



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:22 AM UTC

PDB ID : 6GJV / pdb_00006gjb
Title : apo-structure of IMPDH from Pseudomonas aeruginosa
Authors : Labesse, G.; Haouz, A.; Alexandre, T.; Munier-Lehmann, H.
Deposited on : 2018-05-17
Resolution : 2.11 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

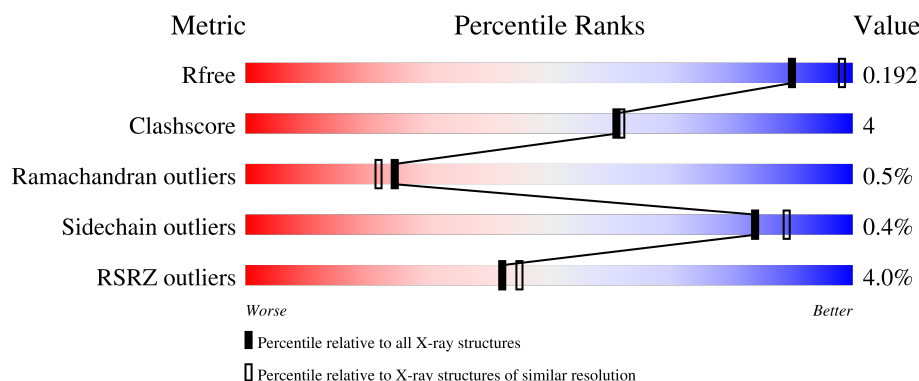
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	509	7% 74% 9% 17%
1	B	509	11% 69% 12% 19%
1	C	509	2% 76% 8% 16%
1	D	509	% 59% 38%
1	E	509	% 77% 6% 17%

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Mol	Chain	Length	Quality of chain
1	F	509	% 75% 9% 16%
1	G	509	% 77% 6% 17%
1	H	509	% 57% 5% 38%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25755 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 Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	1	0
			3150	1988	549	596	17			
1	B	414	Total	C	N	O	S	0	1	0
			3038	1916	531	574	17			
1	C	429	Total	C	N	O	S	0	0	0
			3182	2005	559	601	17			
1	D	318	Total	C	N	O	S	0	0	0
			2315	1453	413	436	13			
1	E	424	Total	C	N	O	S	1	6	0
			3183	2007	558	601	17			
1	F	426	Total	C	N	O	S	0	3	0
			3178	2004	558	599	17			
1	G	424	Total	C	N	O	S	0	3	0
			3172	1999	555	601	17			
1	H	317	Total	C	N	O	S	0	1	0
			2314	1451	414	436	13			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q9HXM5
A	-18	GLY	-	expression tag	UNP Q9HXM5
A	-17	SER	-	expression tag	UNP Q9HXM5
A	-16	SER	-	expression tag	UNP Q9HXM5
A	-15	HIS	-	expression tag	UNP Q9HXM5
A	-14	HIS	-	expression tag	UNP Q9HXM5
A	-13	HIS	-	expression tag	UNP Q9HXM5
A	-12	HIS	-	expression tag	UNP Q9HXM5
A	-11	HIS	-	expression tag	UNP Q9HXM5
A	-10	HIS	-	expression tag	UNP Q9HXM5
A	-9	SER	-	expression tag	UNP Q9HXM5
A	-8	SER	-	expression tag	UNP Q9HXM5
A	-7	GLY	-	expression tag	UNP Q9HXM5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP Q9HXM5
A	-5	VAL	-	expression tag	UNP Q9HXM5
A	-4	PRO	-	expression tag	UNP Q9HXM5
A	-3	ARG	-	expression tag	UNP Q9HXM5
A	-2	GLY	-	expression tag	UNP Q9HXM5
A	-1	SER	-	expression tag	UNP Q9HXM5
A	0	HIS	-	expression tag	UNP Q9HXM5
B	-19	MET	-	initiating methionine	UNP Q9HXM5
B	-18	GLY	-	expression tag	UNP Q9HXM5
B	-17	SER	-	expression tag	UNP Q9HXM5
B	-16	SER	-	expression tag	UNP Q9HXM5
B	-15	HIS	-	expression tag	UNP Q9HXM5
B	-14	HIS	-	expression tag	UNP Q9HXM5
B	-13	HIS	-	expression tag	UNP Q9HXM5
B	-12	HIS	-	expression tag	UNP Q9HXM5
B	-11	HIS	-	expression tag	UNP Q9HXM5
B	-10	HIS	-	expression tag	UNP Q9HXM5
B	-9	SER	-	expression tag	UNP Q9HXM5
B	-8	SER	-	expression tag	UNP Q9HXM5
B	-7	GLY	-	expression tag	UNP Q9HXM5
B	-6	LEU	-	expression tag	UNP Q9HXM5
B	-5	VAL	-	expression tag	UNP Q9HXM5
B	-4	PRO	-	expression tag	UNP Q9HXM5
B	-3	ARG	-	expression tag	UNP Q9HXM5
B	-2	GLY	-	expression tag	UNP Q9HXM5
B	-1	SER	-	expression tag	UNP Q9HXM5
B	0	HIS	-	expression tag	UNP Q9HXM5
C	-19	MET	-	initiating methionine	UNP Q9HXM5
C	-18	GLY	-	expression tag	UNP Q9HXM5
C	-17	SER	-	expression tag	UNP Q9HXM5
C	-16	SER	-	expression tag	UNP Q9HXM5
C	-15	HIS	-	expression tag	UNP Q9HXM5
C	-14	HIS	-	expression tag	UNP Q9HXM5
C	-13	HIS	-	expression tag	UNP Q9HXM5
C	-12	HIS	-	expression tag	UNP Q9HXM5
C	-11	HIS	-	expression tag	UNP Q9HXM5
C	-10	HIS	-	expression tag	UNP Q9HXM5
C	-9	SER	-	expression tag	UNP Q9HXM5
C	-8	SER	-	expression tag	UNP Q9HXM5
C	-7	GLY	-	expression tag	UNP Q9HXM5
C	-6	LEU	-	expression tag	UNP Q9HXM5
C	-5	VAL	-	expression tag	UNP Q9HXM5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP Q9HXM5
C	-3	ARG	-	expression tag	UNP Q9HXM5
C	-2	GLY	-	expression tag	UNP Q9HXM5
C	-1	SER	-	expression tag	UNP Q9HXM5
C	0	HIS	-	expression tag	UNP Q9HXM5
D	-19	MET	-	initiating methionine	UNP Q9HXM5
D	-18	GLY	-	expression tag	UNP Q9HXM5
D	-17	SER	-	expression tag	UNP Q9HXM5
D	-16	SER	-	expression tag	UNP Q9HXM5
D	-15	HIS	-	expression tag	UNP Q9HXM5
D	-14	HIS	-	expression tag	UNP Q9HXM5
D	-13	HIS	-	expression tag	UNP Q9HXM5
D	-12	HIS	-	expression tag	UNP Q9HXM5
D	-11	HIS	-	expression tag	UNP Q9HXM5
D	-10	HIS	-	expression tag	UNP Q9HXM5
D	-9	SER	-	expression tag	UNP Q9HXM5
D	-8	SER	-	expression tag	UNP Q9HXM5
D	-7	GLY	-	expression tag	UNP Q9HXM5
D	-6	LEU	-	expression tag	UNP Q9HXM5
D	-5	VAL	-	expression tag	UNP Q9HXM5
D	-4	PRO	-	expression tag	UNP Q9HXM5
D	-3	ARG	-	expression tag	UNP Q9HXM5
D	-2	GLY	-	expression tag	UNP Q9HXM5
D	-1	SER	-	expression tag	UNP Q9HXM5
D	0	HIS	-	expression tag	UNP Q9HXM5
E	-19	MET	-	initiating methionine	UNP Q9HXM5
E	-18	GLY	-	expression tag	UNP Q9HXM5
E	-17	SER	-	expression tag	UNP Q9HXM5
E	-16	SER	-	expression tag	UNP Q9HXM5
E	-15	HIS	-	expression tag	UNP Q9HXM5
E	-14	HIS	-	expression tag	UNP Q9HXM5
E	-13	HIS	-	expression tag	UNP Q9HXM5
E	-12	HIS	-	expression tag	UNP Q9HXM5
E	-11	HIS	-	expression tag	UNP Q9HXM5
E	-10	HIS	-	expression tag	UNP Q9HXM5
E	-9	SER	-	expression tag	UNP Q9HXM5
E	-8	SER	-	expression tag	UNP Q9HXM5
E	-7	GLY	-	expression tag	UNP Q9HXM5
E	-6	LEU	-	expression tag	UNP Q9HXM5
E	-5	VAL	-	expression tag	UNP Q9HXM5
E	-4	PRO	-	expression tag	UNP Q9HXM5
E	-3	ARG	-	expression tag	UNP Q9HXM5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP Q9HXM5
E	-1	SER	-	expression tag	UNP Q9HXM5
E	0	HIS	-	expression tag	UNP Q9HXM5
F	-19	MET	-	initiating methionine	UNP Q9HXM5
F	-18	GLY	-	expression tag	UNP Q9HXM5
F	-17	SER	-	expression tag	UNP Q9HXM5
F	-16	SER	-	expression tag	UNP Q9HXM5
F	-15	HIS	-	expression tag	UNP Q9HXM5
F	-14	HIS	-	expression tag	UNP Q9HXM5
F	-13	HIS	-	expression tag	UNP Q9HXM5
F	-12	HIS	-	expression tag	UNP Q9HXM5
F	-11	HIS	-	expression tag	UNP Q9HXM5
F	-10	HIS	-	expression tag	UNP Q9HXM5
F	-9	SER	-	expression tag	UNP Q9HXM5
F	-8	SER	-	expression tag	UNP Q9HXM5
F	-7	GLY	-	expression tag	UNP Q9HXM5
F	-6	LEU	-	expression tag	UNP Q9HXM5
F	-5	VAL	-	expression tag	UNP Q9HXM5
F	-4	PRO	-	expression tag	UNP Q9HXM5
F	-3	ARG	-	expression tag	UNP Q9HXM5
F	-2	GLY	-	expression tag	UNP Q9HXM5
F	-1	SER	-	expression tag	UNP Q9HXM5
F	0	HIS	-	expression tag	UNP Q9HXM5
G	-19	MET	-	initiating methionine	UNP Q9HXM5
G	-18	GLY	-	expression tag	UNP Q9HXM5
G	-17	SER	-	expression tag	UNP Q9HXM5
G	-16	SER	-	expression tag	UNP Q9HXM5
G	-15	HIS	-	expression tag	UNP Q9HXM5
G	-14	HIS	-	expression tag	UNP Q9HXM5
G	-13	HIS	-	expression tag	UNP Q9HXM5
G	-12	HIS	-	expression tag	UNP Q9HXM5
G	-11	HIS	-	expression tag	UNP Q9HXM5
G	-10	HIS	-	expression tag	UNP Q9HXM5
G	-9	SER	-	expression tag	UNP Q9HXM5
G	-8	SER	-	expression tag	UNP Q9HXM5
G	-7	GLY	-	expression tag	UNP Q9HXM5
G	-6	LEU	-	expression tag	UNP Q9HXM5
G	-5	VAL	-	expression tag	UNP Q9HXM5
G	-4	PRO	-	expression tag	UNP Q9HXM5
G	-3	ARG	-	expression tag	UNP Q9HXM5
G	-2	GLY	-	expression tag	UNP Q9HXM5
G	-1	SER	-	expression tag	UNP Q9HXM5

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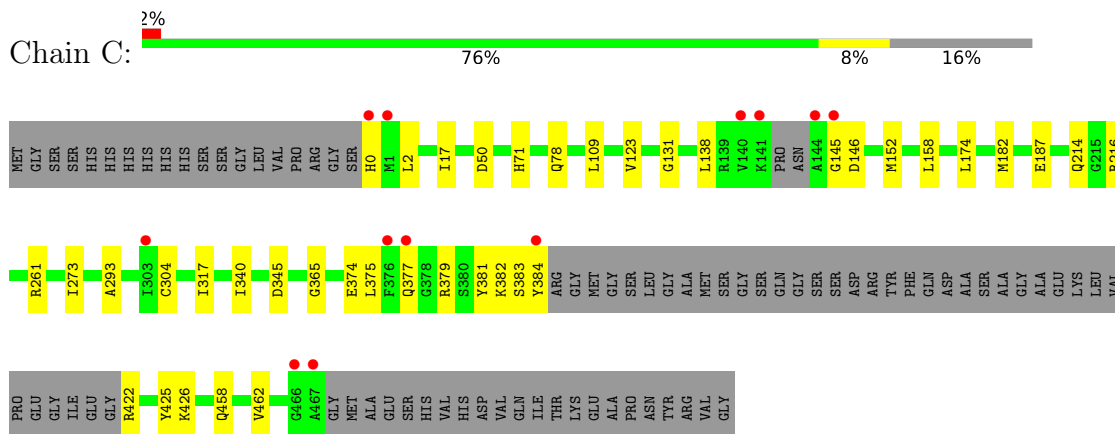
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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP Q9HXM5
H	-19	MET	-	initiating methionine	UNP Q9HXM5
H	-18	GLY	-	expression tag	UNP Q9HXM5
H	-17	SER	-	expression tag	UNP Q9HXM5
H	-16	SER	-	expression tag	UNP Q9HXM5
H	-15	HIS	-	expression tag	UNP Q9HXM5
H	-14	HIS	-	expression tag	UNP Q9HXM5
H	-13	HIS	-	expression tag	UNP Q9HXM5
H	-12	HIS	-	expression tag	UNP Q9HXM5
H	-11	HIS	-	expression tag	UNP Q9HXM5
H	-10	HIS	-	expression tag	UNP Q9HXM5
H	-9	SER	-	expression tag	UNP Q9HXM5
H	-8	SER	-	expression tag	UNP Q9HXM5
H	-7	GLY	-	expression tag	UNP Q9HXM5
H	-6	LEU	-	expression tag	UNP Q9HXM5
H	-5	VAL	-	expression tag	UNP Q9HXM5
H	-4	PRO	-	expression tag	UNP Q9HXM5
H	-3	ARG	-	expression tag	UNP Q9HXM5
H	-2	GLY	-	expression tag	UNP Q9HXM5
H	-1	SER	-	expression tag	UNP Q9HXM5
H	0	HIS	-	expression tag	UNP Q9HXM5

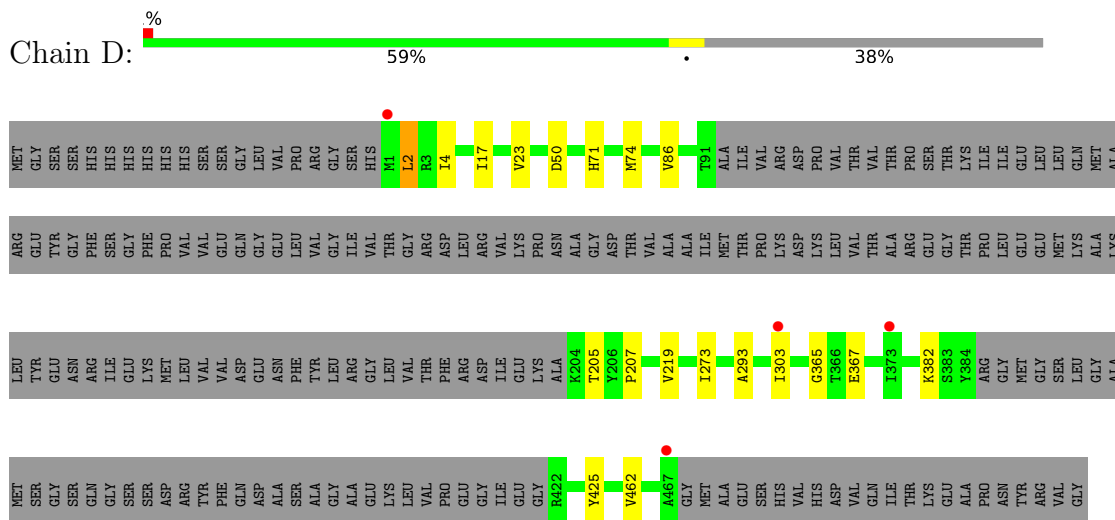
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	240	Total	O	0	0
			240	240		
2	B	256	Total	O	0	0
			256	256		
2	C	307	Total	O	0	0
			307	307		
2	D	211	Total	O	0	0
			211	211		
2	E	350	Total	O	0	0
			350	350		
2	F	289	Total	O	0	0
			289	289		
2	G	315	Total	O	0	0
			315	315		
2	H	255	Total	O	0	0
			255	255		

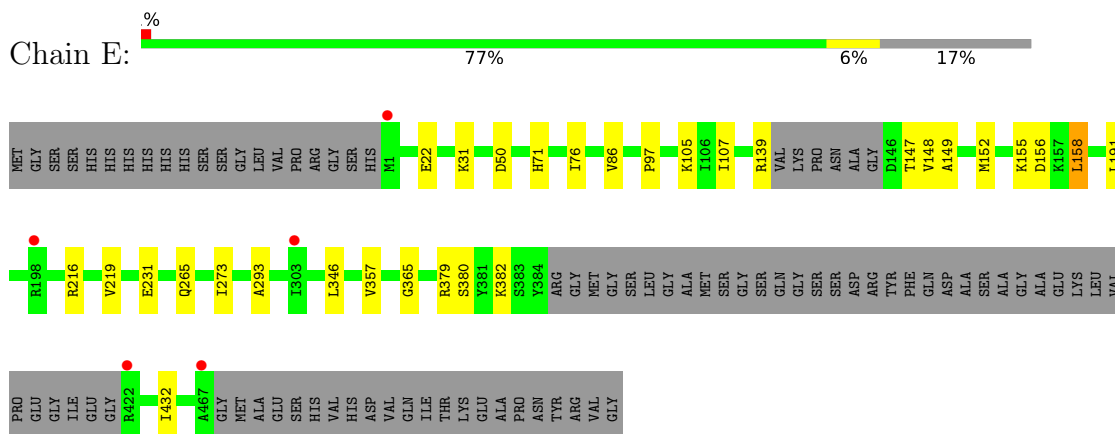
- Molecule 1: Inosine-5'-monophosphate dehydrogenase



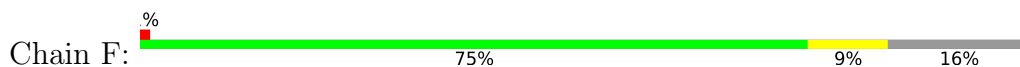
- Molecule 1: Inosine-5'-monophosphate dehydrogenase

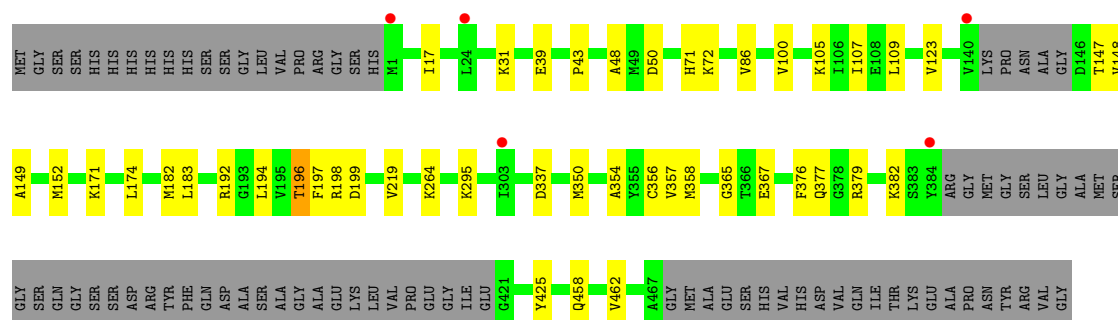


- Molecule 1: Inosine-5'-monophosphate dehydrogenase

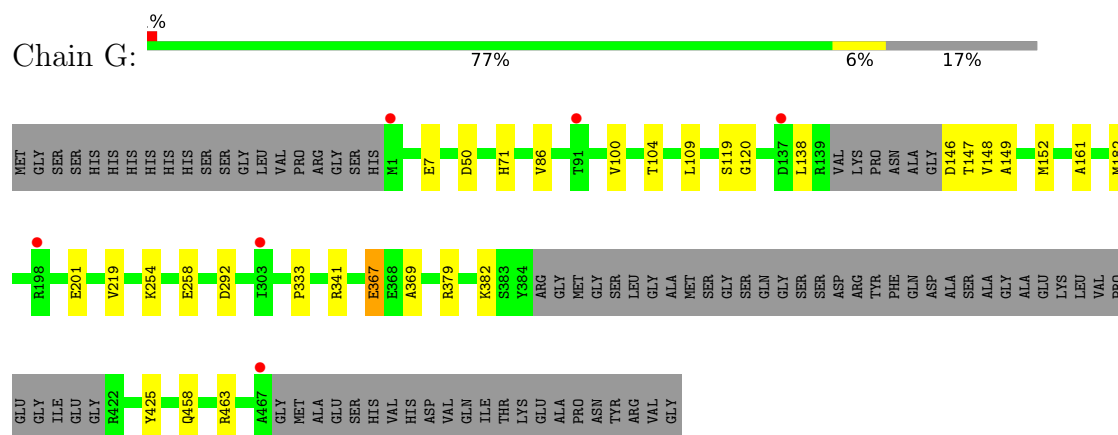


- Molecule 1: Inosine-5'-monophosphate dehydrogenase

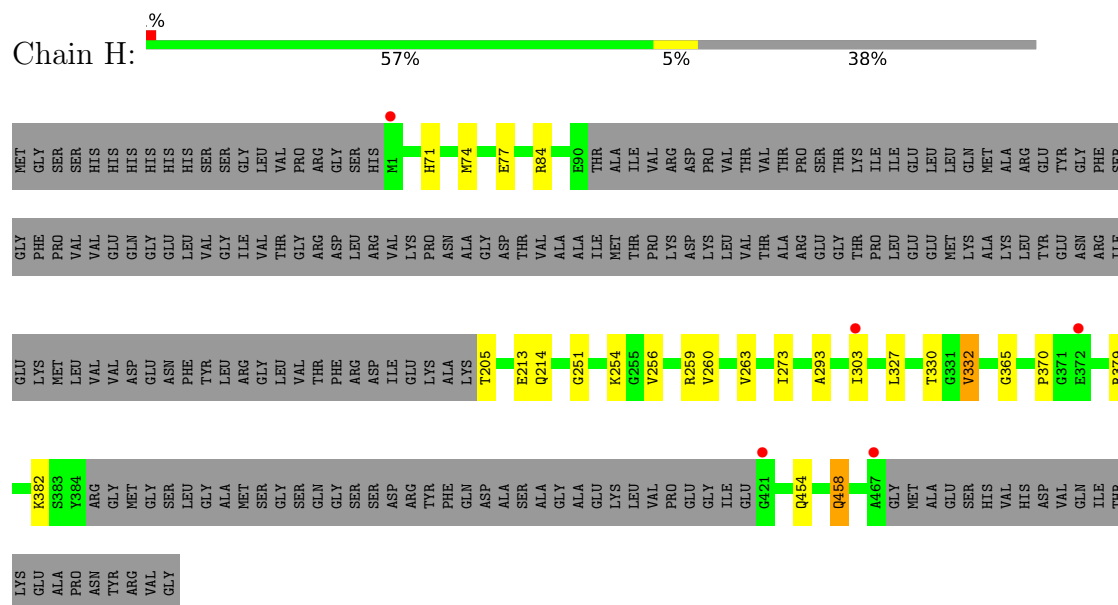




● Molecule 1: Inosine-5'-monophosphate dehydrogenase



● Molecule 1: Inosine-5'-monophosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	115.30Å 194.64Å 122.92Å 90.00° 117.75° 90.00°	Depositor
Resolution (Å)	44.63 – 2.11 44.63 – 2.11	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.63-2.11) 100.0 (44.63-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.160 , 0.191 0.161 , 0.192	Depositor DCC
R_{free} test set	13805 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	25755	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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 [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	0.31	0/3193	0.51	2/4319 (0.0%)
1	B	0.29	0/3078	0.52	1/4158 (0.0%)
1	C	0.31	0/3222	0.51	0/4355
1	D	0.29	0/2343	0.48	0/3166
1	E	0.32	0/3246	0.51	0/4385
1	F	0.29	0/3227	0.48	0/4361
1	G	0.33	0/3218	0.52	0/4348
1	H	0.34	0/2346	0.53	0/3169
All	All	0.31	0/23873	0.51	3/32261 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	PRO	N-CA-CB	6.30	109.93	103.00
1	A	90	GLU	CA-C-N	5.38	131.82	121.54
1	A	90	GLU	C-N-CA	5.38	131.82	121.54

There are no chirality outliers.

There are no planarity outliers.

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	3150	0	3241	36	0
1	B	3038	0	3090	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3182	0	3280	26	0
1	D	2315	0	2384	11	0
1	E	3183	0	3284	22	0
1	F	3178	0	3288	38	0
1	G	3172	0	3273	21	0
1	H	2314	0	2380	19	0
2	A	240	0	0	2	0
2	B	256	0	0	2	0
2	C	307	0	0	10	0
2	D	211	0	0	1	0
2	E	350	0	0	5	0
2	F	289	0	0	6	0
2	G	315	0	0	2	0
2	H	255	0	0	4	0
All	All	25755	0	24220	202	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 4.

All (202) 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:F:350:MET:HE3	1:F:357:VAL:HG23	1.39	1.03
1:A:455:MET:HE3	1:A:459:PRO:HG2	1.46	0.94
1:A:351:VAL:HG22	1:A:455:MET:HE2	1.51	0.90
1:F:337:ASP:CG	1:F:358:MET:HE2	1.98	0.89
1:B:7:GLU:OE2	1:B:463:ARG:NH2	2.09	0.86
1:F:149:ALA:HA	1:F:152:MET:HE3	1.57	0.86
1:C:425:TYR:O	2:C:501:HOH:O	1.96	0.83
1:A:159:VAL:HG12	1:A:182:MET:HE3	1.59	0.83
1:A:455:MET:CE	1:A:459:PRO:HG2	2.09	0.82
1:E:148:VAL:HG12	1:E:152:MET:HE2	1.64	0.80
1:B:198:ARG:HH11	1:B:202:LYS:HD3	1.49	0.78
1:A:90:GLU:HG3	1:A:95:ARG:HH21	1.49	0.78
1:F:350:MET:CE	1:F:357:VAL:HG23	2.15	0.76
1:E:149:ALA:HA	1:E:152:MET:HE3	1.69	0.74
1:F:196:THR:HG22	1:F:199:ASP:H	1.53	0.74
1:A:351:VAL:CG2	1:A:455:MET:HE2	2.17	0.74
1:B:181:LYS:HB3	1:B:194:LEU:HD11	1.69	0.73
1:B:7:GLU:CD	1:B:463:ARG:HH22	1.98	0.72
1:D:365:GLY:HA2	1:D:382:LYS:HG3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:LYS:HA	1:E:158:LEU:HD22	1.72	0.72
1:C:426:LYS:HA	2:C:501:HOH:O	1.91	0.70
1:C:261:ARG:NH1	2:C:504:HOH:O	2.24	0.69
1:A:365:GLY:HA2	1:A:382:LYS:HG3	1.72	0.69
1:G:149:ALA:HA	1:G:152:MET:HE3	1.75	0.69
1:A:367:GLU:HG2	1:A:425:TYR:OH	1.93	0.68
1:D:367:GLU:HG2	1:D:425:TYR:OH	1.94	0.68
1:A:111:GLN:OE1	1:A:114:ARG:NH1	2.27	0.68
1:C:365:GLY:HA2	1:C:382:LYS:HG3	1.77	0.67
1:E:31[B]:LYS:NZ	2:E:501:HOH:O	2.25	0.67
1:B:108:GLU:O	1:B:112:MET:HG3	1.95	0.66
1:C:422:ARG:N	2:C:508:HOH:O	2.28	0.66
1:F:337:ASP:OD2	1:F:358:MET:HE2	1.95	0.66
1:H:379:ARG:NH1	2:H:503:HOH:O	2.29	0.64
1:A:175:TYR:HA	1:B:118:PHE:HE2	1.62	0.63
1:B:379:ARG:NH2	1:B:381:TYR:OH	2.31	0.63
1:C:214:GLN:OE1	1:C:216:ARG:NH1	2.32	0.62
1:F:105:LYS:HD3	1:F:147:THR:HG22	1.80	0.61
1:F:148:VAL:HG12	1:F:152:MET:HE2	1.81	0.61
1:F:196:THR:HG21	2:F:743:HOH:O	2.01	0.61
1:B:198:ARG:NH1	1:B:202:LYS:HD3	2.15	0.61
1:E:97:PRO:HG2	1:E:191:LEU:HD21	1.83	0.61
1:A:86:VAL:HG11	1:A:219:VAL:HB	1.83	0.60
1:A:285:ALA:O	1:A:288:GLU:HG3	2.01	0.60
1:A:130:VAL:HG23	1:A:152:MET:HE1	1.83	0.60
1:C:78:GLN:HG3	2:C:737:HOH:O	2.00	0.60
1:E:216:ARG:NH2	2:E:504:HOH:O	2.30	0.59
2:C:501:HOH:O	1:E:380:SER:N	2.35	0.59
1:A:160:THR:C	1:A:182:MET:HE2	2.27	0.59
1:B:7:GLU:CD	1:B:463:ARG:NH2	2.59	0.59
1:F:365:GLY:HA2	1:F:382:LYS:HG3	1.84	0.59
1:F:198:ARG:NH1	2:F:504:HOH:O	2.36	0.58
1:C:384:TYR:O	2:C:502:HOH:O	2.17	0.58
1:G:148:VAL:HG12	1:G:152:MET:HE2	1.84	0.58
1:F:367:GLU:HG2	1:F:425:TYR:OH	2.04	0.58
1:A:340:ILE:HG23	1:A:345:ASP:HB2	1.86	0.58
1:D:2:LEU:HD13	1:D:4:ILE:HD11	1.87	0.57
1:H:365:GLY:HA2	1:H:382:LYS:HG3	1.86	0.56
1:G:7:GLU:OE1	1:G:463:ARG:NH2	2.30	0.56
1:F:350:MET:HE2	1:F:354:ALA:HB3	1.86	0.56
1:G:369:ALA:O	1:G:382:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:GLU:OE2	1:B:84:ARG:NH1	2.39	0.56
1:C:123:VAL:HG21	1:C:152:MET:SD	2.46	0.56
1:F:337:ASP:OD1	1:F:358:MET:HE2	2.05	0.55
1:A:90:GLU:O	1:A:91:THR:OG1	2.16	0.55
1:H:327:LEU:HD13	1:H:332:VAL:HG22	1.88	0.54
1:G:367[A]:GLU:HG2	1:G:425:TYR:OH	2.07	0.54
1:E:365:GLY:HA2	1:E:382:LYS:HG3	1.90	0.54
1:H:77:GLU:OE1	1:H:84:ARG:NH2	2.41	0.53
1:C:187:GLU:H	1:C:187:GLU:CD	2.16	0.53
1:C:374:GLU:OE1	1:C:383:SER:HB3	2.08	0.53
1:D:303:ILE:HG22	1:D:303:ILE:O	2.09	0.53
1:C:273:ILE:HG12	1:C:293:ALA:HB3	1.90	0.53
1:C:50:ASP:HA	1:C:71:HIS:CD2	2.44	0.53
1:C:374:GLU:OE2	1:C:422:ARG:NE	2.42	0.52
1:H:303:ILE:HD12	1:H:303:ILE:C	2.35	0.52
1:H:454:GLN:HG2	2:H:714:HOH:O	2.09	0.52
1:H:303:ILE:CD1	1:H:303:ILE:O	2.58	0.52
1:B:50:ASP:HA	1:B:71:HIS:CD2	2.45	0.51
1:E:50:ASP:HA	1:E:71:HIS:CD2	2.45	0.51
1:G:119:SER:N	1:G:120[A]:GLY:HA2	2.25	0.51
1:D:50:ASP:HA	1:D:71:HIS:CD2	2.46	0.51
1:F:123:VAL:HG11	1:F:152:MET:HE1	1.91	0.51
1:G:254:LYS:HE3	1:G:258:GLU:OE2	2.11	0.51
1:C:0:HIS:N	2:C:512:HOH:O	2.43	0.51
1:B:86:VAL:HG11	1:B:219:VAL:HB	1.93	0.50
1:B:365:GLY:HA2	1:B:382:LYS:HG3	1.93	0.50
1:A:302:SER:HB3	1:A:303:ILE:HD12	1.92	0.50
1:F:50:ASP:HA	1:F:71:HIS:CD2	2.47	0.49
1:G:119:SER:N	1:G:120[B]:GLY:HA2	2.27	0.49
1:A:340:ILE:HD12	1:A:357:VAL:HG11	1.95	0.49
1:C:379:ARG:HD3	1:E:379:ARG:HH12	1.78	0.49
1:F:48:ALA:HB1	1:F:71:HIS:HA	1.94	0.49
1:G:146:ASP:N	1:G:146:ASP:OD1	2.45	0.49
1:A:2:LEU:HD13	1:A:4:ILE:HD11	1.95	0.48
1:D:273:ILE:HG12	1:D:293:ALA:HB3	1.94	0.48
1:G:50:ASP:HA	1:G:71:HIS:CD2	2.48	0.48
1:A:374:GLU:OE2	1:A:422:ARG:HD3	2.14	0.48
1:D:71:HIS:CE1	1:D:74:MET:HE2	2.48	0.48
1:B:166:PRO:HB2	1:B:169:GLU:HG3	1.95	0.48
1:C:377:GLN:NE2	1:C:381:TYR:OH	2.46	0.48
1:G:86:VAL:HG11	1:G:219:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:109:LEU:HD22	1:G:138:LEU:HD21	1.95	0.48
1:B:1:MET:N	2:B:507:HOH:O	2.42	0.48
1:F:100:VAL:HG11	1:F:109:LEU:HD23	1.96	0.48
1:H:370:PRO:O	1:H:382:LYS:HE3	2.14	0.48
1:F:86:VAL:HG11	1:F:219:VAL:HB	1.95	0.47
1:H:330:THR:OG1	1:H:332:VAL:HG13	2.13	0.47
1:A:1:MET:N	2:A:502:HOH:O	2.29	0.47
1:A:50:ASP:HA	1:A:71:HIS:CD2	2.49	0.47
2:C:501:HOH:O	1:E:380:SER:OG	2.16	0.47
1:B:2:LEU:HD13	1:B:4:ILE:HD11	1.97	0.47
1:F:17:ILE:HD11	1:F:462:VAL:HG13	1.97	0.47
1:F:358:MET:HE1	2:F:580:HOH:O	2.15	0.46
1:B:132:ILE:HG22	1:B:158:LEU:HD21	1.95	0.46
1:A:90:GLU:HG3	1:A:95:ARG:NH2	2.24	0.46
1:A:100:VAL:HG23	1:A:123:VAL:HG22	1.97	0.46
1:F:31:LYS:HE2	1:F:39:GLU:OE1	2.15	0.46
1:F:379:ARG:HD3	1:G:379:ARG:NH2	2.30	0.46
1:B:128:GLU:N	2:B:512:HOH:O	2.48	0.46
1:D:86:VAL:HG11	1:D:219:VAL:HB	1.97	0.46
1:E:105:LYS:HD3	1:E:147:THR:HG22	1.98	0.46
1:F:264:LYS:HA	2:F:531:HOH:O	2.15	0.46
1:F:43:PRO:HB2	1:F:356:CYS:HA	1.96	0.46
1:A:156:ASP:OD1	1:A:156:ASP:N	2.46	0.46
1:E:31[A]:LYS:NZ	2:E:501:HOH:O	2.49	0.45
1:F:183:LEU:HD23	1:F:194:LEU:HD13	1.98	0.45
1:C:304:CYS:HB2	2:C:717:HOH:O	2.15	0.45
1:C:375:LEU:CD2	1:E:432:ILE:HG12	2.47	0.45
1:B:155:LYS:HE2	1:B:189:PHE:CD2	2.52	0.45
1:E:86:VAL:HG11	1:E:219:VAL:HB	1.97	0.45
1:F:295:LYS:NZ	1:F:358:MET:HE1	2.32	0.45
1:B:340:ILE:HG23	1:B:345:ASP:HB2	1.98	0.45
1:H:256:VAL:O	1:H:260:VAL:HG13	2.16	0.45
1:F:196:THR:CG2	1:F:199:ASP:H	2.24	0.45
1:B:284:LYS:O	1:B:288:GLU:HG3	2.17	0.44
1:B:132:ILE:HG23	1:B:153:THR:HB	1.99	0.44
1:H:303:ILE:C	1:H:303:ILE:CD1	2.91	0.44
1:A:384:TYR:O	2:A:501:HOH:O	2.20	0.44
1:B:91:THR:HG22	1:B:92:ALA:H	1.82	0.44
1:C:17:ILE:HD11	1:C:462:VAL:HG13	2.00	0.44
1:F:123:VAL:HG11	1:F:152:MET:CE	2.46	0.44
1:H:205:THR:N	2:H:517:HOH:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:ILE:HG12	2:E:688:HOH:O	2.17	0.44
1:H:273:ILE:HG12	1:H:293:ALA:HB3	1.99	0.44
1:B:306:THR:HG22	1:B:312:VAL:O	2.18	0.43
1:D:205:THR:HG22	1:D:207:PRO:HD3	2.00	0.43
1:E:22:GLU:HG3	1:H:254:LYS:HB2	2.00	0.43
1:E:139:ARG:NH1	2:E:512:HOH:O	2.47	0.43
1:F:358:MET:HE3	2:F:694:HOH:O	2.17	0.43
1:H:251:GLY:HA2	1:H:256:VAL:HG21	2.00	0.43
1:A:110:LEU:HD11	1:A:138:LEU:HD22	2.00	0.43
1:B:370:PRO:O	1:B:382:LYS:HE3	2.19	0.43
1:C:109:LEU:HD22	1:C:138:LEU:HD21	1.99	0.43
1:F:376:PHE:CE2	1:F:377:GLN:HG3	2.53	0.43
1:C:340:ILE:HG23	1:C:345:ASP:HB2	1.99	0.43
1:A:131:GLY:HA3	1:A:152:MET:HE2	2.01	0.43
1:F:105:LYS:HB3	1:F:107:ILE:HG22	2.01	0.43
1:F:350:MET:HE1	1:F:356:CYS:CA	2.48	0.43
1:G:7:GLU:CD	1:G:463:ARG:HH12	2.26	0.43
1:E:273:ILE:HG12	1:E:293:ALA:HB3	2.01	0.43
1:G:341:ARG:HE	1:G:341:ARG:HB2	1.63	0.43
1:F:174:LEU:HD21	1:F:182:MET:HB2	2.01	0.42
1:A:2:LEU:HD11	1:C:317:ILE:HG22	2.01	0.42
1:A:131:GLY:HA2	1:A:158:LEU:HD11	2.00	0.42
1:A:192:ARG:HD3	1:A:192:ARG:HA	1.78	0.42
1:D:17:ILE:HD11	1:D:462:VAL:HG13	2.01	0.42
1:B:71:HIS:CE1	1:B:74:MET:HE2	2.55	0.42
1:B:259:ARG:O	1:B:263:VAL:HG23	2.20	0.42
1:C:174:LEU:HD21	1:C:182:MET:HB2	2.01	0.42
1:B:95:ARG:C	1:B:97:PRO:HD3	2.45	0.42
1:E:156:ASP:OD1	1:E:156:ASP:N	2.53	0.42
1:F:192:ARG:HA	1:F:192:ARG:HD3	1.83	0.42
1:A:340:ILE:HD12	1:A:357:VAL:CG1	2.50	0.41
1:C:131:GLY:HA2	1:C:158:LEU:HD11	2.02	0.41
1:A:303:ILE:HG22	1:A:303:ILE:O	2.20	0.41
1:A:165:THR:HG22	1:A:169:GLU:HB3	2.02	0.41
1:F:72:LYS:HE3	2:F:693:HOH:O	2.20	0.41
1:C:123:VAL:HG22	1:C:131:GLY:C	2.44	0.41
1:G:292:ASP:O	1:G:333:PRO:HD2	2.21	0.41
1:F:171:LYS:HE3	1:F:197:PHE:CZ	2.56	0.41
1:H:71:HIS:CE1	1:H:74:MET:HE2	2.55	0.41
1:G:100:VAL:HG22	1:G:104:THR:CB	2.50	0.41
1:H:458:GLN:HG3	2:H:714:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:LEU:HB2	1:B:191:LEU:HB2	2.03	0.41
1:B:264:LYS:HA	1:B:264:LYS:HD2	1.82	0.41
1:B:458:GLN:HB2	1:B:459:PRO:HD3	2.03	0.41
1:G:120[B]:GLY:HA2	2:G:681:HOH:O	2.20	0.41
1:E:346:LEU:HG	1:E:357:VAL:HG21	2.03	0.40
1:F:295:LYS:HZ3	1:F:358:MET:HE1	1.85	0.40
1:G:120[A]:GLY:HA2	2:G:681:HOH:O	2.20	0.40
1:G:146:ASP:HB2	1:G:147:THR:H	1.69	0.40
1:G:161:ALA:HB2	1:G:182:MET:HE3	2.02	0.40
1:B:273:ILE:HG12	1:B:293:ALA:HB3	2.03	0.40
1:B:327:LEU:HD23	1:B:327:LEU:HA	1.86	0.40
1:D:23:VAL:HB	2:D:525:HOH:O	2.20	0.40
1:E:76:ILE:HD13	1:E:231:GLU:HG2	2.03	0.40
1:B:106:ILE:HD11	1:B:151:ILE:HD13	2.02	0.40
1:A:444:MET:HG2	1:A:455:MET:SD	2.62	0.40
1:B:198:ARG:O	1:B:202:LYS:HG2	2.22	0.40
1:A:17:ILE:HD11	1:A:462:VAL:HG13	2.03	0.40
1:H:213:GLU:OE2	1:H:214:GLN:HG3	2.22	0.40
1:H:259:ARG:O	1:H:263:VAL:HG23	2.22	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	420/509 (82%)	404 (96%)	13 (3%)	3 (1%)	18	15
1	B	405/509 (80%)	386 (95%)	13 (3%)	6 (2%)	8	4
1	C	423/509 (83%)	410 (97%)	10 (2%)	3 (1%)	18	15
1	D	312/509 (61%)	304 (97%)	8 (3%)	0	100	100
1	E	424/509 (83%)	415 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	423/509 (83%)	411 (97%)	11 (3%)	1 (0%)	43	44
1	G	421/509 (83%)	410 (97%)	10 (2%)	1 (0%)	43	44
1	H	312/509 (61%)	304 (97%)	7 (2%)	1 (0%)	36	36
All	All	3140/4072 (77%)	3044 (97%)	81 (3%)	15 (0%)	24	22

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	THR
1	B	327	LEU
1	C	146	ASP
1	A	92	ALA
1	B	328	GLU
1	B	423	VAL
1	B	89	HIS
1	B	103	SER
1	A	120	GLY
1	F	458	GLN
1	C	145	GLY
1	B	93	ILE
1	C	458	GLN
1	H	458	GLN
1	G	458	GLN

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	324/390 (83%)	324 (100%)	0	100	100
1	B	305/390 (78%)	303 (99%)	2 (1%)	76	83
1	C	327/390 (84%)	326 (100%)	1 (0%)	86	91
1	D	233/390 (60%)	232 (100%)	1 (0%)	84	89
1	E	331/390 (85%)	328 (99%)	3 (1%)	70	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	329/390 (84%)	328 (100%)	1 (0%)	86	91
1	G	328/390 (84%)	324 (99%)	4 (1%)	63	71
1	H	233/390 (60%)	232 (100%)	1 (0%)	84	89
All	All	2410/3120 (77%)	2397 (100%)	13 (0%)	84	87

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2	LEU
1	B	205	THR
1	C	2	LEU
1	D	2	LEU
1	E	158	LEU
1	E	265[A]	GLN
1	E	265[B]	GLN
1	F	196	THR
1	G	201[A]	GLU
1	G	201[B]	GLU
1	G	367[A]	GLU
1	G	367[B]	GLU
1	H	332	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	458	GLN
1	C	377	GLN
1	C	458	GLN
1	D	435	GLN
1	E	111	GLN
1	F	214	GLN
1	F	435	GLN

5.3.3 RNA ⓘ

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	425/509 (83%)	0.00	36 (8%) 16 18	22, 35, 98, 133	23 (5%)
1	B	414/509 (81%)	0.29	55 (13%) 7 7	23, 39, 76, 89	108 (26%)
1	C	429/509 (84%)	-0.26	12 (2%) 55 58	24, 34, 78, 137	19 (4%)
1	D	318/509 (62%)	-0.37	4 (1%) 75 77	26, 38, 69, 113	19 (5%)
1	E	424/509 (83%)	-0.46	5 (1%) 76 79	18, 34, 60, 85	27 (6%)
1	F	426/509 (83%)	-0.16	5 (1%) 76 79	25, 41, 69, 102	27 (6%)
1	G	424/509 (83%)	-0.38	6 (1%) 73 76	23, 35, 66, 97	22 (5%)
1	H	317/509 (62%)	-0.49	5 (1%) 70 73	23, 33, 63, 97	21 (6%)
All	All	3177/4072 (78%)	-0.22	128 (4%) 42 45	18, 36, 77, 137	266 (8%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	190	TYR	9.4
1	B	92	ALA	6.0
1	B	186	ASP	5.9
1	B	102	PRO	5.8
1	B	187	GLU	5.7
1	B	91	THR	5.7
1	A	91	THR	5.5
1	B	123	VAL	5.1
1	H	303	ILE	5.0
1	B	149	ALA	5.0
1	B	138	LEU	4.9
1	B	93	ILE	4.8
1	B	103	SER	4.8
1	B	98	VAL	4.8
1	F	1	MET	4.6
1	H	1	MET	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	113	ALA	4.3
1	C	140	VAL	4.3
1	A	1	MET	4.2
1	B	156	ASP	4.2
1	D	1	MET	4.1
1	B	104	THR	4.1
1	C	0	HIS	4.0
1	B	94	VAL	3.9
1	A	140	VAL	3.8
1	B	109	LEU	3.7
1	B	422	ARG	3.7
1	G	1	MET	3.6
1	B	188	ASN	3.6
1	D	303	ILE	3.6
1	E	303	ILE	3.6
1	B	119	SER	3.6
1	A	179	ILE	3.6
1	B	185	VAL	3.4
1	B	118	PHE	3.4
1	A	174	LEU	3.3
1	B	112	MET	3.3
1	A	204	LYS	3.3
1	C	376	PHE	3.3
1	A	197	PHE	3.2
1	A	167	LEU	3.2
1	F	140	VAL	3.1
1	A	303	ILE	3.1
1	H	467	ALA	3.1
1	C	1	MET	3.1
1	A	92	ALA	3.1
1	F	303	ILE	3.1
1	C	145	GLY	3.0
1	C	303	ILE	3.0
1	B	97	PRO	3.0
1	A	194	LEU	2.9
1	B	361	SER	2.9
1	B	99	THR	2.9
1	B	96	ASP	2.9
1	A	88	LYS	2.8
1	B	116	TYR	2.8
1	F	384	TYR	2.8
1	G	467	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	185	VAL	2.7
1	B	129	LEU	2.7
1	E	1	MET	2.7
1	B	195	VAL	2.7
1	E	467	ALA	2.6
1	B	202	LYS	2.6
1	B	303	ILE	2.6
1	G	91	THR	2.6
1	B	194	LEU	2.6
1	G	303	ILE	2.6
1	B	164	GLY	2.6
1	H	421	GLY	2.6
1	C	144	ALA	2.6
1	A	190	TYR	2.6
1	A	161	ALA	2.6
1	B	122	PRO	2.6
1	A	130	VAL	2.5
1	A	133	VAL	2.5
1	A	159	VAL	2.5
1	B	151	ILE	2.5
1	B	1	MET	2.5
1	B	192	ARG	2.5
1	E	198[A]	ARG	2.5
1	F	24	LEU	2.5
1	E	422	ARG	2.5
1	B	165	THR	2.5
1	B	166	PRO	2.5
1	A	124	VAL	2.4
1	B	191	LEU	2.4
1	C	141	LYS	2.4
1	A	90	GLU	2.4
1	A	168	GLU	2.4
1	D	373	ILE	2.4
1	A	89	HIS	2.4
1	B	198	ARG	2.3
1	B	117	GLY	2.3
1	B	203	ALA	2.3
1	B	215	GLY	2.3
1	B	121	PHE	2.3
1	A	94	VAL	2.3
1	A	376	PHE	2.2
1	B	132	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	467	ALA	2.2
1	A	196	THR	2.2
1	A	184	VAL	2.2
1	A	191	LEU	2.2
1	A	166	PRO	2.2
1	A	120	GLY	2.2
1	D	467	ALA	2.2
1	A	183	LEU	2.2
1	B	105	LYS	2.2
1	C	377	GLN	2.1
1	B	110	LEU	2.1
1	B	183	LEU	2.1
1	B	133	VAL	2.1
1	C	466	GLY	2.1
1	G	198	ARG	2.1
1	A	181	LYS	2.1
1	B	95	ARG	2.1
1	G	137	ASP	2.1
1	A	139	ARG	2.1
1	A	175	TYR	2.1
1	C	384	TYR	2.1
1	A	127	GLY	2.1
1	A	467	ALA	2.1
1	H	372	GLU	2.0
1	B	199	ASP	2.0
1	B	180	GLU	2.0
1	A	146	ASP	2.0
1	B	114	ARG	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.