wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 10:01 AM GMT

PDB ID	:	3KHJ
Title	:	C. parvum inosine monophosphate dehydrogenase bound by inhibitor C64
Authors	:	MacPherson, I.S.; Hedstrom, L.K.
Deposited on	:	2009-10-30
Resolution	:	2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

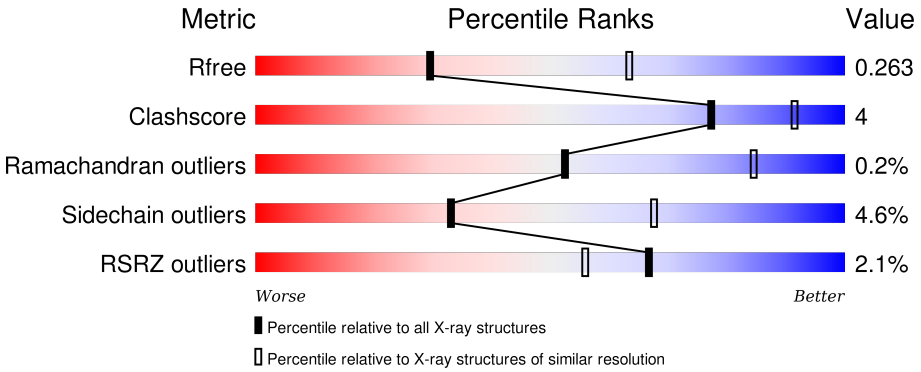
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	361	2% 74% 10% 16%
1	B	361	% 78% 9% • 12%
1	C	361	2% 73% 10% • 15%
1	D	361	79% 9% • 11%
1	E	361	2% 77% • • 17%

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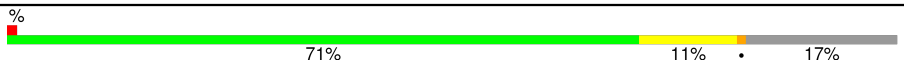
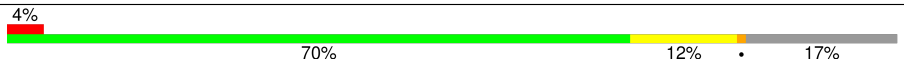
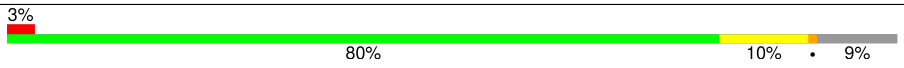
Mol	Chain	Length	Quality of chain
1	F	361	
1	G	361	
1	H	361	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	C64	D	902	-	-	-	X
3	C64	H	903	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 18502 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	302	Total	C	N	O	S	0	0	0
			2221	1404	374	431	12			
1	B	318	Total	C	N	O	S	0	1	0
			2330	1471	390	454	15			
1	C	306	Total	C	N	O	S	0	1	0
			2255	1422	383	438	12			
1	D	321	Total	C	N	O	S	0	0	0
			2322	1463	390	454	15			
1	E	298	Total	C	N	O	S	0	0	0
			2162	1369	365	416	12			
1	F	300	Total	C	N	O	S	0	1	0
			2198	1390	363	433	12			
1	G	300	Total	C	N	O	S	0	0	0
			2188	1379	370	428	11			
1	H	328	Total	C	N	O	S	0	0	0
			2355	1484	397	460	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q5CPK7
A	-1	SER	-	EXPRESSION TAG	UNP Q5CPK7
A	0	HIS	-	EXPRESSION TAG	UNP Q5CPK7
A	90	SER	-	LINKER	UNP Q5CPK7
A	91	GLY	-	LINKER	UNP Q5CPK7
A	92	GLY	-	LINKER	UNP Q5CPK7
B	-2	GLY	-	EXPRESSION TAG	UNP Q5CPK7
B	-1	SER	-	EXPRESSION TAG	UNP Q5CPK7
B	0	HIS	-	EXPRESSION TAG	UNP Q5CPK7
B	90	SER	-	LINKER	UNP Q5CPK7
B	91	GLY	-	LINKER	UNP Q5CPK7
B	92	GLY	-	LINKER	UNP Q5CPK7
C	-2	GLY	-	EXPRESSION TAG	UNP Q5CPK7

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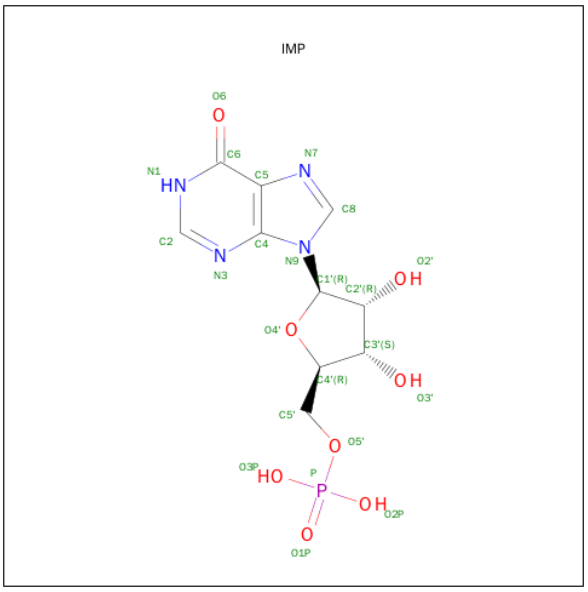
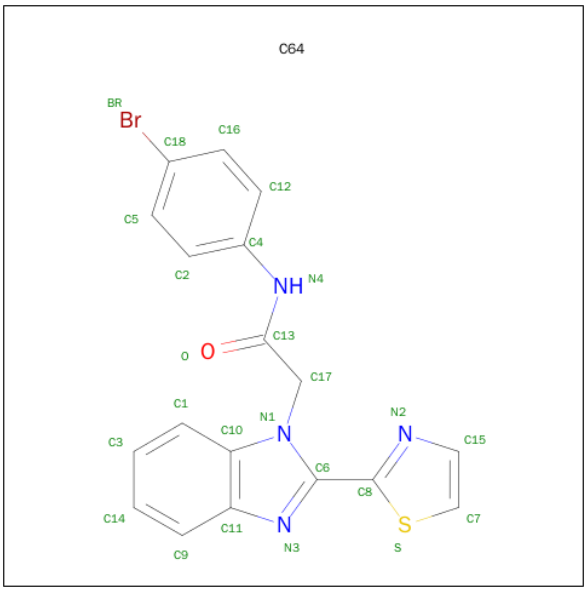
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	EXPRESSION TAG	UNP Q5CPK7
C	0	HIS	-	EXPRESSION TAG	UNP Q5CPK7
C	90	SER	-	LINKER	UNP Q5CPK7
C	91	GLY	-	LINKER	UNP Q5CPK7
C	92	GLY	-	LINKER	UNP Q5CPK7
D	-2	GLY	-	EXPRESSION TAG	UNP Q5CPK7
D	-1	SER	-	EXPRESSION TAG	UNP Q5CPK7
D	0	HIS	-	EXPRESSION TAG	UNP Q5CPK7
D	90	SER	-	LINKER	UNP Q5CPK7
D	91	GLY	-	LINKER	UNP Q5CPK7
D	92	GLY	-	LINKER	UNP Q5CPK7
E	-2	GLY	-	EXPRESSION TAG	UNP Q5CPK7
E	-1	SER	-	EXPRESSION TAG	UNP Q5CPK7
E	0	HIS	-	EXPRESSION TAG	UNP Q5CPK7
E	90	SER	-	LINKER	UNP Q5CPK7
E	91	GLY	-	LINKER	UNP Q5CPK7
E	92	GLY	-	LINKER	UNP Q5CPK7
F	-2	GLY	-	EXPRESSION TAG	UNP Q5CPK7
F	-1	SER	-	EXPRESSION TAG	UNP Q5CPK7
F	0	HIS	-	EXPRESSION TAG	UNP Q5CPK7
F	90	SER	-	LINKER	UNP Q5CPK7
F	91	GLY	-	LINKER	UNP Q5CPK7
F	92	GLY	-	LINKER	UNP Q5CPK7
G	-2	GLY	-	EXPRESSION TAG	UNP Q5CPK7
G	-1	SER	-	EXPRESSION TAG	UNP Q5CPK7
G	0	HIS	-	EXPRESSION TAG	UNP Q5CPK7
G	90	SER	-	LINKER	UNP Q5CPK7
G	91	GLY	-	LINKER	UNP Q5CPK7
G	92	GLY	-	LINKER	UNP Q5CPK7
H	-2	GLY	-	EXPRESSION TAG	UNP Q5CPK7
H	-1	SER	-	EXPRESSION TAG	UNP Q5CPK7
H	0	HIS	-	EXPRESSION TAG	UNP Q5CPK7
H	90	SER	-	LINKER	UNP Q5CPK7
H	91	GLY	-	LINKER	UNP Q5CPK7
H	92	GLY	-	LINKER	UNP Q5CPK7

- Molecule 2 is INOSINIC ACID (three-letter code: IMP) (formula: $C_{10}H_{13}N_4O_8P$).



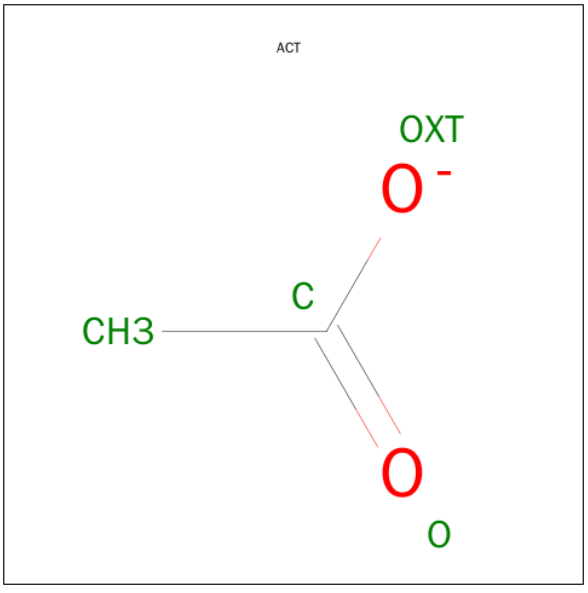
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	E	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	F	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	G	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	H	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 3 is N-(4-BROMOPHENYL)-2-[2-(1,3-THIAZOL-2-YL)-1H-BENZIMIDAZOL-1-YL]ACETAMIDE (three-letter code: C64) (formula: $C_{18}H_{13}BrN_4OS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	Br	C	N	O	S	0	0
			25	1	18	4	1	1		
3	D	1	Total	Br	C	N	O	S	0	0
			25	1	18	4	1	1		
3	H	1	Total	Br	C	N	O	S	0	0
			25	1	18	4	1	1		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	O		0	0
			4	2	2			

- Molecule 5 is water.

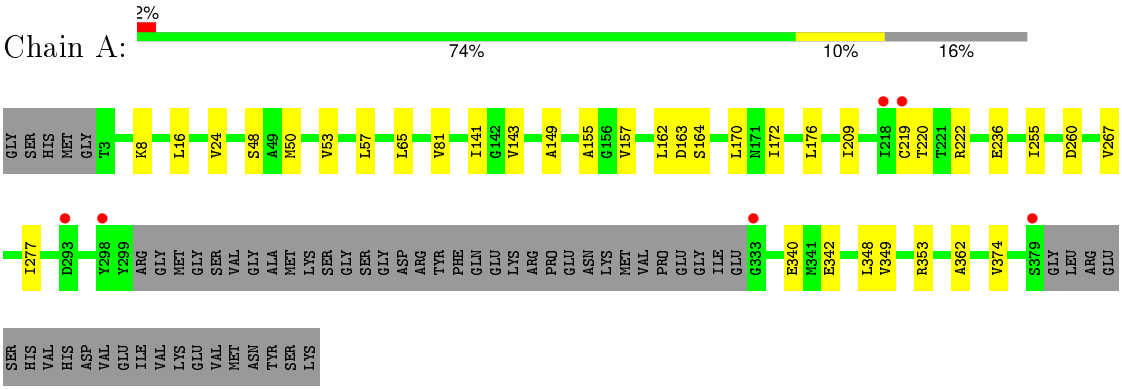
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	37	Total O 37 37	0	0
5	B	38	Total O 38 38	0	0
5	C	41	Total O 41 41	0	0
5	D	40	Total O 40 40	0	0
5	E	13	Total O 13 13	0	0
5	F	17	Total O 17 17	0	0
5	G	9	Total O 9 9	0	0
5	H	13	Total O 13 13	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

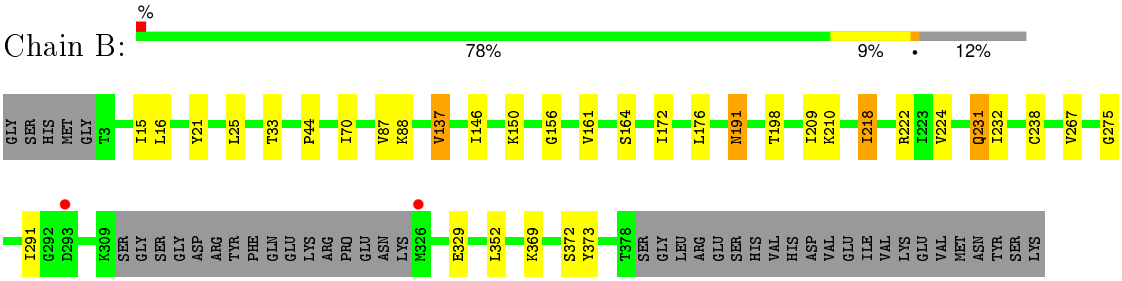
- Molecule 1: Inosine-5-monophosphate dehydrogenase

Chain A:



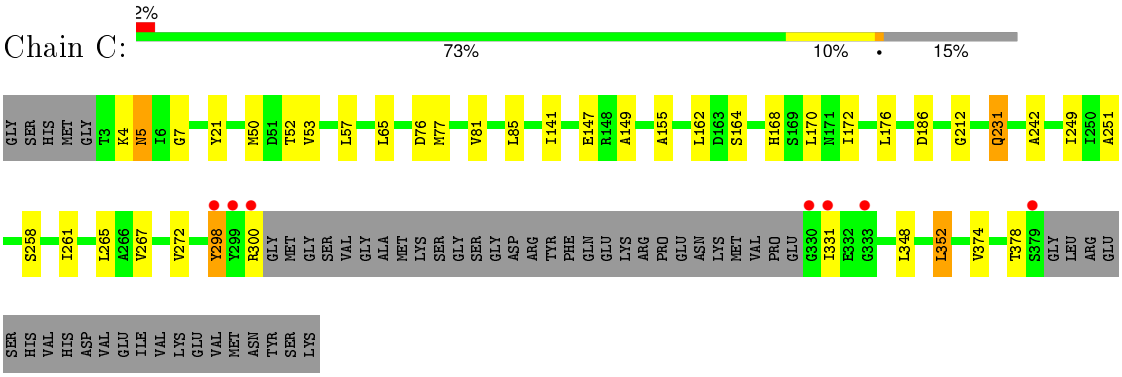
- Molecule 1: Inosine-5-monophosphate dehydrogenase

Chain B:



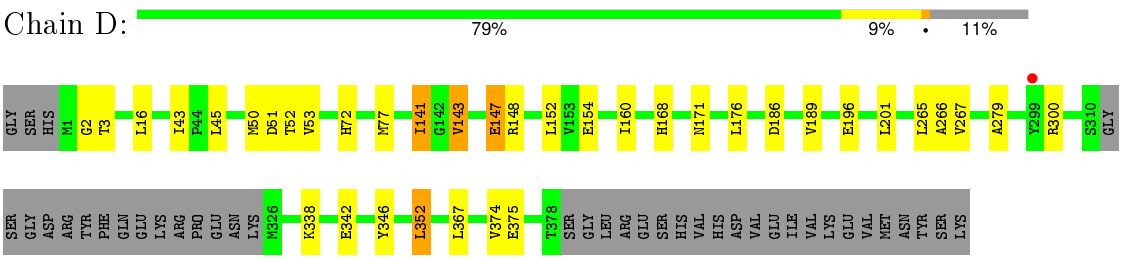
- Molecule 1: Inosine-5-monophosphate dehydrogenase

Chain C:



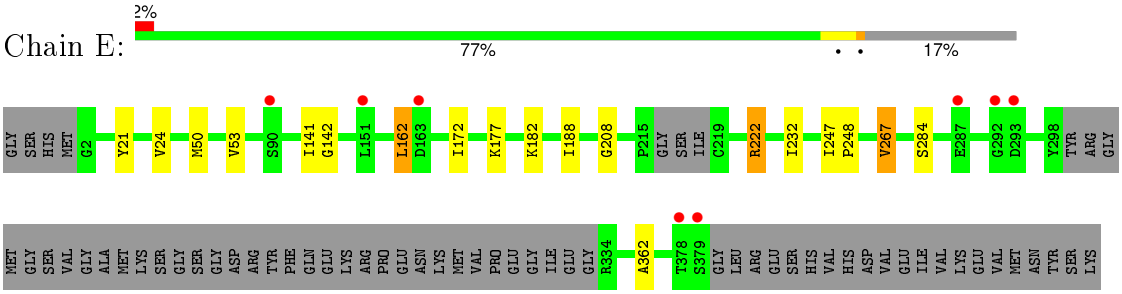
- Molecule 1: Inosine-5-monophosphate dehydrogenase

Chain D:



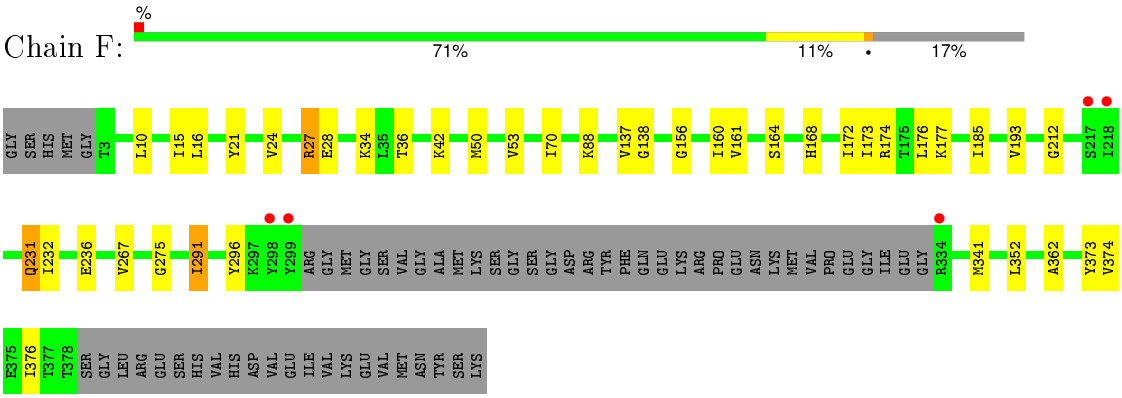
• Molecule 1: Inosine-5-monophosphate dehydrogenase

Chain E:



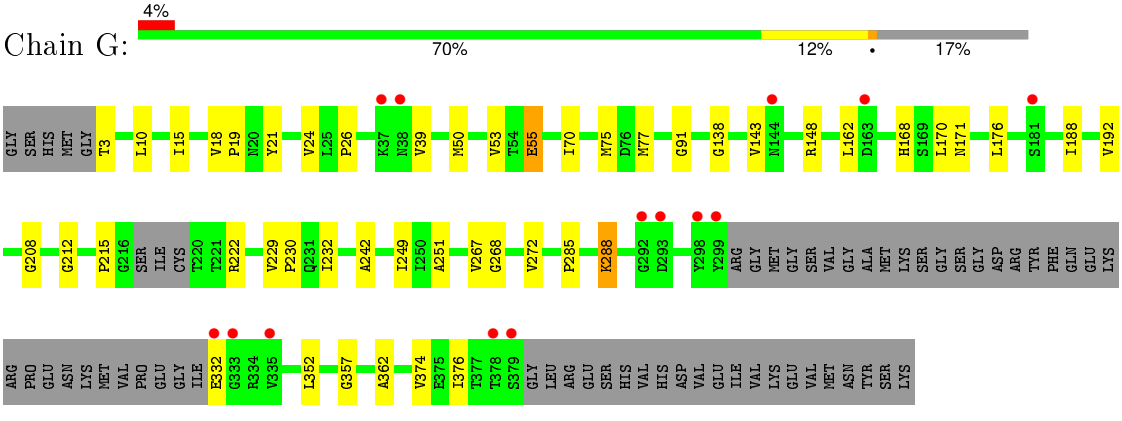
• Molecule 1: Inosine-5-monophosphate dehydrogenase

Chain F:



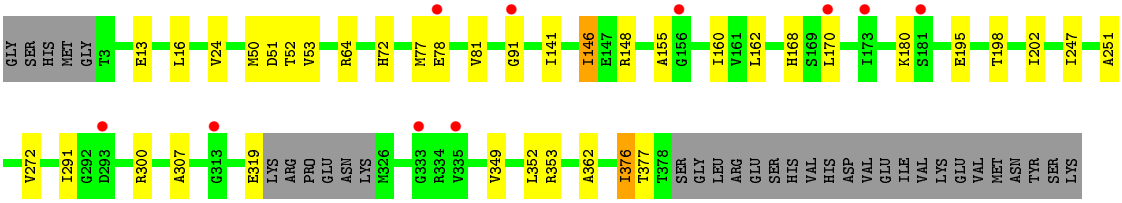
• Molecule 1: Inosine-5-monophosphate dehydrogenase

Chain G:



• Molecule 1: Inosine-5-monophosphate dehydrogenase

Chain H:


GLY SER HIS MET GLY T3 E13 L16 V24 M50 D51 T52 V53 R64 H72 M77 E78 V81 G91 I141 I146 E147 R148 A155 G156 I160 V161 L162 H168 S169 L170 I173 K180 S181 E195 T198 I202 I247 A251
V272 I291 G292 D293 R300 A307 G313 E319 LYS ARG PRO GLU ASN LYS M326 G333 R334 V335 V349 L352 R353 A362 I376 T377 T378 SER GLY LEU ARG GLU SER HIS VAL HIS ASP VAL GLU ILE VAL LYS GLU VAL MET ASN TYR SER LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.48Å 166.14Å 101.29Å 90.00° 105.14° 90.00°	Depositor
Resolution (Å)	42.13 – 2.80 42.13 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (42.13-2.80) 99.2 (42.13-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.15 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.224 , 0.266 0.222 , 0.263	Depositor DCC
R_{free} test set	3301 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	50.7	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 65224 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	18502	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IMP, C64, ACT

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	0/2243	0.49	0/3025
1	B	0.31	0/2356	0.48	0/3176
1	C	0.31	0/2279	0.50	0/3072
1	D	0.30	0/2345	0.48	0/3165
1	E	0.31	0/2181	0.46	0/2941
1	F	0.31	0/2223	0.47	0/3004
1	G	0.30	0/2209	0.46	0/2980
1	H	0.30	0/2380	0.46	0/3216
All	All	0.31	0/18216	0.48	0/24579

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2221	0	2315	17	0
1	B	2330	0	2417	21	0
1	C	2255	0	2349	20	0
1	D	2322	0	2382	19	0
1	E	2162	0	2252	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2198	0	2262	24	0
1	G	2188	0	2241	19	0
1	H	2355	0	2380	16	0
2	A	23	0	11	0	0
2	B	23	0	11	0	0
2	C	23	0	11	0	0
2	D	23	0	11	0	0
2	E	23	0	11	0	0
2	F	23	0	11	0	0
2	G	23	0	11	0	0
2	H	23	0	11	0	0
3	B	25	0	13	2	0
3	D	25	0	13	1	0
3	H	25	0	13	2	0
4	D	4	0	3	0	0
5	A	37	0	0	1	0
5	B	38	0	0	0	0
5	C	41	0	0	0	0
5	D	40	0	0	0	0
5	E	13	0	0	0	0
5	F	17	0	0	0	0
5	G	9	0	0	0	0
5	H	13	0	0	0	0
All	All	18502	0	18728	137	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.

The worst 5 of 137 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:C:231:GLN:HA	1:C:231:GLN:HE21	1.45	0.82
1:C:50:MET:HB2	1:C:53:VAL:HG12	1.64	0.79
1:D:143:VAL:HG11	1:D:171:ASN:HB3	1.66	0.77
1:C:242:ALA:HB3	1:C:249:ILE:HD11	1.67	0.75
1:E:50:MET:HB2	1:E:53:VAL:HG22	1.71	0.73

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	298/361 (82%)	288 (97%)	10 (3%)	0	100	100
1	B	315/361 (87%)	304 (96%)	10 (3%)	1 (0%)	46	79
1	C	303/361 (84%)	290 (96%)	13 (4%)	0	100	100
1	D	317/361 (88%)	307 (97%)	10 (3%)	0	100	100
1	E	292/361 (81%)	278 (95%)	14 (5%)	0	100	100
1	F	297/361 (82%)	285 (96%)	11 (4%)	1 (0%)	46	79
1	G	294/361 (81%)	279 (95%)	12 (4%)	3 (1%)	19	52
1	H	324/361 (90%)	300 (93%)	23 (7%)	1 (0%)	46	79
All	All	2440/2888 (84%)	2331 (96%)	103 (4%)	6 (0%)	52	84

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	91	GLY
1	H	91	GLY
1	G	212	GLY
1	G	268	GLY
1	B	275	GLY

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	243/295 (82%)	232 (96%)	11 (4%)	34	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	253/295 (86%)	243 (96%)	10 (4%)	38 73
1	C	246/295 (83%)	231 (94%)	15 (6%)	23 55
1	D	248/295 (84%)	238 (96%)	10 (4%)	38 73
1	E	233/295 (79%)	227 (97%)	6 (3%)	54 86
1	F	239/295 (81%)	228 (95%)	11 (5%)	33 67
1	G	234/295 (79%)	219 (94%)	15 (6%)	22 52
1	H	247/295 (84%)	236 (96%)	11 (4%)	34 68
All	All	1943/2360 (82%)	1854 (95%)	89 (5%)	33 67

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	154	GLU
1	E	222	ARG
1	H	162	LEU
1	D	176	LEU
1	D	374	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	204	ASN
1	C	231	GLN
1	G	5	ASN
1	C	171	ASN
1	F	231	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	IMP	A	801	-	20,25,25	1.41	3 (15%)	22,38,38	2.76	3 (13%)
2	IMP	B	804	-	20,25,25	1.37	3 (15%)	22,38,38	2.66	3 (13%)
3	C64	B	901	-	24,28,28	1.40	3 (12%)	28,39,39	0.84	2 (7%)
2	IMP	C	803	-	20,25,25	1.36	3 (15%)	22,38,38	2.69	3 (13%)
4	ACT	D	401	-	1,3,3	1.21	0	0,3,3	0.00	-
2	IMP	D	802	-	20,25,25	1.39	3 (15%)	22,38,38	2.66	3 (13%)
3	C64	D	902	-	24,28,28	1.39	3 (12%)	28,39,39	0.92	3 (10%)
2	IMP	E	805	-	20,25,25	1.41	3 (15%)	22,38,38	2.74	2 (9%)
2	IMP	F	808	-	20,25,25	1.43	3 (15%)	22,38,38	2.78	3 (13%)
2	IMP	G	807	-	20,25,25	1.39	3 (15%)	22,38,38	2.77	3 (13%)
2	IMP	H	806	-	20,25,25	1.35	3 (15%)	22,38,38	2.59	3 (13%)
3	C64	H	903	-	24,28,28	1.40	3 (12%)	28,39,39	0.85	2 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IMP	A	801	-	-	0/6/26/26	0/3/3/3
2	IMP	B	804	-	-	0/6/26/26	0/3/3/3
3	C64	B	901	-	-	0/8/12/12	0/4/4/4
2	IMP	C	803	-	-	0/6/26/26	0/3/3/3
4	ACT	D	401	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IMP	D	802	-	-	0/6/26/26	0/3/3/3
3	C64	D	902	-	-	0/8/12/12	0/4/4/4
2	IMP	E	805	-	-	0/6/26/26	0/3/3/3
2	IMP	F	808	-	-	0/6/26/26	0/3/3/3
2	IMP	G	807	-	-	0/6/26/26	0/3/3/3
2	IMP	H	806	-	-	0/6/26/26	0/3/3/3
3	C64	H	903	-	-	0/8/12/12	0/4/4/4

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	901	C64	C4-N4	-2.67	1.36	1.41
3	H	903	C64	C4-N4	-2.62	1.36	1.41
3	D	902	C64	C4-N4	-2.51	1.36	1.41
3	D	902	C64	C8-N2	2.44	1.35	1.31
3	H	903	C64	C8-N2	2.52	1.35	1.31

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	808	IMP	N3-C2-N1	-11.84	119.83	128.89
2	G	807	IMP	N3-C2-N1	-11.82	119.84	128.89
2	A	801	IMP	N3-C2-N1	-11.80	119.86	128.89
2	E	805	IMP	N3-C2-N1	-11.73	119.91	128.89
2	D	802	IMP	N3-C2-N1	-11.55	120.05	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	901	C64	2	0
3	D	902	C64	1	0
3	H	903	C64	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	302/361 (83%)	-0.24	6 (1%)	68	58	28, 38, 55, 68	0
1	B	318/361 (88%)	-0.15	2 (0%)	90	86	31, 40, 59, 63	0
1	C	306/361 (84%)	-0.24	7 (2%)	64	52	23, 37, 55, 64	0
1	D	321/361 (88%)	-0.25	1 (0%)	94	92	28, 38, 58, 70	0
1	E	298/361 (82%)	0.05	8 (2%)	58	45	50, 64, 86, 88	0
1	F	300/361 (83%)	0.01	5 (1%)	73	63	50, 62, 76, 77	0
1	G	300/361 (83%)	0.29	14 (4%)	35	24	57, 73, 93, 94	0
1	H	328/361 (90%)	0.18	10 (3%)	54	41	52, 66, 84, 85	0
All	All	2473/2888 (85%)	-0.04	53 (2%)	67	56	23, 54, 83, 94	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	218	ILE	6.2
1	C	331	ILE	5.5
1	F	299	TYR	4.5
1	F	298	TYR	4.1
1	A	379	SER	3.9

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	C64	H	903	25/25	0.83	0.41	5.38	51,52,52,52	25
3	C64	D	902	25/25	0.80	0.37	3.16	50,50,50,51	25
3	C64	B	901	25/25	0.89	0.29	1.48	54,54,54,54	25
2	IMP	G	807	23/23	0.84	0.20	0.36	104,105,105,105	0
2	IMP	E	805	23/23	0.83	0.21	0.10	79,81,82,82	0
2	IMP	A	801	23/23	0.91	0.17	-0.04	57,61,62,62	0
2	IMP	F	808	23/23	0.87	0.19	-0.15	56,59,61,61	0
2	IMP	C	803	23/23	0.94	0.16	-0.36	44,49,50,50	0
2	IMP	H	806	23/23	0.96	0.14	-1.06	51,52,52,53	0
2	IMP	B	804	23/23	0.96	0.12	-1.07	46,48,49,49	0
2	IMP	D	802	23/23	0.96	0.13	-1.25	39,41,41,41	0
4	ACT	D	401	4/4	0.78	0.17	-1.46	95,95,95,95	0

6.5 Other polymers

There are no such residues in this entry.