wwPDB X-ray Structure Validation Summary Report (i)

Apr 29, 2024 – 05:00 am BST

PDB ID	:	4ZDA
Title	:	Crystal structure of isocitrate dehydrogenase in complex with isocitrate and Mn from M. smegmatis
Authors	:	Pojer, F.; Murima, P.; McKinney, J.D.
Deposited on	:	2015-04-17
Resolution	:	2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

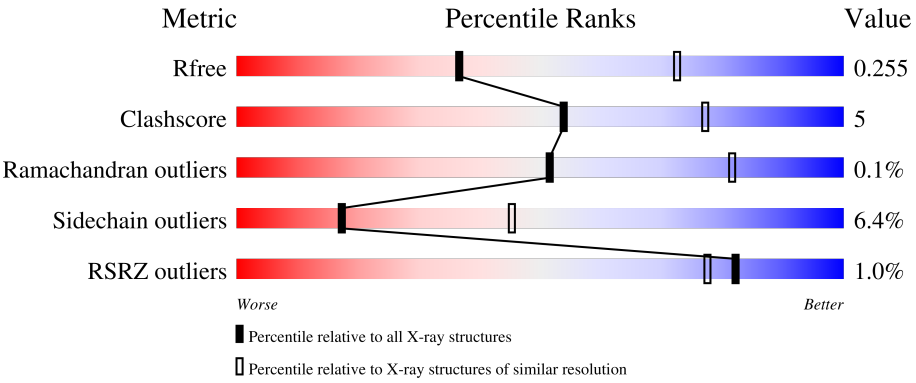
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	767	79% 15%
1	B	767	78% 16%
1	C	767	81% 13%
1	D	767	79% 15%
1	E	767	81% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	767	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 34561 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 Isocitrate dehydrogenase (NADP) Icd2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	735	Total	C	N	O	S	0	1	0
			5752	3635	984	1106	27			
1	B	735	Total	C	N	O	S	0	0	0
			5745	3630	982	1106	27			
1	C	735	Total	C	N	O	S	0	0	0
			5745	3630	982	1106	27			
1	D	735	Total	C	N	O	S	0	0	0
			5745	3630	982	1106	27			
1	E	735	Total	C	N	O	S	0	0	0
			5745	3630	982	1106	27			
1	F	735	Total	C	N	O	S	0	0	0
			5745	3630	982	1106	27			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	744	PRO	-	expression tag	UNP A0QSZ3
A	745	ARG	-	expression tag	UNP A0QSZ3
A	746	TYR	-	expression tag	UNP A0QSZ3
A	747	PRO	-	expression tag	UNP A0QSZ3
A	748	TYR	-	expression tag	UNP A0QSZ3
A	749	ASP	-	expression tag	UNP A0QSZ3
A	750	VAL	-	expression tag	UNP A0QSZ3
A	751	PRO	-	expression tag	UNP A0QSZ3
A	752	ASP	-	expression tag	UNP A0QSZ3
A	753	TYR	-	expression tag	UNP A0QSZ3
A	754	ALA	-	expression tag	UNP A0QSZ3
A	755	LYS	-	expression tag	UNP A0QSZ3
A	756	LEU	-	expression tag	UNP A0QSZ3
A	757	ALA	-	expression tag	UNP A0QSZ3
A	758	ALA	-	expression tag	UNP A0QSZ3
A	759	ALA	-	expression tag	UNP A0QSZ3
A	760	LEU	-	expression tag	UNP A0QSZ3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	761	GLU	-	expression tag	UNP A0QSZ3
A	762	HIS	-	expression tag	UNP A0QSZ3
A	763	HIS	-	expression tag	UNP A0QSZ3
A	764	HIS	-	expression tag	UNP A0QSZ3
A	765	HIS	-	expression tag	UNP A0QSZ3
A	766	HIS	-	expression tag	UNP A0QSZ3
A	767	HIS	-	expression tag	UNP A0QSZ3
B	744	PRO	-	expression tag	UNP A0QSZ3
B	745	ARG	-	expression tag	UNP A0QSZ3
B	746	TYR	-	expression tag	UNP A0QSZ3
B	747	PRO	-	expression tag	UNP A0QSZ3
B	748	TYR	-	expression tag	UNP A0QSZ3
B	749	ASP	-	expression tag	UNP A0QSZ3
B	750	VAL	-	expression tag	UNP A0QSZ3
B	751	PRO	-	expression tag	UNP A0QSZ3
B	752	ASP	-	expression tag	UNP A0QSZ3
B	753	TYR	-	expression tag	UNP A0QSZ3
B	754	ALA	-	expression tag	UNP A0QSZ3
B	755	LYS	-	expression tag	UNP A0QSZ3
B	756	LEU	-	expression tag	UNP A0QSZ3
B	757	ALA	-	expression tag	UNP A0QSZ3
B	758	ALA	-	expression tag	UNP A0QSZ3
B	759	ALA	-	expression tag	UNP A0QSZ3
B	760	LEU	-	expression tag	UNP A0QSZ3
B	761	GLU	-	expression tag	UNP A0QSZ3
B	762	HIS	-	expression tag	UNP A0QSZ3
B	763	HIS	-	expression tag	UNP A0QSZ3
B	764	HIS	-	expression tag	UNP A0QSZ3
B	765	HIS	-	expression tag	UNP A0QSZ3
B	766	HIS	-	expression tag	UNP A0QSZ3
B	767	HIS	-	expression tag	UNP A0QSZ3
C	744	PRO	-	expression tag	UNP A0QSZ3
C	745	ARG	-	expression tag	UNP A0QSZ3
C	746	TYR	-	expression tag	UNP A0QSZ3
C	747	PRO	-	expression tag	UNP A0QSZ3
C	748	TYR	-	expression tag	UNP A0QSZ3
C	749	ASP	-	expression tag	UNP A0QSZ3
C	750	VAL	-	expression tag	UNP A0QSZ3
C	751	PRO	-	expression tag	UNP A0QSZ3
C	752	ASP	-	expression tag	UNP A0QSZ3
C	753	TYR	-	expression tag	UNP A0QSZ3
C	754	ALA	-	expression tag	UNP A0QSZ3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	755	LYS	-	expression tag	UNP A0QSZ3
C	756	LEU	-	expression tag	UNP A0QSZ3
C	757	ALA	-	expression tag	UNP A0QSZ3
C	758	ALA	-	expression tag	UNP A0QSZ3
C	759	ALA	-	expression tag	UNP A0QSZ3
C	760	LEU	-	expression tag	UNP A0QSZ3
C	761	GLU	-	expression tag	UNP A0QSZ3
C	762	HIS	-	expression tag	UNP A0QSZ3
C	763	HIS	-	expression tag	UNP A0QSZ3
C	764	HIS	-	expression tag	UNP A0QSZ3
C	765	HIS	-	expression tag	UNP A0QSZ3
C	766	HIS	-	expression tag	UNP A0QSZ3
C	767	HIS	-	expression tag	UNP A0QSZ3
D	744	PRO	-	expression tag	UNP A0QSZ3
D	745	ARG	-	expression tag	UNP A0QSZ3
D	746	TYR	-	expression tag	UNP A0QSZ3
D	747	PRO	-	expression tag	UNP A0QSZ3
D	748	TYR	-	expression tag	UNP A0QSZ3
D	749	ASP	-	expression tag	UNP A0QSZ3
D	750	VAL	-	expression tag	UNP A0QSZ3
D	751	PRO	-	expression tag	UNP A0QSZ3
D	752	ASP	-	expression tag	UNP A0QSZ3
D	753	TYR	-	expression tag	UNP A0QSZ3
D	754	ALA	-	expression tag	UNP A0QSZ3
D	755	LYS	-	expression tag	UNP A0QSZ3
D	756	LEU	-	expression tag	UNP A0QSZ3
D	757	ALA	-	expression tag	UNP A0QSZ3
D	758	ALA	-	expression tag	UNP A0QSZ3
D	759	ALA	-	expression tag	UNP A0QSZ3
D	760	LEU	-	expression tag	UNP A0QSZ3
D	761	GLU	-	expression tag	UNP A0QSZ3
D	762	HIS	-	expression tag	UNP A0QSZ3
D	763	HIS	-	expression tag	UNP A0QSZ3
D	764	HIS	-	expression tag	UNP A0QSZ3
D	765	HIS	-	expression tag	UNP A0QSZ3
D	766	HIS	-	expression tag	UNP A0QSZ3
D	767	HIS	-	expression tag	UNP A0QSZ3
E	744	PRO	-	expression tag	UNP A0QSZ3
E	745	ARG	-	expression tag	UNP A0QSZ3
E	746	TYR	-	expression tag	UNP A0QSZ3
E	747	PRO	-	expression tag	UNP A0QSZ3
E	748	TYR	-	expression tag	UNP A0QSZ3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	749	ASP	-	expression tag	UNP A0QSZ3
E	750	VAL	-	expression tag	UNP A0QSZ3
E	751	PRO	-	expression tag	UNP A0QSZ3
E	752	ASP	-	expression tag	UNP A0QSZ3
E	753	TYR	-	expression tag	UNP A0QSZ3
E	754	ALA	-	expression tag	UNP A0QSZ3
E	755	LYS	-	expression tag	UNP A0QSZ3
E	756	LEU	-	expression tag	UNP A0QSZ3
E	757	ALA	-	expression tag	UNP A0QSZ3
E	758	ALA	-	expression tag	UNP A0QSZ3
E	759	ALA	-	expression tag	UNP A0QSZ3
E	760	LEU	-	expression tag	UNP A0QSZ3
E	761	GLU	-	expression tag	UNP A0QSZ3
E	762	HIS	-	expression tag	UNP A0QSZ3
E	763	HIS	-	expression tag	UNP A0QSZ3
E	764	HIS	-	expression tag	UNP A0QSZ3
E	765	HIS	-	expression tag	UNP A0QSZ3
E	766	HIS	-	expression tag	UNP A0QSZ3
E	767	HIS	-	expression tag	UNP A0QSZ3
F	744	PRO	-	expression tag	UNP A0QSZ3
F	745	ARG	-	expression tag	UNP A0QSZ3
F	746	TYR	-	expression tag	UNP A0QSZ3
F	747	PRO	-	expression tag	UNP A0QSZ3
F	748	TYR	-	expression tag	UNP A0QSZ3
F	749	ASP	-	expression tag	UNP A0QSZ3
F	750	VAL	-	expression tag	UNP A0QSZ3
F	751	PRO	-	expression tag	UNP A0QSZ3
F	752	ASP	-	expression tag	UNP A0QSZ3
F	753	TYR	-	expression tag	UNP A0QSZ3
F	754	ALA	-	expression tag	UNP A0QSZ3
F	755	LYS	-	expression tag	UNP A0QSZ3
F	756	LEU	-	expression tag	UNP A0QSZ3
F	757	ALA	-	expression tag	UNP A0QSZ3
F	758	ALA	-	expression tag	UNP A0QSZ3
F	759	ALA	-	expression tag	UNP A0QSZ3
F	760	LEU	-	expression tag	UNP A0QSZ3
F	761	GLU	-	expression tag	UNP A0QSZ3
F	762	HIS	-	expression tag	UNP A0QSZ3
F	763	HIS	-	expression tag	UNP A0QSZ3
F	764	HIS	-	expression tag	UNP A0QSZ3
F	765	HIS	-	expression tag	UNP A0QSZ3
F	766	HIS	-	expression tag	UNP A0QSZ3

Continued on next page...

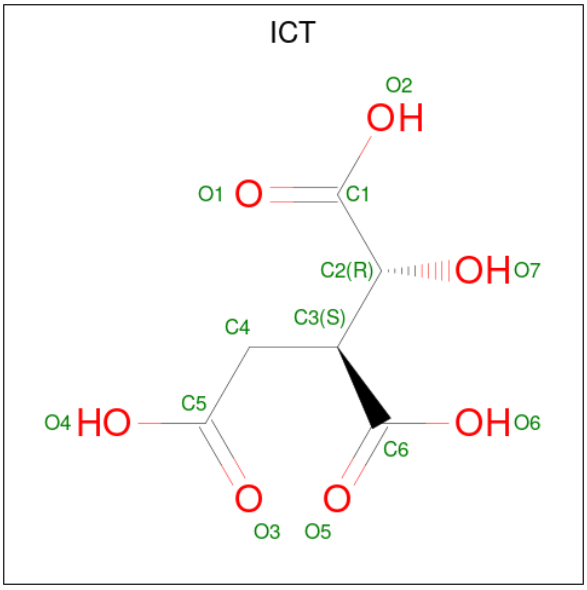
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	767	HIS	-	expression tag	UNP A0QSZ3

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	E	1	Total Mn 1 1	0	0
2	F	1	Total Mn 1 1	0	0

- Molecule 3 is ISOCITRIC ACID (three-letter code: ICT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 6 7	0	0
3	B	1	Total C O 13 6 7	0	0
3	C	1	Total C O 13 6 7	0	0

Continued on next page...

Continued from previous page...

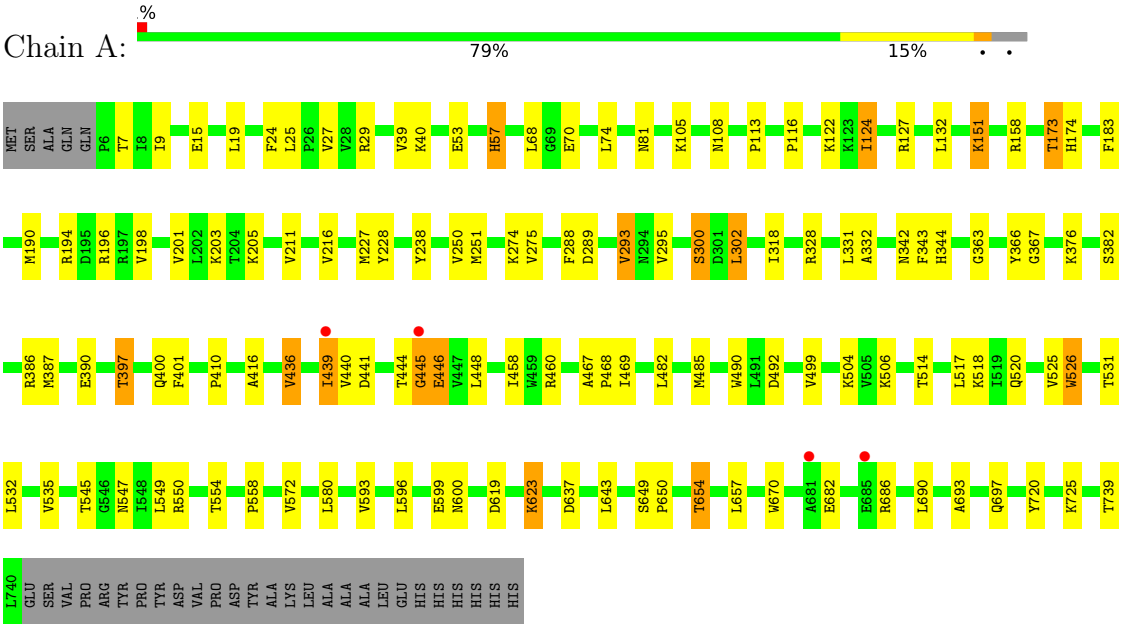
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 13 6 7	0	0
3	E	1	Total C O 13 6 7	0	0
3	F	1	Total C O 13 6 7	0	0

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.

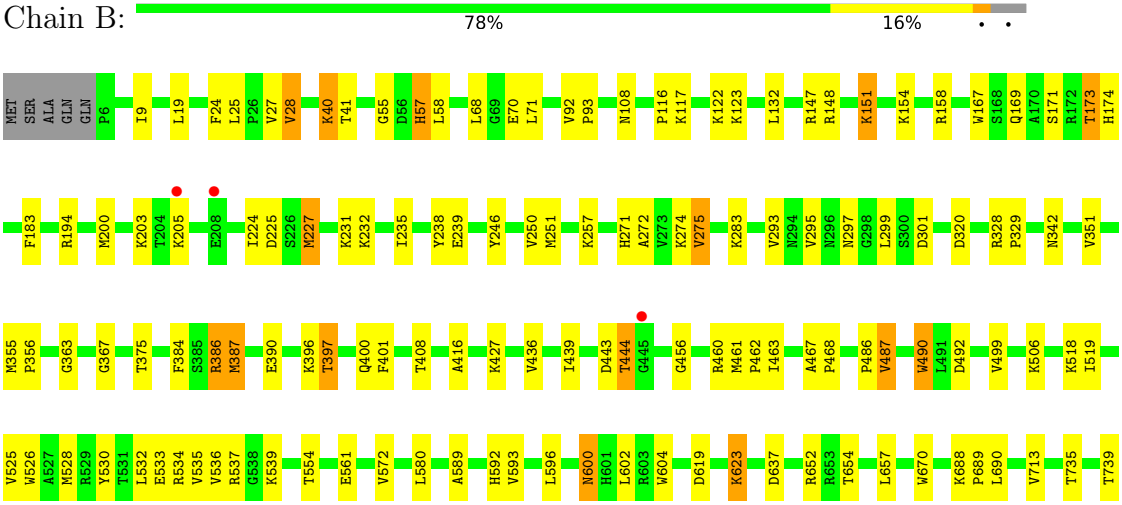
• Molecule 1: Isocitrate dehydrogenase (NADP) Icd2

Chain A:



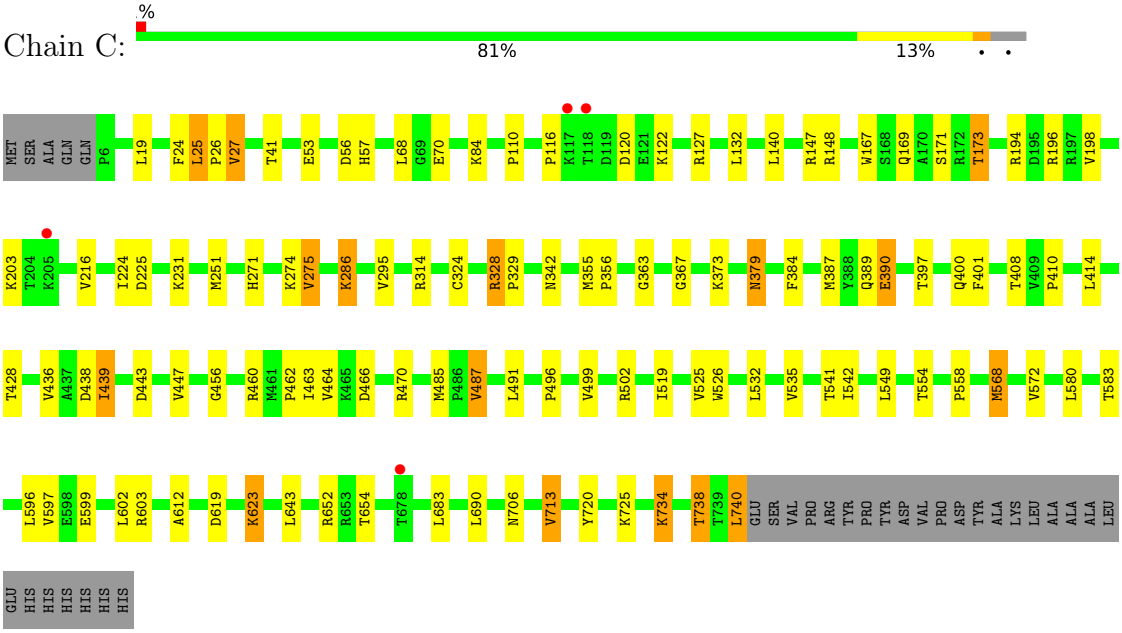
• Molecule 1: Isocitrate dehydrogenase (NADP) Icd2

Chain B:



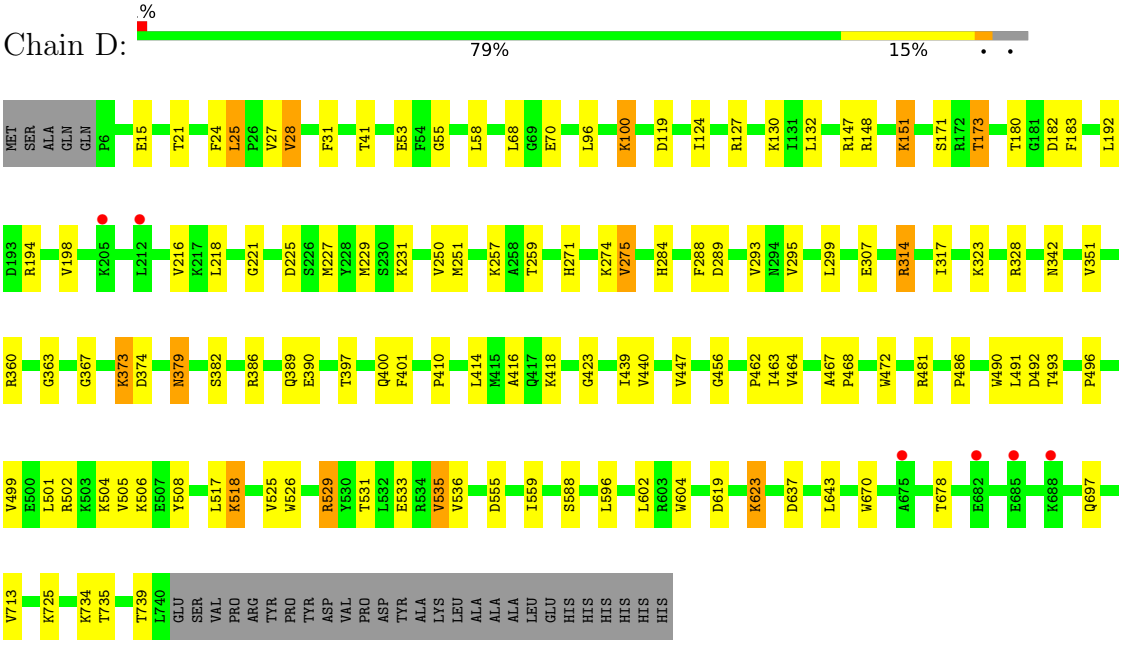
• Molecule 1: Isocitrate dehydrogenase (NADP) Icd2

Chain C:



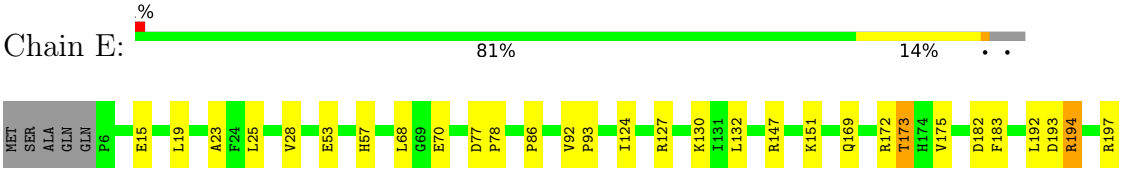
• Molecule 1: Isocitrate dehydrogenase (NADP) Icd2

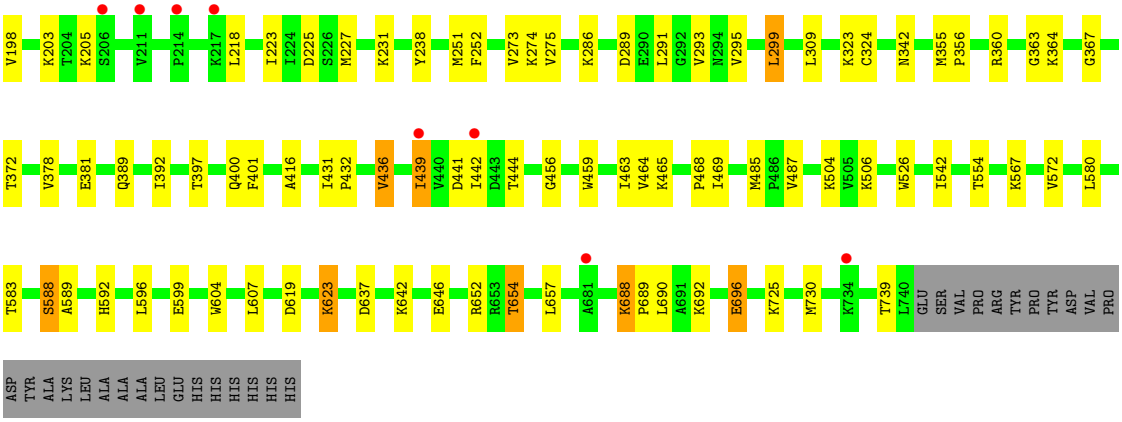
Chain D:



• Molecule 1: Isocitrate dehydrogenase (NADP) Icd2

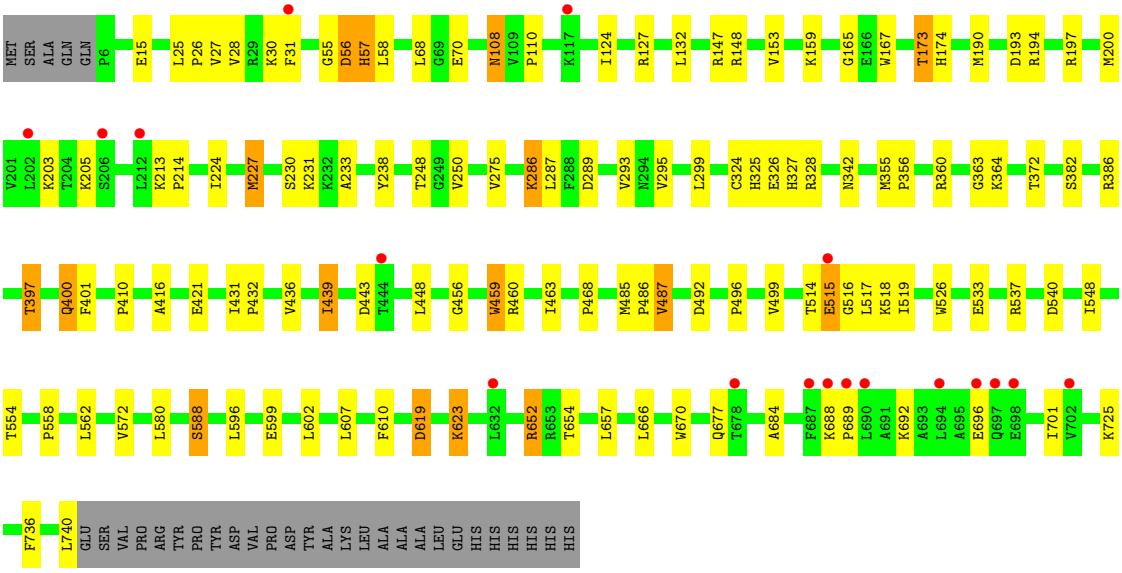
Chain E:





• Molecule 1: Isocitrate dehydrogenase (NADP) Icd2

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	201.77Å 206.16Å 145.60Å 90.00° 90.97° 90.00°	Depositor
Resolution (Å)	48.59 – 2.80 48.59 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.59-2.80) 99.2 (48.59-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.214 , 0.257 0.211 , 0.255	Depositor DCC
R_{free} test set	7271 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	68.2	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 26.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -1/2*h-1/2*k-l,1/2*h+1/2*k-l,1/2*h-1/2*k 0.028 for -1/2*h-1/2*k+l,1/2*h+1/2*k+l,-1/2*h+1/2*k 0.023 for -1/2*h+1/2*k+l,-1/2*h+1/2*k-l,-1/2*h-1/2*k 0.029 for -1/2*h+1/2*k-l,-1/2*h+1/2*k+l,1/2*h+1/2*k 0.013 for k,h,-l 0.014 for -k,-h,-l 0.017 for -1/2*h+1/2*k-l,1/2*h-1/2*k-l,-1/2*h-1/2*k 0.010 for -1/2*h-1/2*k-l,-1/2*h-1/2*k+l,-1/2*h+1/2*k 0.011 for -1/2*h+1/2*k+l,1/2*h-1/2*k+l,1/2*h+1/2*k 0.017 for -1/2*h-1/2*k+l,-1/2*h-1/2*k-l,1/2*h-1/2*k 0.021 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	34561	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

[1] Intensities estimated from amplitudes.

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

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ICT, MN

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	0.41	2/5870 (0.0%)	0.52	0/7936
1	B	0.42	5/5859 (0.1%)	0.52	0/7921
1	C	0.41	2/5859 (0.0%)	0.55	1/7921 (0.0%)
1	D	0.42	4/5859 (0.1%)	0.51	0/7921
1	E	0.42	3/5859 (0.1%)	0.50	0/7921
1	F	0.42	3/5859 (0.1%)	0.50	0/7921
All	All	0.42	19/35165 (0.1%)	0.52	1/47541 (0.0%)

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	604	TRP	CD2-CE2	5.41	1.47	1.41
1	B	604	TRP	CD2-CE2	5.29	1.47	1.41
1	B	526	TRP	CD2-CE2	5.21	1.47	1.41
1	D	490	TRP	CD2-CE2	5.19	1.47	1.41
1	D	670	TRP	CD2-CE2	5.14	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	740	LEU	CA-C-O	-17.14	84.12	120.10

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	5752	0	5752	74	0
1	B	5745	0	5745	73	0
1	C	5745	0	5745	52	0
1	D	5745	0	5745	61	0
1	E	5745	0	5745	50	0
1	F	5745	0	5745	64	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	13	0	5	0	0
3	B	13	0	5	0	0
3	C	13	0	5	0	0
3	D	13	0	5	0	0
3	E	13	0	5	0	0
3	F	13	0	4	0	0
All	All	34561	0	34506	367	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 367 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:E:251:MET:HE1	1:E:367:GLY:HA2	1.45	0.98
1:A:251:MET:CE	1:A:367:GLY:HA2	1.93	0.98
1:C:485:MET:HE2	1:C:542:ILE:HG13	1.48	0.96
1:A:400:GLN:HE21	1:A:401:PHE:H	1.16	0.94
1:A:173:THR:HG21	1:A:363:GLY:O	1.69	0.92

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	734/767 (96%)	713 (97%)	19 (3%)	2 (0%)	41 72
1	B	733/767 (96%)	708 (97%)	23 (3%)	2 (0%)	41 72
1	C	733/767 (96%)	712 (97%)	21 (3%)	0	100 100
1	D	733/767 (96%)	707 (96%)	26 (4%)	0	100 100
1	E	733/767 (96%)	708 (97%)	24 (3%)	1 (0%)	51 81
1	F	733/767 (96%)	706 (96%)	26 (4%)	1 (0%)	51 81
All	All	4399/4602 (96%)	4254 (97%)	139 (3%)	6 (0%)	51 81

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	444	THR
1	B	600	ASN
1	E	444	THR
1	F	515	GLU
1	A	445	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	620/646 (96%)	584 (94%)	36 (6%)	20 50
1	B	619/646 (96%)	579 (94%)	40 (6%)	17 44
1	C	619/646 (96%)	579 (94%)	40 (6%)	17 44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	619/646 (96%)	574 (93%)	45 (7%)	14 38
1	E	619/646 (96%)	578 (93%)	41 (7%)	16 44
1	F	619/646 (96%)	584 (94%)	35 (6%)	20 50
All	All	3715/3876 (96%)	3478 (94%)	237 (6%)	17 45

5 of 237 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	740	LEU
1	F	325	HIS
1	D	379	ASN
1	F	299	LEU
1	F	725	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	400	GLN
1	E	400	GLN
1	D	592	HIS
1	E	108	ASN
1	E	672	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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	$\#\|Z\| > 2$
3	ICT	E	802	2	12,12,12	1.06	0	13,16,16	1.19	2 (15%)
3	ICT	D	802	2	12,12,12	1.08	0	13,16,16	1.18	0
3	ICT	F	802	2	12,12,12	1.12	0	13,16,16	1.22	2 (15%)
3	ICT	A	802	2	12,12,12	1.09	0	13,16,16	1.33	3 (23%)
3	ICT	B	802	2	12,12,12	1.15	0	13,16,16	1.04	0
3	ICT	C	802	2	12,12,12	1.13	0	13,16,16	1.08	1 (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
3	ICT	E	802	2	-	2/16/16/16	-
3	ICT	D	802	2	-	3/16/16/16	-
3	ICT	F	802	2	-	9/16/16/16	-
3	ICT	A	802	2	-	4/16/16/16	-
3	ICT	B	802	2	-	2/16/16/16	-
3	ICT	C	802	2	-	3/16/16/16	-

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	802	ICT	O2-C1-C2	2.49	120.01	113.27
3	A	802	ICT	O6-C6-C3	2.40	120.64	114.03
3	F	802	ICT	O2-C1-C2	2.07	118.86	113.27
3	A	802	ICT	O5-C6-C3	-2.05	117.80	122.95
3	E	802	ICT	O4-C5-C4	2.05	120.65	114.07

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	802	ICT	C4-C3-C6-O5
3	F	802	ICT	C1-C2-C3-C4
3	F	802	ICT	O7-C2-C3-C4
3	B	802	ICT	O1-C1-C2-O7
3	B	802	ICT	O2-C1-C2-O7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	735/767 (95%)	-0.16	4 (0%)	91	88	37, 57, 86, 116	0
1	B	735/767 (95%)	-0.14	3 (0%)	92	91	41, 61, 91, 112	0
1	C	735/767 (95%)	-0.14	4 (0%)	91	88	42, 64, 95, 127	0
1	D	735/767 (95%)	-0.07	6 (0%)	86	81	39, 68, 102, 118	0
1	E	735/767 (95%)	0.05	8 (1%)	80	75	49, 71, 97, 126	0
1	F	735/767 (95%)	0.07	18 (2%)	59	49	48, 73, 105, 135	0
All	All	4410/4602 (95%)	-0.07	43 (0%)	82	77	37, 66, 98, 135	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	690	LEU	5.2
1	B	445	GLY	3.2
1	D	205	LYS	3.1
1	E	206	SER	3.1
1	E	734	LYS	3.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

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. 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	B-factors(Å^2)	Q<0.9
3	ICT	F	802	13/13	0.93	0.24	70,75,79,80	0
3	ICT	D	802	13/13	0.94	0.17	60,64,71,73	0
3	ICT	B	802	13/13	0.95	0.22	57,58,61,61	0
3	ICT	E	802	13/13	0.95	0.22	64,68,72,74	0
3	ICT	C	802	13/13	0.95	0.20	58,59,63,63	0
2	MN	C	801	1/1	0.96	0.19	68,68,68,68	0
2	MN	E	801	1/1	0.96	0.20	86,86,86,86	0
3	ICT	A	802	13/13	0.96	0.20	57,59,60,61	0
2	MN	B	801	1/1	0.96	0.16	65,65,65,65	0
2	MN	D	801	1/1	0.98	0.21	70,70,70,70	0
2	MN	A	801	1/1	0.98	0.23	66,66,66,66	0
2	MN	F	801	1/1	0.98	0.22	80,80,80,80	0

6.5 Other polymers (i)

There are no such residues in this entry.