



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:26 AM UTC

PDB ID : 7OY9 / pdb_00007oy9
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

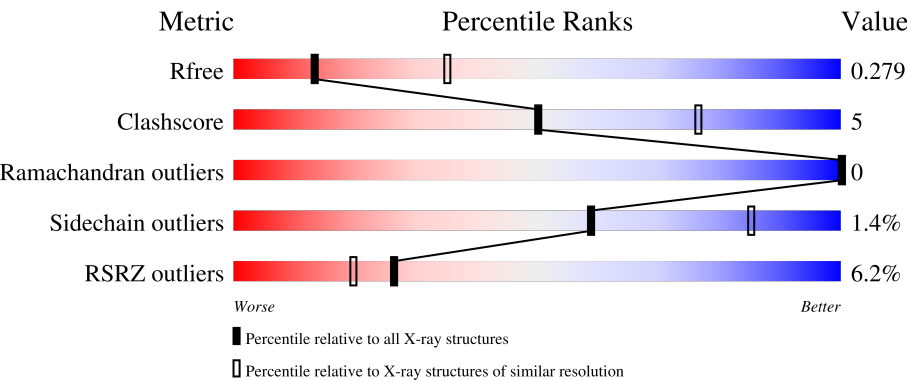
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	496	4% 80% 12% 8%
1	B	496	4% 82% 9% 8%
1	C	496	7% 81% 10% 8%
1	D	496	5% 81% 11% 8%
1	E	496	7% 78% 12% 8%

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Mol	Chain	Length	Quality of chain
1	F	496	 5% 77% 15% 8%
1	G	496	 6% 79% 12% 8%
1	H	496	 8% 82% 10% 8%

2 Entry composition

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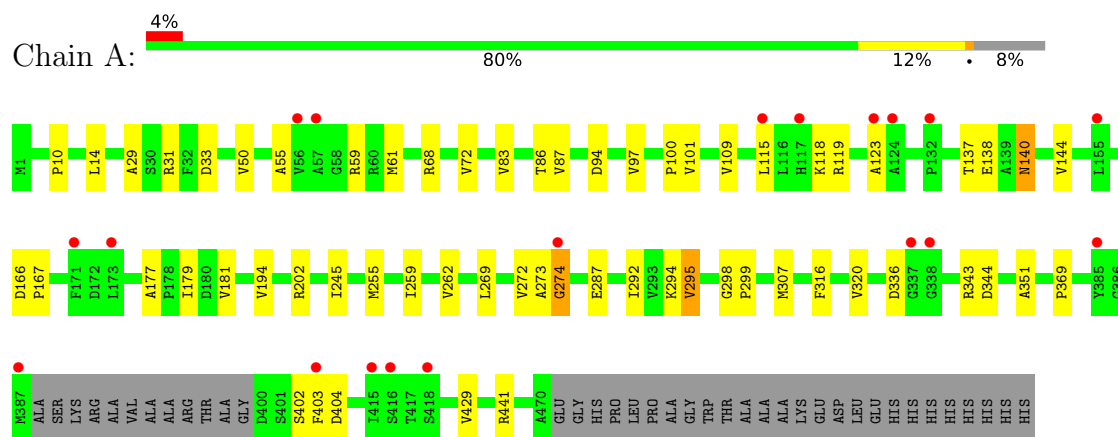
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Chain	Residue	Modelled	Actual	Comment	Reference
H	492	HIS	-	expression tag	UNP A0A0D6IET0
H	493	HIS	-	expression tag	UNP A0A0D6IET0
H	494	HIS	-	expression tag	UNP A0A0D6IET0
H	495	HIS	-	expression tag	UNP A0A0D6IET0
H	496	HIS	-	expression tag	UNP A0A0D6IET0

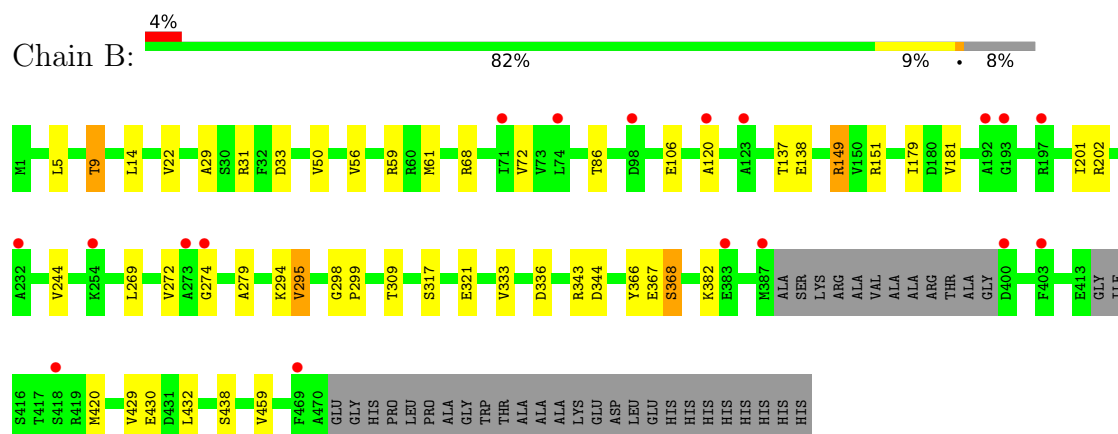
3 Residue-property plots [i](#)

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.

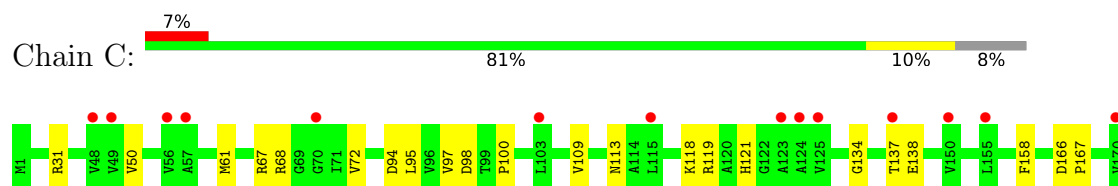
- Molecule 1: Guanosine 5'-monophosphate reductase



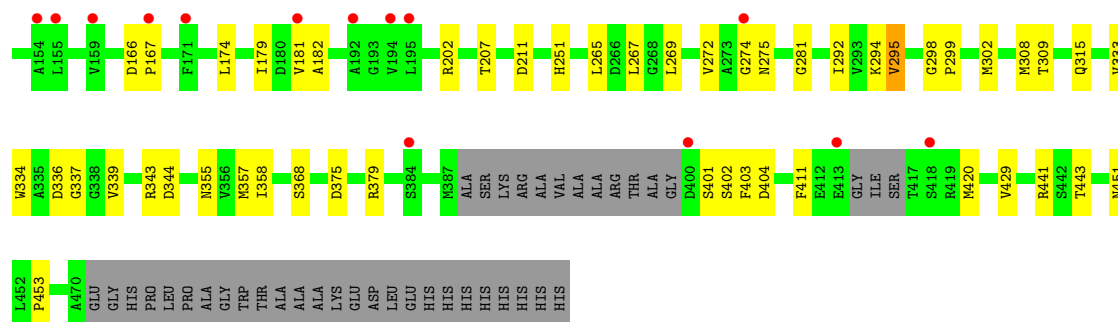
- Molecule 1: Guanosine 5'-monophosphate reductase



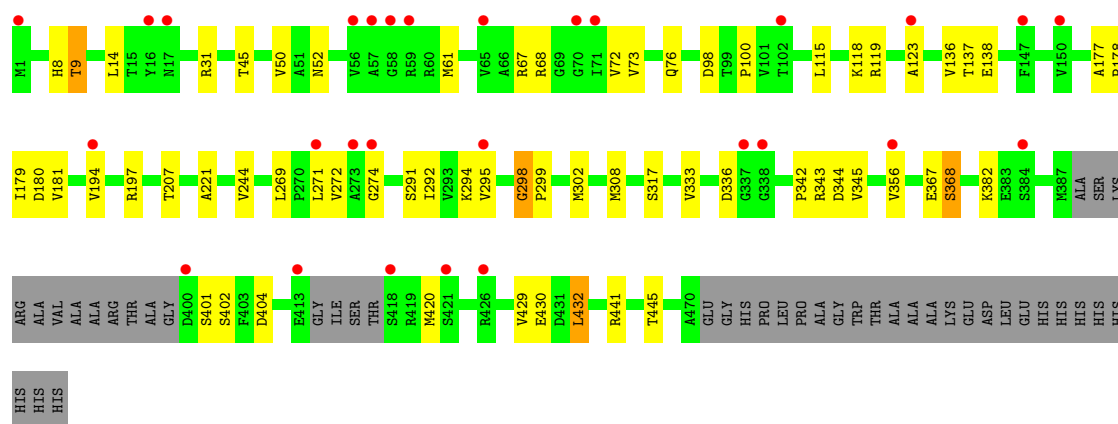
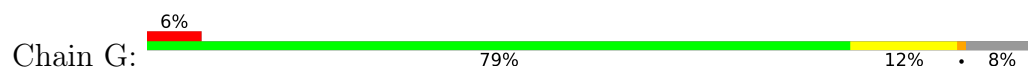
- Molecule 1: Guanosine 5'-monophosphate reductase



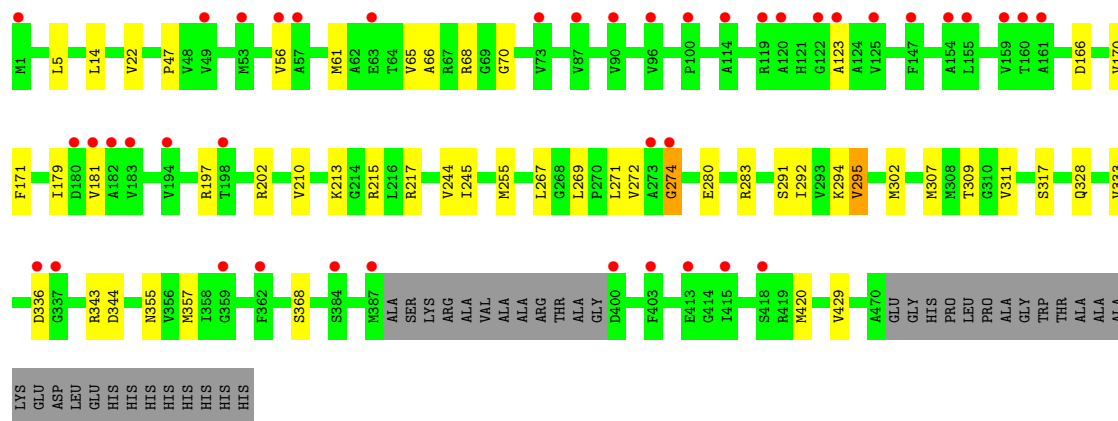
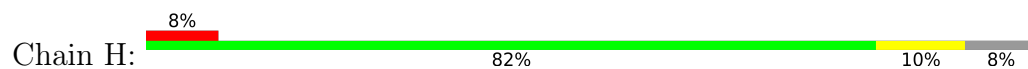




• Molecule 1: Guanosine 5'-monophosphate reductase



• Molecule 1: Guanosine 5'-monophosphate reductase



4 Data and refinement statistics

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 43.73 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.73-2.80) 100.0 (43.73-2.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.234 , 0.275 0.241 , 0.279	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)	0.31 , 75.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.68	0/3288	0.99	6/4497 (0.1%)
1	B	0.61	0/3296	0.92	7/4502 (0.2%)
1	C	0.62	0/3280	0.94	6/4481 (0.1%)
1	D	0.64	0/3296	0.99	9/4505 (0.2%)
1	E	0.74	0/3280	1.01	10/4480 (0.2%)
1	F	0.69	0/3277	1.03	10/4478 (0.2%)
1	G	0.64	0/3259	0.93	7/4456 (0.2%)
1	H	0.61	0/3287	0.96	5/4496 (0.1%)
All	All	0.65	0/26263	0.97	60/35895 (0.2%)

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

There are no bond length outliers.

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	274	GLY	CA-C-N	-8.62	110.84	122.99
1	H	274	GLY	C-N-CA	-8.62	110.84	122.99
1	D	274	GLY	CA-C-N	-8.29	111.31	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	274	GLY	C-N-CA	-8.29	111.31	122.99
1	F	56	VAL	N-CA-C	8.10	118.99	111.45
1	F	274	GLY	CA-C-N	-7.91	111.84	122.99
1	F	274	GLY	C-N-CA	-7.91	111.84	122.99
1	H	56	VAL	N-CA-C	7.80	118.39	110.82
1	E	274	GLY	CA-C-N	-7.15	113.14	123.00
1	E	274	GLY	C-N-CA	-7.15	113.14	123.00
1	C	368	SER	CA-C-N	7.13	127.74	119.47
1	C	368	SER	C-N-CA	7.13	127.74	119.47
1	A	402	SER	N-CA-C	6.98	120.80	111.30
1	D	177	ALA	CA-C-N	6.92	126.89	119.28
1	D	177	ALA	C-N-CA	6.92	126.89	119.28
1	H	368	SER	CA-C-N	6.85	127.42	119.47
1	H	368	SER	C-N-CA	6.85	127.42	119.47
1	G	402	SER	N-CA-C	6.58	119.05	111.02
1	E	56	VAL	N-CA-C	6.58	118.55	111.58
1	B	56	VAL	N-CA-C	6.44	117.44	111.45
1	C	274	GLY	CA-C-N	-6.33	114.06	122.99
1	C	274	GLY	C-N-CA	-6.33	114.06	122.99
1	B	274	GLY	CA-C-N	-6.27	114.14	122.99
1	B	274	GLY	C-N-CA	-6.27	114.14	122.99
1	C	309	THR	N-CA-C	6.20	121.01	113.38
1	D	56	VAL	N-CA-C	6.17	117.19	111.45
1	B	368	SER	CA-C-N	6.04	126.48	119.47
1	B	368	SER	C-N-CA	6.04	126.48	119.47
1	C	402	SER	N-CA-C	6.00	118.59	111.33
1	G	274	GLY	CA-C-N	-5.97	114.75	123.00
1	G	274	GLY	C-N-CA	-5.97	114.75	123.00
1	A	274	GLY	N-CA-C	5.93	127.23	113.18
1	E	166	ASP	CA-C-N	5.89	126.31	119.47
1	E	166	ASP	C-N-CA	5.89	126.31	119.47
1	D	368	SER	CA-C-N	5.89	126.30	119.47
1	D	368	SER	C-N-CA	5.89	126.30	119.47
1	F	309	THR	N-CA-C	5.86	120.71	113.50
1	F	69	GLY	CA-C-N	-5.79	116.54	122.27
1	F	69	GLY	C-N-CA	-5.79	116.54	122.27
1	B	459	VAL	N-CA-C	5.66	116.91	109.21
1	F	53	MET	N-CA-C	5.57	118.31	110.23
1	G	368	SER	CA-C-N	5.51	125.86	119.47
1	G	368	SER	C-N-CA	5.51	125.86	119.47
1	F	368	SER	CA-C-N	5.48	125.83	119.47
1	F	368	SER	C-N-CA	5.48	125.83	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	404	ASP	N-CA-C	-5.48	105.47	111.82
1	E	295	VAL	N-CA-C	5.41	116.33	107.24
1	E	298	GLY	CA-C-N	5.40	124.73	118.85
1	E	298	GLY	C-N-CA	5.40	124.73	118.85
1	B	309	THR	N-CA-C	5.36	119.97	113.38
1	F	275	ASN	N-CA-C	5.25	117.45	108.90
1	E	452	LEU	CA-C-N	-5.21	113.26	119.05
1	E	452	LEU	C-N-CA	-5.21	113.26	119.05
1	G	298	GLY	CA-C-N	5.15	124.46	118.85
1	G	298	GLY	C-N-CA	5.15	124.46	118.85
1	A	320	VAL	CB-CA-C	-5.15	105.29	111.88
1	D	309	THR	N-CA-C	5.13	119.69	113.38
1	A	177	ALA	CA-C-N	5.06	124.84	119.28
1	A	177	ALA	C-N-CA	5.06	124.84	119.28
1	D	275	ASN	N-CA-C	5.05	117.13	108.90

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 ⓘ

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	30	0
1	C	3227	0	3140	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3243	0	3159	36	0
1	E	3227	0	3143	39	0
1	F	3224	0	3140	51	0
1	G	3206	0	3109	42	0
1	H	3233	0	3136	31	0
All	All	25837	0	25130	269	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 (269) 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:D:61:MET:HE1	1:D:429:VAL:HG21	1.50	0.93
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	1.62	0.82
1:D:343:ARG:NH1	1:D:344:ASP:OD1	2.15	0.79
1:H:61:MET:HE1	1:H:429:VAL:HG21	1.67	0.77
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:G:61:MET:HE1	1:G:429:VAL:HG21	1.69	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: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:A:255:MET:HE3	1:A:274:GLY:HA3	1.77	0.65
1:B:59:ARG:HG2	1:B:86:THR:HG23	1.79	0.65
1:B:61:MET:HE1	1:B:429:VAL:HG21	1.79	0.65
1:B:294:LYS:HG2	1:B:336:ASP:HB2	1.79	0.65
1:C:61:MET:HE1	1:C:429:VAL:HG21	1.79	0.64
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:14:LEU:H	1:H:317:SER:HB2	1.69	0.58
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: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	1.88	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:F:343:ARG:HH21	1:H:307:MET:HE1	1.72	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:F:61:MET:HE1	1:F:429:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:59:ARG:HG2	1:D:86:THR:HG23	1.94	0.50
1:G:61:MET:CE	1:G:429:VAL:HG21	2.40	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:D:247:THR:HG22	1:D:255:MET:HE2	1.95	0.48
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:H:255:MET:HE3	1:H:274:GLY:HA3	1.94	0.48
1:E:61:MET:HE1	1:E:429:VAL:CG2	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:61:MET:HE1	1:G:429:VAL:CG2	2.42	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: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:D:61:MET:CE	1:D:429:VAL:HG21	2.34	0.47
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:45:THR:OG1	1:G:207:THR:O	2.30	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:308:MET:HB2	1:F:308:MET:HE2	1.79	0.46
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:C:247:THR:HG22	1:C:255:MET:HE2	1.98	0.46
1:F:443:THR:OG1	1:H:309:THR:O	2.33	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:C:61:MET:CE	1:C:429:VAL:HG21	2.47	0.45
1:F:137:THR:HG22	1:F:138:GLU:N	2.32	0.45
1:G:61:MET:HE1	1:G:429:VAL:HG11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:180:ASP:OD1	1:G:197:ARG:HG3	2.16	0.45
1:H:61:MET:HE3	1:H:65:VAL:CG2	2.47	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:302:MET:HA	1:D:307:MET:HE3	1.98	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:A:61:MET:CE	1:A:429:VAL:HG21	2.47	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:G:244:VAL:HG22	1:G:272:VAL:CB	2.46	0.44
1:D:61:MET:HE3	1:D:65:VAL:CG2	2.48	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
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: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:G:308:MET:HE2	1:G:308:MET:HB2	1.88	0.43
1:H:420:MET:HE3	1:H:420:MET:HB3	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:ALA:O	1:G:8:HIS:HA	2.19	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:G:420:MET:HE3	1:G:420:MET:HB3	1.76	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: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:G:368:SER:O	1:G:382:LYS:NZ	2.52	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:F:420:MET:HE3	1:F:420:MET:HB3	1.88	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:B:420:MET:HB3	1:B:420:MET:HE3	1.82	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:294:LYS:NZ	1:F:357:MET:HE1	2.36	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:D:301:ALA:O	1:D:307:MET:HE2	2.20	0.41
1:E:339:VAL:O	1:E:339:VAL:HG23	2.20	0.41
1:E:420:MET:HE3	1:E:420:MET:HB3	1.92	0.41
1:H:166:ASP:O	1:H:170:VAL:HG23	2.21	0.41
1:H:245:ILE:HG22	1:H:255:MET:HE1	2.02	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: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
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
1:F:61:MET:HE1	1:F:429:VAL:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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%)	320 (99%)	3 (1%)	70	89
1	B	325/372 (87%)	319 (98%)	6 (2%)	51	82
1	C	322/372 (87%)	318 (99%)	4 (1%)	63	87
1	D	324/372 (87%)	321 (99%)	3 (1%)	70	89
1	E	323/372 (87%)	318 (98%)	5 (2%)	57	84
1	F	322/372 (87%)	317 (98%)	5 (2%)	55	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	319/372 (86%)	313 (98%)	6 (2%)	50	81
1	H	322/372 (87%)	317 (98%)	5 (2%)	55	83
All	All	2580/2976 (87%)	2543 (99%)	37 (1%)	59	85

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	269	LEU
1	A	295	VAL
1	B	9	THR
1	B	149	ARG
1	B	269	LEU
1	B	295	VAL
1	B	333	VAL
1	B	432	LEU
1	C	269	LEU
1	C	295	VAL
1	C	333	VAL
1	C	432	LEU
1	D	269	LEU
1	D	295	VAL
1	D	333	VAL
1	E	267	LEU
1	E	269	LEU
1	E	295	VAL
1	E	333	VAL
1	E	355	ASN
1	F	9	THR
1	F	269	LEU
1	F	295	VAL
1	F	302	MET
1	F	333	VAL
1	G	9	THR
1	G	269	LEU
1	G	295	VAL
1	G	302	MET
1	G	333	VAL
1	G	432	LEU
1	H	267	LEU
1	H	269	LEU

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Mol	Chain	Res	Type
1	H	295	VAL
1	H	302	MET
1	H	333	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	456	HIS
1	B	341	HIS
1	C	52	ASN
1	D	251	HIS
1	D	341	HIS
1	E	121	HIS
1	E	332	HIS
1	E	355	ASN
1	E	456	HIS
1	F	315	GLN
1	F	332	HIS
1	G	233	GLN
1	G	341	HIS
1	H	113	ASN
1	H	341	HIS

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 oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	458/496 (92%)	0.39	19 (4%)	41	33	66, 104, 160, 176	0
1	B	456/496 (91%)	0.54	18 (3%)	43	34	73, 119, 156, 178	0
1	C	454/496 (91%)	0.73	33 (7%)	21	15	68, 118, 158, 170	0
1	D	458/496 (92%)	0.47	26 (5%)	29	22	66, 108, 168, 188	0
1	E	454/496 (91%)	0.53	36 (7%)	18	13	61, 98, 162, 185	0
1	F	455/496 (91%)	0.45	24 (5%)	32	24	65, 100, 162, 188	0
1	G	454/496 (91%)	0.65	28 (6%)	26	20	63, 118, 155, 174	0
1	H	458/496 (92%)	0.79	42 (9%)	14	10	66, 123, 174, 190	0
All	All	3647/3968 (91%)	0.57	226 (6%)	26	20	61, 112, 163, 190	0

All (226) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	181	VAL	5.2
1	B	98	ASP	4.8
1	B	192	ALA	4.5
1	C	123	ALA	4.4
1	E	136	VAL	4.4
1	B	120	ALA	4.3
1	H	274	GLY	4.3
1	G	274	GLY	4.2
1	D	90	VAL	4.1
1	C	383	GLU	4.1
1	B	274	GLY	4.1
1	E	123	ALA	3.9
1	G	123	ALA	3.9
1	H	400	ASP	3.9
1	E	337	GLY	3.8
1	F	195	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	400	ASP	3.8
1	H	387	MET	3.6
1	C	384	SER	3.6
1	A	337	GLY	3.6
1	G	400	ASP	3.5
1	E	181	VAL	3.5
1	E	182	ALA	3.5
1	G	418	SER	3.5
1	C	194	VAL	3.4
1	F	413	GLU	3.4
1	F	274	GLY	3.4
1	D	274	GLY	3.3
1	C	315	GLN	3.3
1	H	90	VAL	3.3
1	C	193	GLY	3.3
1	H	182	ALA	3.3
1	C	195	LEU	3.3
1	B	123	ALA	3.3
1	D	155	LEU	3.2
1	G	16	TYR	3.2
1	E	98	ASP	3.2
1	E	155	LEU	3.2
1	F	155	LEU	3.2
1	A	274	GLY	3.2
1	E	124	ALA	3.1
1	D	102	THR	3.1
1	A	155	LEU	3.1
1	F	384	SER	3.1
1	H	96	VAL	3.0
1	C	115	LEU	3.0
1	E	132	PRO	3.0
1	G	413	GLU	3.0
1	G	384	SER	3.0
1	H	122	GLY	3.0
1	H	120	ALA	3.0
1	E	180	ASP	3.0
1	F	400	ASP	3.0
1	E	122	GLY	3.0
1	E	135	LEU	2.9
1	A	123	ALA	2.9
1	E	274	GLY	2.9
1	E	192	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	128	PHE	2.9
1	E	197	ARG	2.9
1	F	123	ALA	2.9
1	F	136	VAL	2.9
1	H	181	VAL	2.9
1	H	73	VAL	2.9
1	E	179	ILE	2.9
1	C	192	ALA	2.8
1	H	49	VAL	2.8
1	A	403	PHE	2.8
1	D	115	LEU	2.8
1	E	115	LEU	2.8
1	A	338	GLY	2.8
1	G	59	ARG	2.8
1	H	119	ARG	2.8
1	C	182	ALA	2.8
1	H	415	ILE	2.8
1	E	183	VAL	2.7
1	A	124	ALA	2.7
1	B	387	MET	2.7
1	E	413	GLU	2.7
1	H	403	PHE	2.7
1	G	338	GLY	2.7
1	D	96	VAL	2.7
1	G	56	VAL	2.7
1	H	114	ALA	2.7
1	E	403	PHE	2.7
1	H	384	SER	2.7
1	B	469	PHE	2.6
1	F	192	ALA	2.6
1	G	70	GLY	2.6
1	H	154	ALA	2.6
1	E	195	LEU	2.6
1	H	100	PRO	2.6
1	C	155	LEU	2.6
1	H	125	VAL	2.6
1	A	418	SER	2.6
1	C	274	GLY	2.6
1	D	136	VAL	2.6
1	G	194	VAL	2.6
1	D	161	ALA	2.6
1	H	161	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	273	ALA	2.6
1	C	400	ASP	2.5
1	D	173	LEU	2.5
1	A	387	MET	2.5
1	F	167	PRO	2.5
1	A	56	VAL	2.5
1	C	125	VAL	2.5
1	D	418	SER	2.5
1	F	133	ILE	2.5
1	H	418	SER	2.5
1	D	56	VAL	2.5
1	H	183	VAL	2.5
1	E	57	ALA	2.5
1	E	112	ALA	2.5
1	E	114	ALA	2.5
1	H	160	THR	2.5
1	D	400	ASP	2.4
1	F	132	PRO	2.4
1	F	125	VAL	2.4
1	F	418	SER	2.4
1	G	150	VAL	2.4
1	B	403	PHE	2.4
1	G	57	ALA	2.4
1	C	103	LEU	2.4
1	F	115	LEU	2.4
1	G	1	MET	2.4
1	C	241	ASP	2.4
1	C	240	ALA	2.4
1	H	57	ALA	2.4
1	G	71	ILE	2.4
1	E	125	VAL	2.4
1	E	400	ASP	2.4
1	B	418	SER	2.4
1	B	193	GLY	2.4
1	E	56	VAL	2.4
1	G	295	VAL	2.4
1	C	171	PHE	2.4
1	G	273	ALA	2.4
1	G	147	PHE	2.3
1	C	57	ALA	2.3
1	F	171	PHE	2.3
1	C	413	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	95	LEU	2.3
1	F	159	VAL	2.3
1	H	159	VAL	2.3
1	A	57	ALA	2.3
1	D	1	MET	2.3
1	D	51	ALA	2.3
1	D	123	ALA	2.3
1	D	273	ALA	2.3
1	H	123	ALA	2.3
1	G	426	ARG	2.3
1	D	101	VAL	2.3
1	G	337	GLY	2.3
1	B	383	GLU	2.2
1	D	135	LEU	2.2
1	B	197	ARG	2.2
1	C	56	VAL	2.2
1	C	150	VAL	2.2
1	G	421	SER	2.2
1	E	121	HIS	2.2
1	C	49	VAL	2.2
1	D	137	THR	2.2
1	C	387	MET	2.2
1	C	124	ALA	2.2
1	D	195	LEU	2.2
1	H	63	GLU	2.2
1	A	117	HIS	2.2
1	D	132	PRO	2.2
1	A	385	TYR	2.2
1	E	116	LEU	2.2
1	B	273	ALA	2.2
1	A	415	ILE	2.2
1	F	121	HIS	2.2
1	F	194	VAL	2.2
1	H	337	GLY	2.2
1	C	170	VAL	2.1
1	G	271	LEU	2.1
1	F	154	ALA	2.1
1	C	426	ARG	2.1
1	H	413	GLU	2.1
1	C	218	ILE	2.1
1	E	133	ILE	2.1
1	E	52	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	359	GLY	2.1
1	B	232	ALA	2.1
1	E	366	TYR	2.1
1	A	416	SER	2.1
1	B	254	LYS	2.1
1	E	387	MET	2.1
1	H	87	VAL	2.1
1	H	155	LEU	2.1
1	A	171	PHE	2.1
1	H	336	ASP	2.1
1	H	362	PHE	2.1
1	D	154	ALA	2.1
1	F	181	VAL	2.1
1	A	132	PRO	2.1
1	F	78	LEU	2.1
1	H	198	THR	2.1
1	H	1	MET	2.0
1	D	181	VAL	2.0
1	E	90	VAL	2.0
1	A	173	LEU	2.0
1	G	58	GLY	2.0
1	H	147	PHE	2.0
1	E	99	THR	2.0
1	G	102	THR	2.0
1	H	53	MET	2.0
1	D	159	VAL	2.0
1	G	65	VAL	2.0
1	G	356	VAL	2.0
1	H	194	VAL	2.0
1	A	115	LEU	2.0
1	B	74	LEU	2.0
1	F	135	LEU	2.0
1	G	17	ASN	2.0
1	C	70	GLY	2.0
1	C	337	GLY	2.0
1	D	147	PHE	2.0
1	B	71	ILE	2.0
1	C	137	THR	2.0
1	E	137	THR	2.0
1	H	180	ASP	2.0
1	C	48	VAL	2.0
1	H	56	VAL	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 oligosaccharides 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.