wwPDB X-ray Structure Validation Summary Report (i)

Nov 21, 2023 – 01:38 AM JST

PDB ID	:	7EBE
Title	:	Crystal structure of Isocitrate lyase-1 from Candida albicans
Authors	:	Hiragi, K.; Nishio, K.; Moriyama, S.; Hamaguchi, T.; Mizoguchi, A.; Yonekura, K.; Tani, K.; Mizushima, T.
Deposited on	:	2021-03-09
Resolution	:	2.69 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:

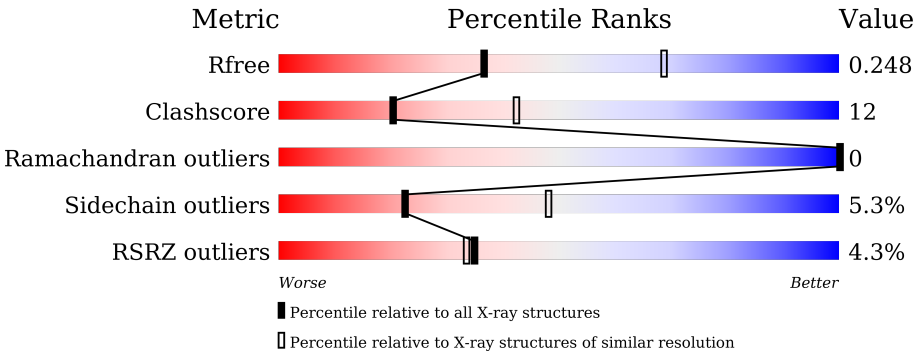
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.69 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	556	4% 78% 18%
1	B	556	3% 76% 19%
1	C	556	3% 79% 16%
1	D	556	3% 77% 18%
1	E	556	6% 74% 19%
1	F	556	6% 74% 21%

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Mol	Chain	Length	Quality of chain
1	G	556	4% 74% 19%
1	H	556	4% 78% 16%

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	FMT	B	603	-	-	X	-
3	FMT	H	603	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 34327 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 lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	544	Total	C	N	O	S	0	0	0
			4289	2728	736	810	15			
1	B	540	Total	C	N	O	S	0	0	0
			4252	2703	730	805	14			
1	C	535	Total	C	N	O	S	0	0	0
			4219	2683	725	797	14			
1	D	541	Total	C	N	O	S	0	0	0
			4265	2712	733	806	14			
1	E	542	Total	C	N	O	S	0	0	0
			4276	2720	734	808	14			
1	F	543	Total	C	N	O	S	0	0	0
			4281	2723	735	809	14			
1	G	535	Total	C	N	O	S	0	0	0
			4212	2677	725	796	14			
1	H	533	Total	C	N	O	S	0	0	0
			4191	2665	723	789	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q59RB8
A	-4	HIS	-	expression tag	UNP Q59RB8
A	-3	HIS	-	expression tag	UNP Q59RB8
A	-2	HIS	-	expression tag	UNP Q59RB8
A	-1	HIS	-	expression tag	UNP Q59RB8
A	0	HIS	-	expression tag	UNP Q59RB8
B	-5	HIS	-	expression tag	UNP Q59RB8
B	-4	HIS	-	expression tag	UNP Q59RB8
B	-3	HIS	-	expression tag	UNP Q59RB8
B	-2	HIS	-	expression tag	UNP Q59RB8
B	-1	HIS	-	expression tag	UNP Q59RB8
B	0	HIS	-	expression tag	UNP Q59RB8
C	-5	HIS	-	expression tag	UNP Q59RB8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP Q59RB8
C	-3	HIS	-	expression tag	UNP Q59RB8
C	-2	HIS	-	expression tag	UNP Q59RB8
C	-1	HIS	-	expression tag	UNP Q59RB8
C	0	HIS	-	expression tag	UNP Q59RB8
D	-5	HIS	-	expression tag	UNP Q59RB8
D	-4	HIS	-	expression tag	UNP Q59RB8
D	-3	HIS	-	expression tag	UNP Q59RB8
D	-2	HIS	-	expression tag	UNP Q59RB8
D	-1	HIS	-	expression tag	UNP Q59RB8
D	0	HIS	-	expression tag	UNP Q59RB8
E	-5	HIS	-	expression tag	UNP Q59RB8
E	-4	HIS	-	expression tag	UNP Q59RB8
E	-3	HIS	-	expression tag	UNP Q59RB8
E	-2	HIS	-	expression tag	UNP Q59RB8
E	-1	HIS	-	expression tag	UNP Q59RB8
E	0	HIS	-	expression tag	UNP Q59RB8
F	-5	HIS	-	expression tag	UNP Q59RB8
F	-4	HIS	-	expression tag	UNP Q59RB8
F	-3	HIS	-	expression tag	UNP Q59RB8
F	-2	HIS	-	expression tag	UNP Q59RB8
F	-1	HIS	-	expression tag	UNP Q59RB8
F	0	HIS	-	expression tag	UNP Q59RB8
G	-5	HIS	-	expression tag	UNP Q59RB8
G	-4	HIS	-	expression tag	UNP Q59RB8
G	-3	HIS	-	expression tag	UNP Q59RB8
G	-2	HIS	-	expression tag	UNP Q59RB8
G	-1	HIS	-	expression tag	UNP Q59RB8
G	0	HIS	-	expression tag	UNP Q59RB8
H	-5	HIS	-	expression tag	UNP Q59RB8
H	-4	HIS	-	expression tag	UNP Q59RB8
H	-3	HIS	-	expression tag	UNP Q59RB8
H	-2	HIS	-	expression tag	UNP Q59RB8
H	-1	HIS	-	expression tag	UNP Q59RB8
H	0	HIS	-	expression tag	UNP Q59RB8

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

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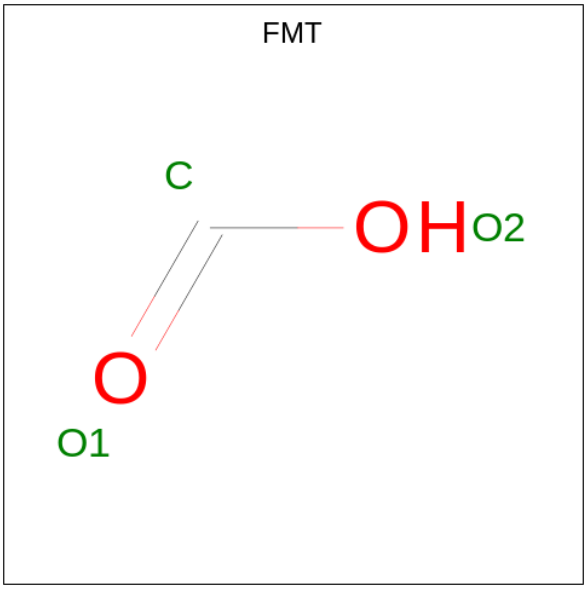
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	G	1	Total C O 3 1 2	0	0
3	G	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0

- Molecule 4 is water.

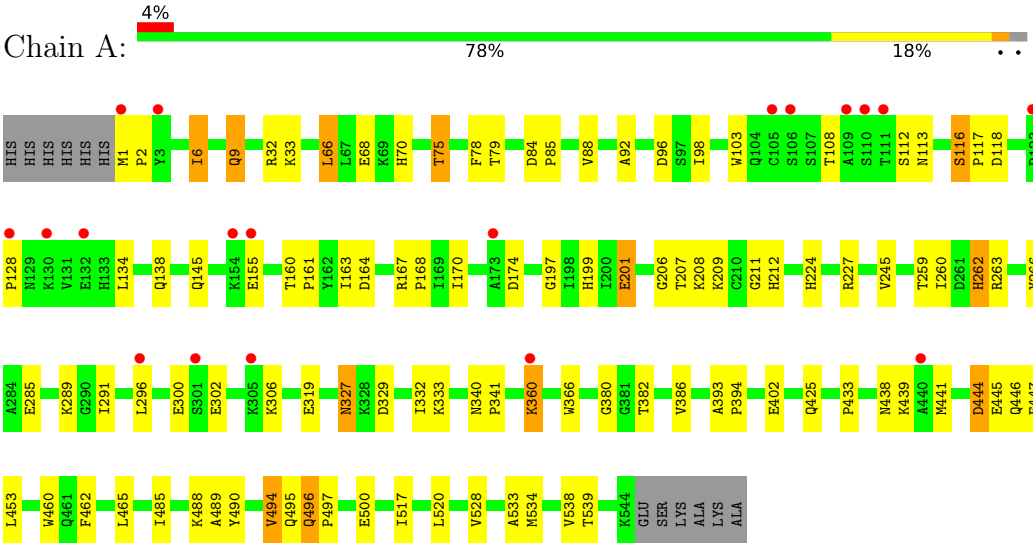
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	32	Total O 32 32	0	0
4	B	38	Total O 38 38	0	0
4	C	56	Total O 56 56	0	0
4	D	29	Total O 29 29	0	0
4	E	29	Total O 29 29	0	0
4	F	22	Total O 22 22	0	0
4	G	52	Total O 52 52	0	0
4	H	40	Total O 40 40	0	0

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.

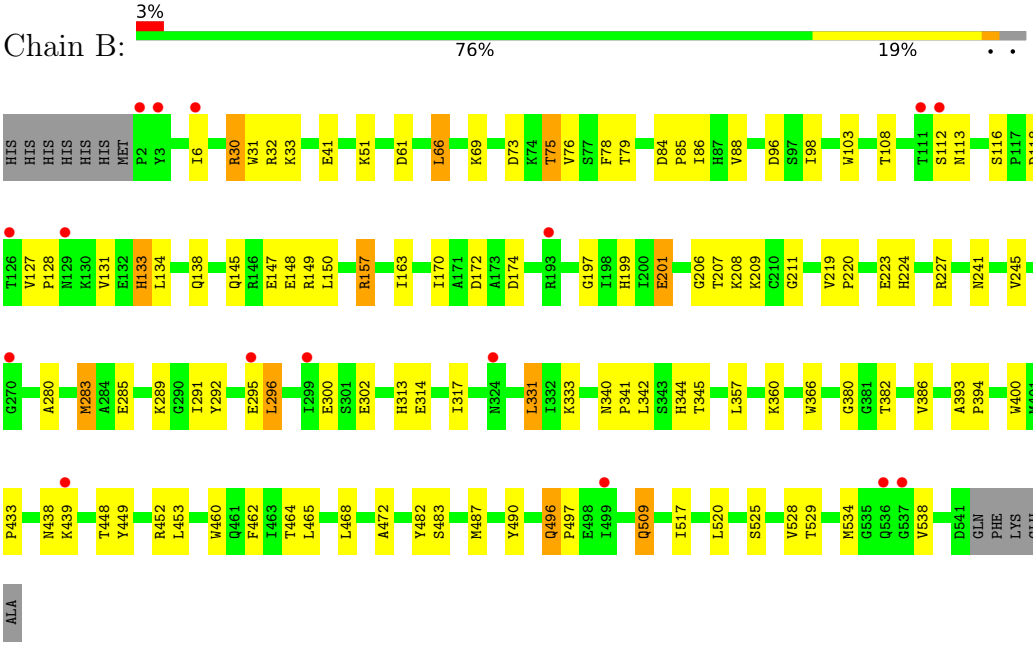
• Molecule 1: Isocitrate lyase

Chain A:

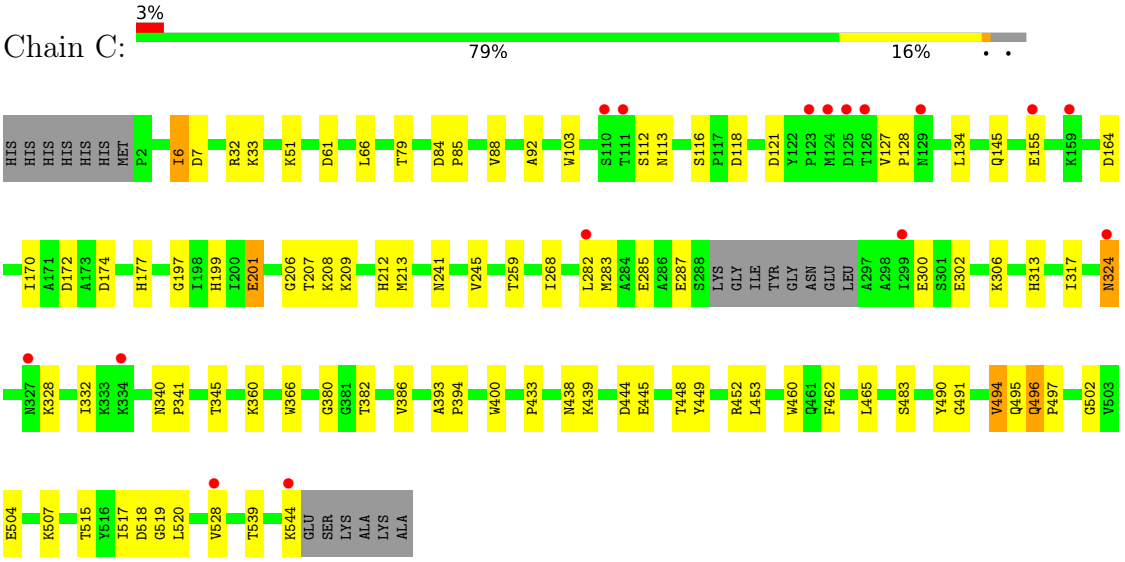


• Molecule 1: Isocitrate lyase

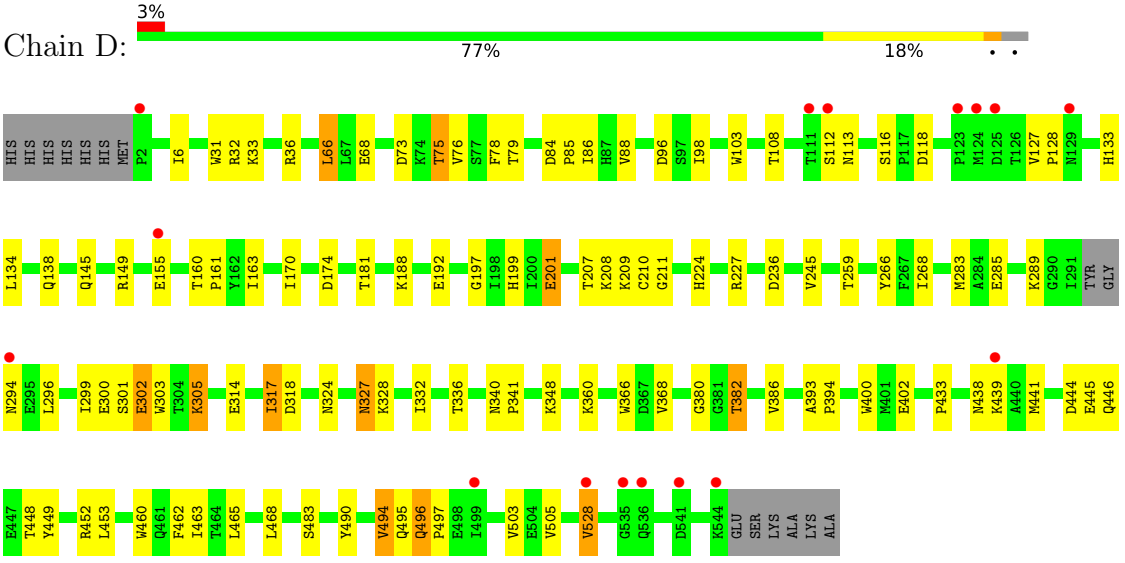
Chain B:



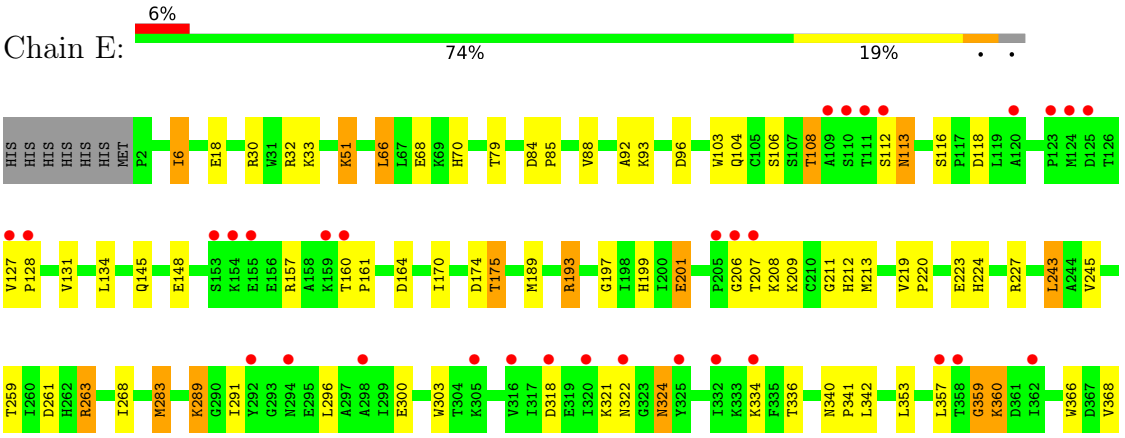
• Molecule 1: Isocitrate lyase

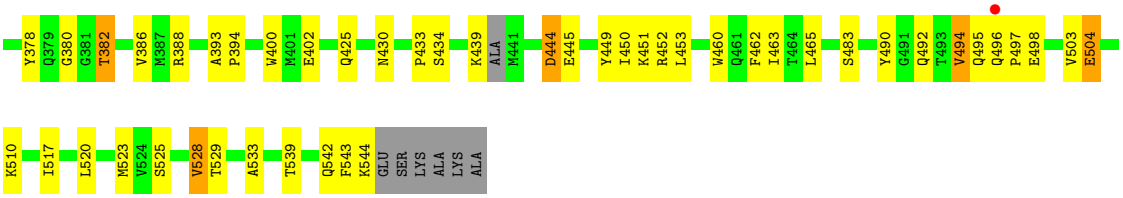


• Molecule 1: Isocitrate lyase

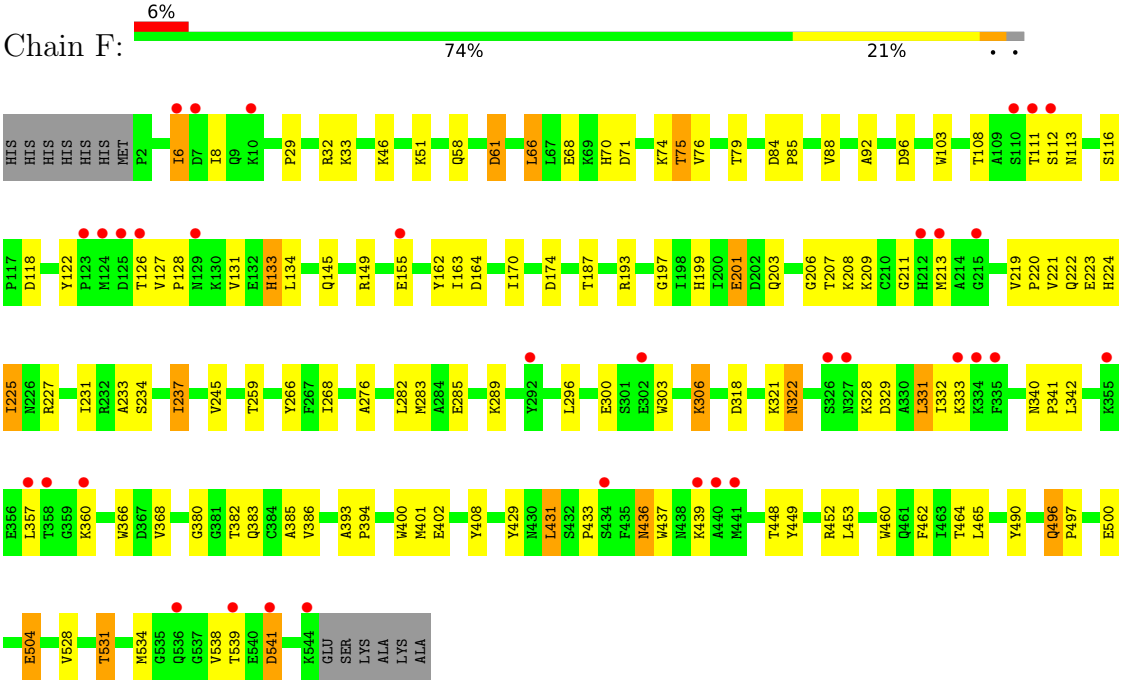


• Molecule 1: Isocitrate lyase

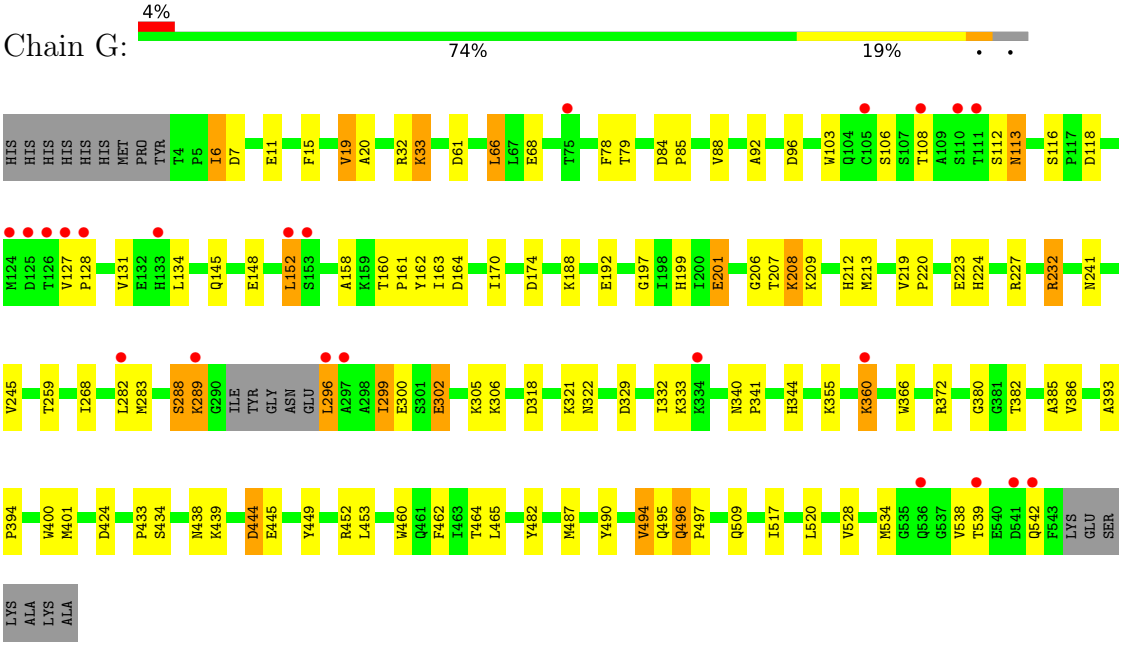




• Molecule 1: Isocitrate lyase

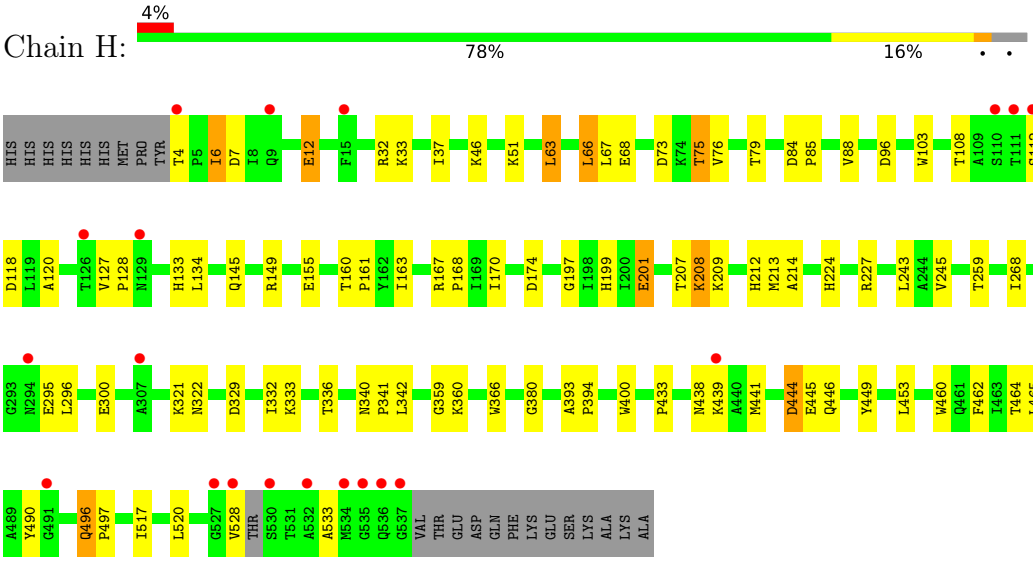


• Molecule 1: Isocitrate lyase



• Molecule 1: Isocitrate lyase

Chain H:


4%
78%
16%
HIS HIS HIS HIS HIS HIS MET PRO TYR T4 P5 I6 D7 I8 Q9 E12 F15 R32 K33 I37 K46 K51 L63 L66 L67 E68 D73 K74 T75 V76 T79 D84 P85 V88 D96 W103 T108 A109 S110 T111 S112 N113 S116 P117
D118 L119 A120 T126 V127 P128 N129 H133 L134 Q145 R149 E155 T160 P161 Y162 I163 R167 P168 I169 I170 D174 G197 I198 H199 I200 E201 T207 K208 K209 H212 M213 A214 H224 R227 L243 A244 V245 T259 I268 M283 I291 Y292
G293 N294 E295 L296 E300 A307 K321 N322 D329 I332 K333 T336 N340 P341 L342 G359 K360 W366 G380 A393 P394 W400 P433 N438 K439 A440 M441 D444 E445 Q446 Y449 L453 W460 Q461 F462 I463 T464 L465 L473 K488
A489 Y490 G491 Q496 P497 I517 L520 G527 V528 THR S530 T531 A532 A533 M534 G535 Q536 G537 VAL THR GLU ASP GLN PHE LYS GLU SER LYS ALA LYS ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.97Å 139.91Å 200.30Å 90.00° 92.55° 90.00°	Depositor
Resolution (Å)	47.11 – 2.69 48.27 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.11-2.69) 99.5 (48.27-2.69)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.215 , 0.248 0.217 , 0.248	Depositor DCC
R_{free} test set	6148 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	67.1	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	34327	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.85% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: MG, FMT

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	0.21	0/4389	0.34	0/5938
1	B	0.22	0/4351	0.35	0/5888
1	C	0.21	0/4317	0.34	0/5840
1	D	0.21	0/4363	0.34	0/5901
1	E	0.21	0/4375	0.36	0/5917
1	F	0.21	0/4381	0.35	0/5927
1	G	0.21	0/4308	0.34	0/5827
1	H	0.21	0/4287	0.34	0/5798
All	All	0.21	0/34771	0.35	0/47036

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	3
1	B	0	3
1	C	0	4
1	D	0	2
1	E	0	4
1	F	0	3
1	G	0	3
1	H	0	3
All	All	0	25

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	GLY	Peptide
1	A	360	LYS	Peptide
1	A	380	GLY	Peptide
1	B	206	GLY	Peptide
1	B	360	LYS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4289	0	4239	100	1
1	B	4252	0	4198	132	1
1	C	4219	0	4165	76	0
1	D	4265	0	4215	106	1
1	E	4276	0	4222	150	0
1	F	4281	0	4228	143	1
1	G	4212	0	4162	136	0
1	H	4191	0	4143	99	2
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
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	6	0	2	0	0
3	B	6	0	2	2	0
3	C	6	0	2	0	0
3	D	6	0	2	1	0
3	G	6	0	2	1	0
3	H	6	0	2	2	0
4	A	32	0	0	2	0
4	B	38	0	0	2	0
4	C	56	0	0	6	0
4	D	29	0	0	0	0
4	E	29	0	0	0	0
4	F	22	0	0	2	0
4	G	52	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	40	0	0	1	0
All	All	34327	0	33584	837	3

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 12.

The worst 5 of 837 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:B:149:ARG:O	1:B:157:ARG:NH1	1.65	1.28
1:F:29:PRO:O	1:F:32:ARG:HD3	1.41	1.21
1:G:219:VAL:HG22	1:G:220:PRO:HD2	1.32	1.11
1:E:219:VAL:HG22	1:E:220:PRO:HD2	1.32	1.10
1:B:296:LEU:CD2	1:D:528:VAL:HG21	1.79	1.10

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:GLU:OE1	1:H:321:LYS:NZ[1_565]	1.54	0.66
1:D:324:ASN:N	1:H:322:ASN:O[2_555]	2.04	0.16
1:B:289:LYS:CG	1:F:282:LEU:CD1[2_456]	2.10	0.10

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	542/556 (98%)	532 (98%)	10 (2%)	0	100	100
1	B	538/556 (97%)	528 (98%)	10 (2%)	0	100	100
1	C	531/556 (96%)	520 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	537/556 (97%)	527 (98%)	10 (2%)	0	100	100
1	E	538/556 (97%)	526 (98%)	12 (2%)	0	100	100
1	F	541/556 (97%)	531 (98%)	10 (2%)	0	100	100
1	G	531/556 (96%)	521 (98%)	10 (2%)	0	100	100
1	H	529/556 (95%)	516 (98%)	13 (2%)	0	100	100
All	All	4287/4448 (96%)	4201 (98%)	86 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	446/456 (98%)	429 (96%)	17 (4%)	33	62
1	B	442/456 (97%)	416 (94%)	26 (6%)	19	43
1	C	439/456 (96%)	422 (96%)	17 (4%)	32	61
1	D	444/456 (97%)	420 (95%)	24 (5%)	22	47
1	E	445/456 (98%)	417 (94%)	28 (6%)	18	40
1	F	445/456 (98%)	418 (94%)	27 (6%)	18	41
1	G	438/456 (96%)	410 (94%)	28 (6%)	17	39
1	H	434/456 (95%)	412 (95%)	22 (5%)	24	50
All	All	3533/3648 (97%)	3344 (95%)	189 (5%)	22	48

5 of 189 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	61	ASP
1	G	66	LEU
1	F	133	HIS
1	F	366	TRP
1	G	232	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	436	ASN
1	F	508	HIS
1	H	113	ASN
1	E	53	ASN
1	D	327	ASN

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 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	FMT	C	602	-	2,2,2	0.68	0	1,1,1	0.72	0
3	FMT	H	602	-	2,2,2	0.72	0	1,1,1	0.69	0
3	FMT	H	603	-	2,2,2	0.71	0	1,1,1	0.69	0
3	FMT	A	603	-	2,2,2	0.70	0	1,1,1	0.70	0
3	FMT	C	603	-	2,2,2	0.67	0	1,1,1	0.71	0
3	FMT	G	603	-	2,2,2	0.67	0	1,1,1	0.71	0
3	FMT	A	602	-	2,2,2	0.70	0	1,1,1	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FMT	D	602	2	2,2,2	0.70	0	1,1,1	0.70	0
3	FMT	B	602	-	2,2,2	0.73	0	1,1,1	0.68	0
3	FMT	G	602	-	2,2,2	0.71	0	1,1,1	0.68	0
3	FMT	D	603	-	2,2,2	0.69	0	1,1,1	0.70	0
3	FMT	B	603	-	2,2,2	0.70	0	1,1,1	0.70	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	603	FMT	2	0
3	G	603	FMT	1	0
3	D	603	FMT	1	0
3	B	603	FMT	2	0

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	544/556 (97%)	0.16	23 (4%)	36	35	43, 66, 103, 132	0
1	B	540/556 (97%)	0.13	18 (3%)	46	46	42, 67, 101, 121	0
1	C	535/556 (96%)	0.15	16 (2%)	50	51	39, 66, 111, 127	0
1	D	541/556 (97%)	0.10	16 (2%)	50	51	39, 63, 98, 123	0
1	E	542/556 (97%)	0.34	33 (6%)	21	20	54, 82, 116, 136	0
1	F	543/556 (97%)	0.45	34 (6%)	20	19	50, 80, 113, 132	0
1	G	535/556 (96%)	0.26	23 (4%)	35	33	40, 74, 117, 138	0
1	H	533/556 (95%)	0.19	21 (3%)	39	38	48, 71, 113, 140	0
All	All	4313/4448 (96%)	0.22	184 (4%)	35	33	39, 71, 111, 140	0

The worst 5 of 184 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	544	LYS	6.3
1	G	296	LEU	5.1
1	H	532	ALA	4.5
1	E	294	ASN	4.5
1	D	536	GLN	4.3

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	FMT	B	602	3/3	0.89	0.25	78,78,83,84	0
3	FMT	B	603	3/3	0.89	0.28	75,75,80,81	0
3	FMT	H	603	3/3	0.90	0.25	76,76,81,84	0
3	FMT	H	602	3/3	0.93	0.22	68,68,71,76	0
3	FMT	D	603	3/3	0.93	0.42	75,75,83,83	0
3	FMT	G	602	3/3	0.94	0.19	69,69,76,80	0
3	FMT	D	602	3/3	0.94	0.17	63,63,63,72	0
3	FMT	C	602	3/3	0.94	0.27	68,68,69,73	0
2	MG	H	601	1/1	0.95	0.20	70,70,70,70	0
2	MG	D	601	1/1	0.96	0.24	66,66,66,66	0
3	FMT	C	603	3/3	0.97	0.15	63,63,67,72	0
3	FMT	A	602	3/3	0.97	0.14	70,70,72,76	0
2	MG	B	601	1/1	0.97	0.23	63,63,63,63	0
2	MG	G	601	1/1	0.98	0.33	62,62,62,62	0
3	FMT	G	603	3/3	0.98	0.12	74,74,74,75	0
2	MG	A	601	1/1	0.98	0.25	46,46,46,46	0
2	MG	E	601	1/1	0.98	0.39	69,69,69,69	0
2	MG	C	601	1/1	0.99	0.22	52,52,52,52	0
3	FMT	A	603	3/3	0.99	0.39	76,76,82,84	0
2	MG	F	601	1/1	0.99	0.35	71,71,71,71	0

6.5 Other polymers (i)

There are no such residues in this entry.