01	0.42
1:A:68:ARG:NH1	1:A:202:ARG:HG2	2.35	0.42
1:A:97:VAL:HG13	1:A:194:VAL:O	2.20	0.42
1:G:177:ALA:HA	1:G:178:PRO:HD3	1.96	0.42
1:D:137:THR:HG22	1:D:138:GLU:N	2.34	0.42
1:H:171:PHE:CE2	1:H:197:ARG:HD2	2.54	0.42
1:A:307:MET:CE	1:D:343:ARG:HE	2.33	0.42
1:E:38:THR:HG21	1:E:355:ASN:ND2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:LEU:HD13	1:C:452:LEU:HD22	2.02	0.41
1:F:166:ASP:HA	1:F:167:PRO:HD3	1.95	0.41
1:F:443:THR:OG1	1:H:309:THR:O	2.33	0.41
1:A:287:GLU:OE1	1:E:328:GLN:HG2	2.20	0.41
1:B:120:ALA:HB2	1:B:366:TYR:HD2	1.85	0.41
1:C:432:LEU:HD13	1:C:432:LEU:HA	1.89	0.41
1:D:66:ALA:HA	1:D:70:GLY:O	2.21	0.41
1:E:137:THR:HG22	1:E:138:GLU:H	1.85	0.41
1:G:368:SER:O	1:G:382:LYS:NZ	2.52	0.41
1:H:244:VAL:HA	1:H:272:VAL:HB	2.01	0.41
1:B:50:VAL:HB	1:B:72:VAL:HG22	2.02	0.41
1:D:31:ARG:NH1	1:D:438:SER:OG	2.53	0.41
1:A:202:ARG:HH11	1:A:202:ARG:HD3	1.74	0.41
1:B:244:VAL:HG22	1:B:272:VAL:HB	2.01	0.41
1:D:276:VAL:O	1:D:295:VAL:HG23	2.21	0.41
1:E:53:MET:HB2	1:E:56:VAL:HG23	2.02	0.41
1:E:67:ARG:HG3	1:E:95:LEU:O	2.21	0.41
1:E:342:PRO:HB2	1:G:308:MET:O	2.20	0.41
1:G:137:THR:HG22	1:G:138:GLU:N	2.35	0.41
1:A:29:ALA:HB3	1:A:33:ASP:OD2	2.20	0.41
1:E:179:ILE:HG22	1:E:181:VAL:H	1.85	0.41
1:C:166:ASP:HA	1:C:167:PRO:HD3	1.96	0.41
1:D:255:MET:O	1:D:259:ILE:HG13	2.20	0.41
1:A:166:ASP:HA	1:A:167:PRO:HD3	1.89	0.41
1:D:68:ARG:NH1	1:D:202:ARG:HG2	2.36	0.41
1:H:166:ASP:O	1:H:170:VAL:HG23	2.21	0.41
1:F:339:VAL:HG21	1:F:358:ILE:HG12	2.03	0.41
1:H:66:ALA:HA	1:H:70:GLY:O	2.20	0.41
1:G:61:MET:CE	1:G:429:VAL:HG11	2.51	0.40
1:H:123:ALA:HB3	1:H:181:VAL:HG21	2.03	0.40
1:H:272:VAL:HG22	1:H:292:ILE:HB	2.02	0.40
1:B:201:ILE:HG21	1:D:407:ARG:HA	2.03	0.40
1:H:68:ARG:NH1	1:H:202:ARG:HG2	2.35	0.40
1:C:298:GLY:N	1:C:299:PRO:HD3	2.36	0.40
1:D:349:LEU:HD13	1:D:452:LEU:HD22	2.03	0.40
1:G:432:LEU:HD13	1:G:432:LEU:HA	1.92	0.40
1:H:61:MET:CE	1:H:429:VAL:HG21	2.50	0.40
1:A:109:VAL:HG11	1:A:144:VAL:HG13	2.03	0.40
1:A:245:ILE:HD11	1:A:262:VAL:HG21	2.04	0.40
1:B:294:LYS:HE3	1:B:336:ASP:OD2	2.21	0.40
1:E:97:VAL:HG13	1:E:194:VAL:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:308:MET:O	1:G:342:PRO:HB2	2.22	0.40
1:A:298:GLY:N	1:A:299:PRO:HD3	2.35	0.40
1:C:134:GLY:HA2	1:C:158:PHE:CE2	2.56	0.40
1:E:294:LYS:HD2	1:E:357:MET:SD	2.62	0.40

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

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	9	THR
1	C	269	LEU
1	C	295	VAL
1	D	269	LEU
1	D	295	VAL
1	E	269	LEU
1	E	295	VAL
1	E	333	VAL
1	E	343	ARG
1	E	355	ASN
1	F	9	THR
1	F	295	VAL
1	F	302	MET
1	G	295	VAL
1	H	269	LEU
1	H	295	VAL
1	H	302	MET

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 [\(i\)](#)

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	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

All (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
1	F	134	GLY	6.6
1	H	416	SER	6.4
1	H	153	ILE	6.2
1	H	103	LEU	6.1
1	H	125	VAL	5.9
1	B	383	GLU	5.8
1	H	417	THR	5.7
1	E	173	LEU	5.3
1	H	95	LEU	5.2
1	H	90	VAL	5.2
1	E	124	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
1	H	183	VAL	5.1
1	B	192	ALA	5.0
1	E	384	SER	5.0
1	H	96	VAL	5.0
1	H	384	SER	5.0
1	H	191	LEU	4.9
1	H	414	GLY	4.9
1	G	384	SER	4.9
1	B	191	LEU	4.8
1	F	384	SER	4.8
1	D	174	LEU	4.8
1	E	182	ALA	4.7
1	E	123	ALA	4.6
1	A	124	ALA	4.6
1	F	173	LEU	4.4
1	E	183	VAL	4.3
1	H	127	VAL	4.3
1	D	173	LEU	4.2
1	F	152	ASP	4.0
1	F	376	ARG	4.0
1	E	134	GLY	4.0
1	E	195	LEU	3.9
1	A	125	VAL	3.9
1	H	182	ALA	3.9
1	F	135	LEU	3.9
1	H	130	GLY	3.9
1	G	383	GLU	3.9
1	H	173	LEU	3.9
1	E	136	VAL	3.9
1	D	195	LEU	3.8
1	E	372	LEU	3.8
1	C	181	VAL	3.7
1	E	181	VAL	3.7
1	C	182	ALA	3.6
1	H	128	PHE	3.6
1	A	117	HIS	3.6
1	H	157	ASP	3.6
1	B	98	ASP	3.6
1	G	147	PHE	3.5
1	D	156	SER	3.5
1	C	195	LEU	3.5
1	H	126	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	128	PHE	3.5
1	F	184	MET	3.5
1	H	160	THR	3.4
1	G	156	SER	3.4
1	E	109	VAL	3.4
1	A	183	VAL	3.4
1	D	274	GLY	3.4
1	F	383	GLU	3.3
1	D	170	VAL	3.3
1	E	125	VAL	3.3
1	F	128	PHE	3.3
1	A	135	LEU	3.3
1	B	120	ALA	3.2
1	G	235	LEU	3.2
1	H	158	PHE	3.2
1	A	123	ALA	3.2
1	F	123	ALA	3.2
1	C	372	LEU	3.1
1	D	271	LEU	3.1
1	D	160	THR	3.1
1	A	193	GLY	3.1
1	C	413	GLU	3.1
1	A	416	SER	3.1
1	H	193	GLY	3.1
1	G	228	VAL	3.1
1	H	387	MET	3.1
1	B	123	ALA	3.0
1	E	377	ASP	3.0
1	H	415	ILE	3.0
1	H	156	SER	3.0
1	F	117	HIS	3.0
1	D	181	VAL	3.0
1	B	181	VAL	3.0
1	D	183	VAL	3.0
1	G	240	ALA	3.0
1	H	154	ALA	3.0
1	E	184	MET	3.0
1	F	256	LEU	3.0
1	E	180	ASP	3.0
1	H	274	GLY	2.9
1	G	123	ALA	2.9
1	G	418	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	366	TYR	2.9
1	H	133	ILE	2.9
1	H	190	THR	2.9
1	B	184	MET	2.9
1	A	192	ALA	2.9
1	G	128	PHE	2.9
1	D	418	SER	2.9
1	E	117	HIS	2.9
1	E	381	TYR	2.9
1	F	181	VAL	2.9
1	C	25	ARG	2.9
1	B	133	ILE	2.9
1	E	127	VAL	2.9
1	H	100	PRO	2.8
1	D	182	ALA	2.8
1	H	192	ALA	2.8
1	A	128	PHE	2.8
1	B	135	LEU	2.8
1	B	418	SER	2.8
1	E	113	ASN	2.8
1	A	376	ARG	2.8
1	A	156	SER	2.8
1	E	156	SER	2.8
1	E	374	PHE	2.8
1	F	377	ASP	2.8
1	E	376	ARG	2.8
1	C	245	ILE	2.8
1	E	153	ILE	2.8
1	C	153	ILE	2.7
1	E	132	PRO	2.7
1	B	195	LEU	2.7
1	A	174	LEU	2.7
1	B	193	GLY	2.7
1	B	128	PHE	2.7
1	D	158	PHE	2.7
1	F	113	ASN	2.7
1	D	240	ALA	2.7
1	E	122	GLY	2.7
1	F	126	VAL	2.7
1	H	216	LEU	2.7
1	C	240	ALA	2.7
1	E	385	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	115	LEU	2.7
1	E	160	THR	2.7
1	G	239	GLY	2.7
1	C	124	ALA	2.6
1	H	124	ALA	2.6
1	D	374	PHE	2.6
1	C	117	HIS	2.6
1	D	373	LEU	2.6
1	G	96	VAL	2.6
1	A	133	ILE	2.6
1	E	115	LEU	2.6
1	A	136	VAL	2.6
1	B	156	SER	2.6
1	D	383	GLU	2.6
1	F	125	VAL	2.6
1	G	262	VAL	2.6
1	G	32	PHE	2.6
1	D	90	VAL	2.5
1	E	135	LEU	2.5
1	E	413	GLU	2.5
1	H	63	GLU	2.5
1	G	374	PHE	2.5
1	C	123	ALA	2.5
1	A	402	SER	2.5
1	B	173	LEU	2.5
1	A	97	VAL	2.5
1	D	228	VAL	2.5
1	B	134	GLY	2.5
1	C	103	LEU	2.5
1	H	373	LEU	2.5
1	D	95	LEU	2.4
1	H	147	PHE	2.4
1	E	150	VAL	2.4
1	G	243	LEU	2.4
1	D	157	ASP	2.4
1	C	110	SER	2.3
1	C	171	PHE	2.3
1	F	274	GLY	2.3
1	A	184	MET	2.3
1	B	376	ARG	2.3
1	C	134	GLY	2.3
1	A	96	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	218	ILE	2.3
1	E	373	LEU	2.3
1	F	417	THR	2.3
1	H	135	LEU	2.3
1	A	132	PRO	2.3
1	F	132	PRO	2.3
1	A	191	LEU	2.3
1	C	173	LEU	2.3
1	H	181	VAL	2.3
1	B	381	TYR	2.3
1	C	374	PHE	2.3
1	A	377	ASP	2.3
1	G	114	ALA	2.3
1	F	153	ILE	2.3
1	G	174	LEU	2.3
1	D	243	LEU	2.3
1	G	387	MET	2.3
1	G	413	GLU	2.3
1	A	134	GLY	2.3
1	D	203	ALA	2.3
1	E	200	ALA	2.2
1	H	194	VAL	2.2
1	B	216	LEU	2.2
1	A	379	ARG	2.2
1	D	96	VAL	2.2
1	E	194	VAL	2.2
1	F	194	VAL	2.2
1	G	289	GLY	2.2
1	H	195	LEU	2.2
1	H	381	TYR	2.2
1	E	193	GLY	2.2
1	B	416	SER	2.2
1	C	381	TYR	2.2
1	C	224	ILE	2.2
1	G	381	TYR	2.2
1	C	180	ASP	2.2
1	A	374	PHE	2.2
1	H	383	GLU	2.2
1	D	239	GLY	2.2
1	H	271	LEU	2.2
1	G	224	ILE	2.2
1	H	259	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	159	VAL	2.1
1	B	74	LEU	2.1
1	B	147	PHE	2.1
1	B	174	LEU	2.1
1	H	32	PHE	2.1
1	H	374	PHE	2.1
1	A	375	ASP	2.1
1	D	115	LEU	2.1
1	D	154	ALA	2.1
1	G	195	LEU	2.1
1	A	130	GLY	2.1
1	F	166	ASP	2.1
1	B	125	VAL	2.1
1	G	150	VAL	2.1
1	C	115	LEU	2.1
1	F	127	VAL	2.1
1	H	67	ARG	2.1
1	H	242	LEU	2.1
1	D	184	MET	2.1
1	D	135	LEU	2.1
1	H	98	ASP	2.1
1	E	96	VAL	2.0
1	E	98	ASP	2.0
1	E	274	GLY	2.0
1	B	185	THR	2.0
1	D	125	VAL	2.0
1	D	381	TYR	2.0
1	H	377	ASP	2.0
1	D	416	SER	2.0
1	H	240	ALA	2.0

## 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 monosaccharides 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.