



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:37 PM GMT

PDB ID : 1L5J
Title : CRYSTAL STRUCTURE OF E. COLI ACONITASE B.
Authors : Williams, C.H.; Stillman, T.J.; Barynin, V.V.; Sedelnikova, S.E.; Tang, Y.;
Green, J.; Guest, J.R.; Artymiuk, P.J.
Deposited on : 2002-03-07
Resolution : 2.40 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 ⓘ symbol.

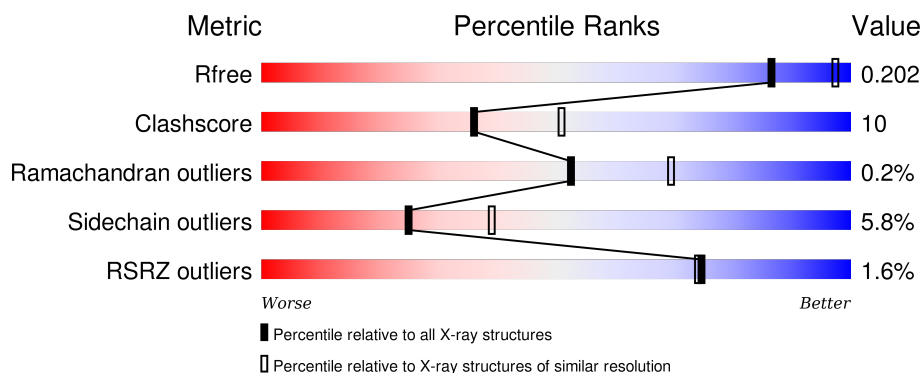
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

i

X-RAY DIFFRACTION

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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 $\leq 5\%$. 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	865	<div> <div>2%</div> <div>79%</div> <div>18%</div> <div></div> </div>
1	B	865	<div> <div>%</div> <div>79%</div> <div>18%</div> <div></div> </div>

2 Entry composition [i](#)

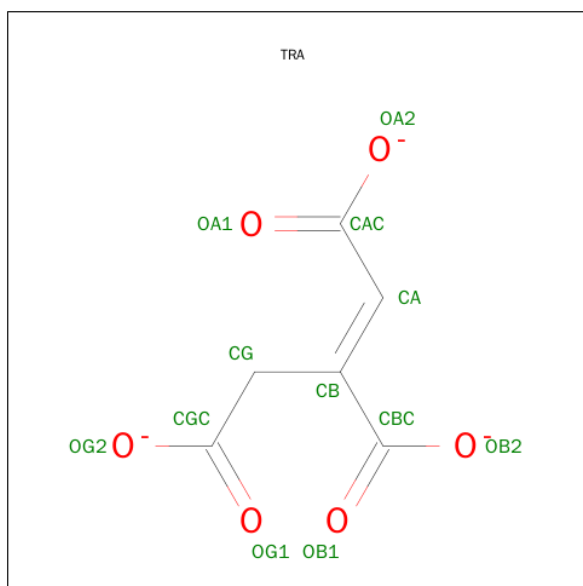
There are 4 unique types of molecules in this entry. The entry contains 13712 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aconitate hydratase 2.

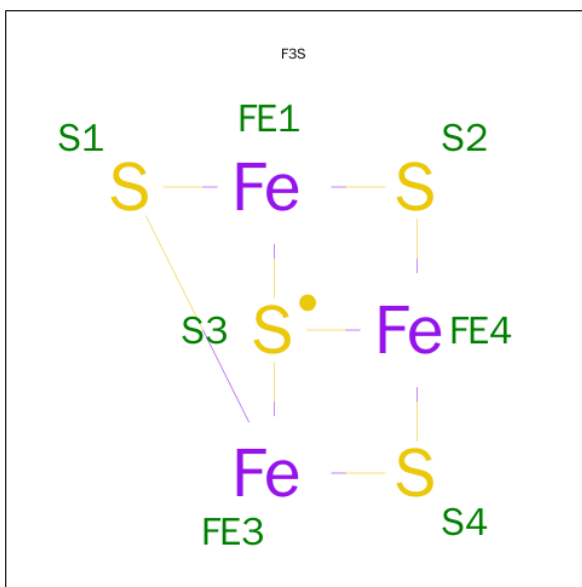
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	862	Total	C	N	O	S	0	0	0
			6552	4152	1122	1245	33			
1	B	862	Total	C	N	O	S	0	0	0
			6552	4152	1122	1245	33			

- Molecule 2 is ACONITATE ION (three-letter code: TRA) (formula: $C_6H_3O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

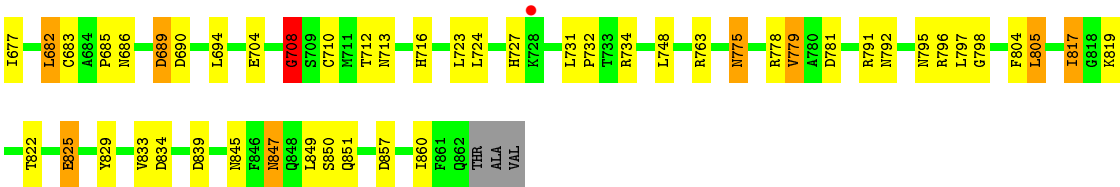
- Molecule 3 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			7	3	4		
3	B	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	294	Total	O	0	0
			294	294		
4	B	276	Total	O	0	0
			276	276		



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	138.97Å 169.63Å 113.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.10 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.00-2.40) 96.0 (20.10-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.151 , 0.203 0.155 , 0.202	Depositor DCC
R_{free} test set	5019 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 40.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 100794 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13712	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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, 0.375 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: TRA, F3S

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	0.34	0/6686	0.75	26/9076 (0.3%)
1	B	0.35	0/6686	0.77	36/9076 (0.4%)
All	All	0.35	0/13372	0.76	62/18152 (0.3%)

There are no bond length outliers.

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	ASP	CB-CG-OD2	6.52	124.16	118.30
1	B	637	ASP	CB-CG-OD2	6.48	124.13	118.30
1	B	104	ASP	CB-CG-OD2	6.27	123.94	118.30
1	A	676	ASP	CB-CG-OD2	6.25	123.92	118.30
1	B	476	ASP	CB-CG-OD2	5.97	123.68	118.30

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	6552	0	6569	129	0
1	B	6552	0	6569	122	0
2	A	12	0	3	2	0
2	B	12	0	3	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	7	0	0	0	0
3	B	7	0	0	0	0
4	A	294	0	0	15	0
4	B	276	0	0	11	0
All	All	13712	0	13144	251	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 10.

The worst 5 of 251 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:530:GLU:OE2	1:B:577:ARG:NH1	1.79	1.15
1:A:439:MET:HE2	4:A:1105:HOH:O	1.56	1.06
1:B:465:MET:SD	1:B:636:GLY:HA3	1.98	1.03
1:B:178:ASN:ND2	1:B:180:ASP:H	1.55	1.03
1:A:439:MET:HB3	4:A:1105:HOH:O	1.60	1.00

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	860/865 (99%)	831 (97%)	26 (3%)	3 (0%)	46	63
1	B	860/865 (99%)	828 (96%)	31 (4%)	1 (0%)	56	74
All	All	1720/1730 (99%)	1659 (96%)	57 (3%)	4 (0%)	52	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	PRO
1	A	94	GLN
1	A	708	GLY
1	B	708	GLY

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	690/692 (100%)	654 (95%)	36 (5%)	29	45
1	B	690/692 (100%)	646 (94%)	44 (6%)	22	34
All	All	1380/1384 (100%)	1300 (94%)	80 (6%)	25	39

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2	LEU
1	B	157	LEU
1	B	797	LEU
1	B	12	ARG
1	B	52	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	847	ASN
1	B	178	ASN
1	B	832	GLN
1	A	848	GLN
1	B	148	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 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	TRA	A	866	-	3,11,11	1.63	1 (33%)	3,14,14	3.49	3 (100%)
3	F3S	A	868	1	0,9,9	0.00	-	0,15,15	0.00	-
2	TRA	B	867	-	3,11,11	1.87	1 (33%)	3,14,14	2.87	3 (100%)
3	F3S	B	869	1	0,9,9	0.00	-	0,15,15	0.00	-

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	TRA	A	866	-	-	0/4/12/12	0/0/0/0
3	F3S	A	868	1	-	0/0/24/24	0/0/3/3
2	TRA	B	867	-	-	0/4/12/12	0/0/0/0
3	F3S	B	869	1	-	0/0/24/24	0/0/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	867	TRA	CA-CB	-2.56	1.32	1.34
2	A	866	TRA	CA-CB	-2.31	1.32	1.34

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	866	TRA	CAC-CA-CB	-4.66	116.68	127.14
2	B	867	TRA	CAC-CA-CB	-3.52	119.23	127.14
2	A	866	TRA	CGC-CG-CB	-2.77	107.06	114.00
2	A	866	TRA	CG-CB-CA	-2.67	118.95	125.70
2	B	867	TRA	CG-CB-CA	-2.57	119.21	125.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	866	TRA	2	0
2	B	867	TRA	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	862/865 (99%)	-0.69	15 (1%) 73 72	17, 32, 71, 97	0
1	B	862/865 (99%)	-0.74	12 (1%) 78 77	18, 32, 66, 96	0
All	All	1724/1730 (99%)	-0.72	27 (1%) 74 74	17, 32, 68, 97	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	377	GLU	7.7
1	A	377	GLU	7.1
1	B	376	ALA	6.4
1	B	375	VAL	4.7
1	A	138	ALA	4.4

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 carbohydrates 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. 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, 95th 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(\AA^2)	Q<0.9
2	TRA	A	866	12/12	0.97	0.12	0.89	18,26,31,37	0
2	TRA	B	867	12/12	0.97	0.11	0.77	25,31,40,65	0
3	F3S	A	868	7/7	0.98	0.06	-1.07	19,26,30,30	0
3	F3S	B	869	7/7	0.98	0.04	-2.32	21,26,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.