wwPDB X-ray Structure Validation Summary Report (i)

Nov 6, 2023 – 09:30 PM EST

PDB ID	:	1F8M
Title	:	CRYSTAL STRUCTURE OF 3-BROMOPYRUVATE MODIFIED ISOCITRATE LYASE (ICL) FROM MYCOBACTERIUM TUBERCULOSIS
Authors	:	Sharma, V.; Sharma, S.; Hoener zu Bentrup, K.; McKinney, J.D.; Russell, D.G.; Jacobs Jr., W.R.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)
Deposited on	:	2000-06-30
Resolution	:	1.80 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:

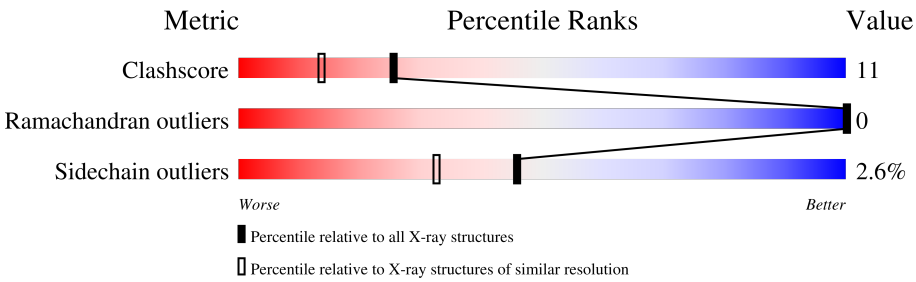
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 1.80 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))
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	429	81% 17% •
1	B	429	82% 17% •
1	C	429	80% 18% •
1	D	429	77% 21% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14276 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
			Total	C	N	O	S			
1	A	427	3308	2078	575	646	9	0	0	0
1	B	427	3308	2078	575	646	9	0	0	0
1	C	427	3308	2078	575	646	9	0	0	0
1	D	427	3308	2078	575	646	9	0	0	0

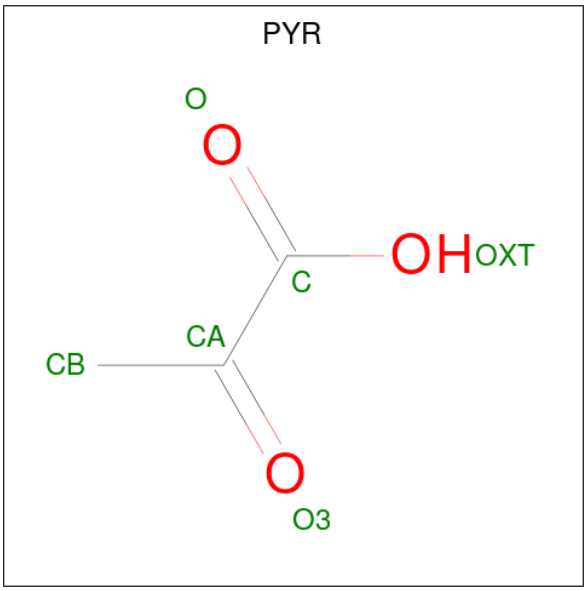
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	insertion	UNP P0A5H3
B	1	ALA	-	insertion	UNP P0A5H3
C	1	ALA	-	insertion	UNP P0A5H3
D	1	ALA	-	insertion	UNP P0A5H3

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

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

- Molecule 3 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	238	238	238	0	0
4	B	282	282	282	0	0
4	C	272	272	272	0	0
4	D	224	224	224	0	0

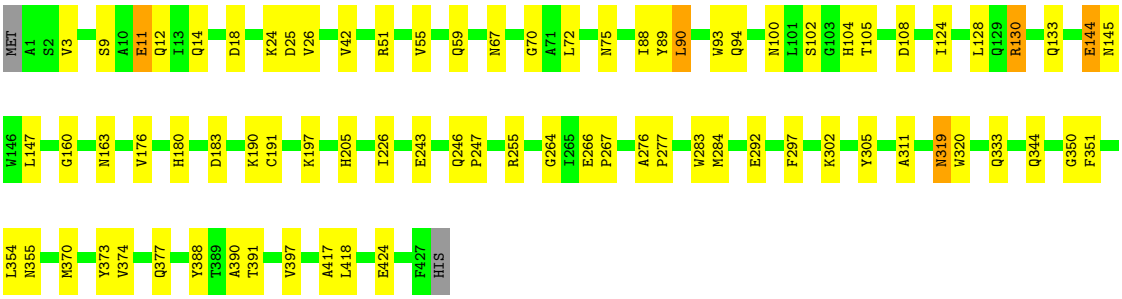
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

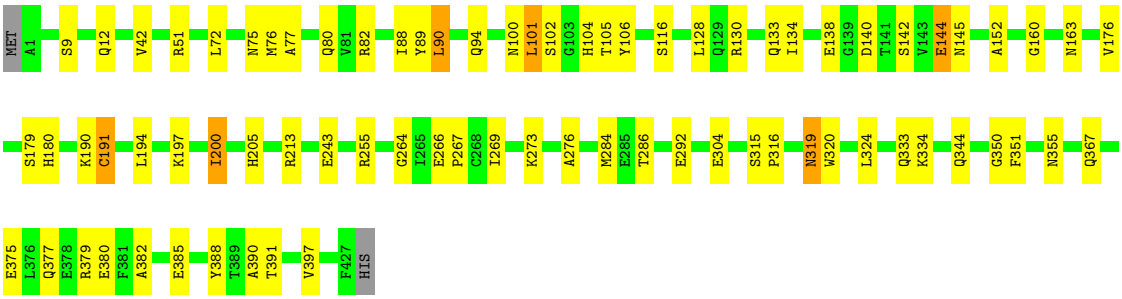
• Molecule 1: ISOCITRATE LYASE

Chain A:



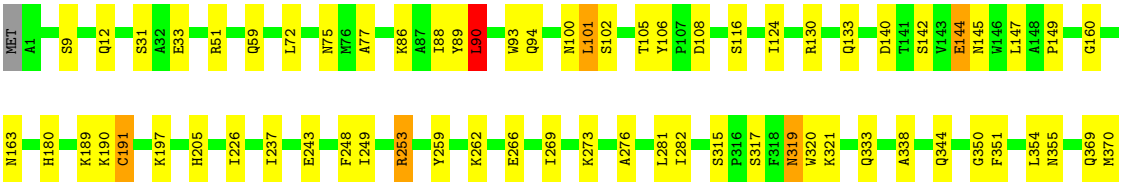
• Molecule 1: ISOCITRATE LYASE

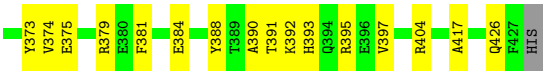
Chain B:



• Molecule 1: ISOCITRATE LYASE

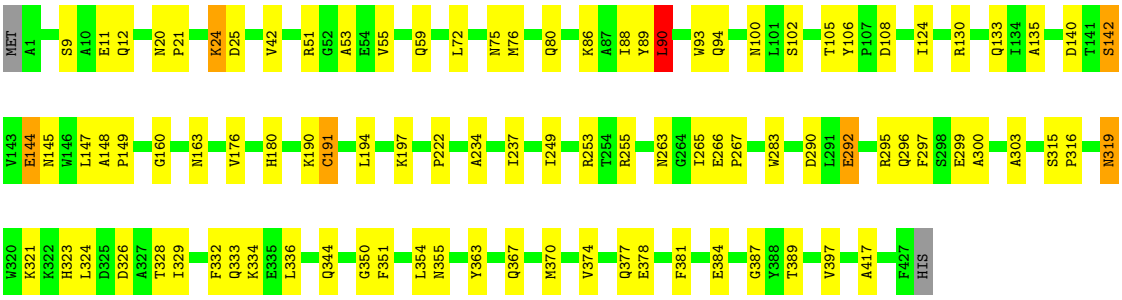
Chain C:





- Molecule 1: ISOCITRATE LYASE

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.31Å 129.04Å 166.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.86 – 1.80	Depositor
% Data completeness (in resolution range)	87.2 (19.86-1.80)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.203 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14276	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.65	0/3379	0.77	3/4595 (0.1%)
1	B	0.66	0/3379	0.77	1/4595 (0.0%)
1	C	0.64	0/3379	0.76	2/4595 (0.0%)
1	D	0.62	0/3379	0.77	2/4595 (0.0%)
All	All	0.64	0/13516	0.77	8/18380 (0.0%)

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	1
1	C	0	1
All	All	0	2

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})
1	C	90	LEU	CA-CB-CG	5.50	127.96	115.30
1	A	130	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	D	417	ALA	N-CA-C	5.23	125.12	111.00
1	A	183	ASP	CB-CG-OD1	5.22	123.00	118.30
1	B	90	LEU	CA-CB-CG	5.17	127.18	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	373	TYR	Sidechain
1	C	373	TYR	Sidechain

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	3308	0	3192	62	0
1	B	3308	0	3192	75	0
1	C	3308	0	3192	82	0
1	D	3308	0	3192	89	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
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
4	A	238	0	0	5	0
4	B	282	0	0	13	0
4	C	272	0	0	10	0
4	D	224	0	0	6	0
All	All	14276	0	12768	275	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 11.

The worst 5 of 275 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:ARG:HH12	1:D:145:ASN:HD21	1.07	0.99
1:B:9:SER:OG	1:B:12:GLN:HG3	1.68	0.94
1:C:130:ARG:HH11	1:C:133:GLN:HE22	1.21	0.86
1:D:51:ARG:HH12	1:D:145:ASN:ND2	1.74	0.85
1:B:77:ALA:HB1	1:B:88:ILE:HD13	1.60	0.83

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	425/429 (99%)	415 (98%)	10 (2%)	0	100	100
1	B	425/429 (99%)	415 (98%)	10 (2%)	0	100	100
1	C	425/429 (99%)	417 (98%)	8 (2%)	0	100	100
1	D	425/429 (99%)	413 (97%)	12 (3%)	0	100	100
All	All	1700/1716 (99%)	1660 (98%)	40 (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	337/339 (99%)	327 (97%)	10 (3%)	41	27
1	B	337/339 (99%)	329 (98%)	8 (2%)	49	36
1	C	337/339 (99%)	330 (98%)	7 (2%)	53	42
1	D	337/339 (99%)	327 (97%)	10 (3%)	41	27
All	All	1348/1356 (99%)	1313 (97%)	35 (3%)	46	32

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	142	SER
1	D	144	GLU
1	D	283	TRP
1	B	101	LEU
1	B	90	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	377	GLN
1	D	377	GLN
1	C	133	GLN
1	D	367	GLN
1	D	145	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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	PYR	A	500	1	5,5,5	1.14	0	3,6,6	2.10	1 (33%)
3	PYR	C	500	1	5,5,5	1.32	0	3,6,6	1.10	0
3	PYR	B	500	1	5,5,5	1.23	0	3,6,6	1.27	0
3	PYR	D	500	1	5,5,5	1.21	0	3,6,6	1.32	0

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	PYR	A	500	1	-	0/4/4/4	-
3	PYR	C	500	1	-	0/4/4/4	-
3	PYR	B	500	1	-	0/4/4/4	-
3	PYR	D	500	1	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	500	PYR	OXT-C-CA	3.13	122.53	113.97

There are no chirality outliers.

There are no torsion outliers.

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.