wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 12:23 AM GMT

PDB ID	:	2A5H
Title	:	2.1 Angstrom X-ray crystal structure of lysine-2,3-aminomutase from Clostridium subterminale SB4, with Michaelis analog (L-alpha-lysine external aldimine form of pyridoxal-5'-phosphate).
Authors	:	Lepore, B.W.; Ruzicka, F.J.; Frey, P.A.; Ringe, D.
Deposited on	:	2005-06-30
Resolution	:	2.10 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:

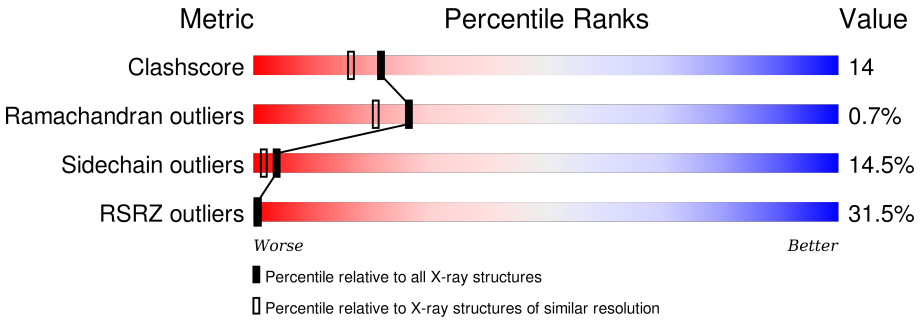
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.10 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	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	416	31% 68% 22% 7%
1	B	416	42% 67% 24% 6%
1	C	416	24% 67% 23% 7%
1	D	416	24% 66% 24% 7%

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	SO4	A	592	-	-	-	X
3	SO4	B	495	-	-	-	X
3	SO4	C	593	-	-	-	X
3	SO4	D	494	-	-	-	X
4	SAM	C	417	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14034 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 L-lysine 2,3-aminomutase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	Se	28	9	0
			3285	2067	591	607	11	9			
1	B	410	Total	C	N	O	S	Se	21	8	0
			3288	2071	589	608	11	9			
1	C	409	Total	C	N	O	S	Se	23	8	0
			3280	2065	588	607	11	9			
1	D	410	Total	C	N	O	S	Se	17	9	0
			3297	2074	595	608	11	9			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	GB 5410603
A	57	MSE	MET	MODIFIED RESIDUE	GB 5410603
A	124	MSE	MET	MODIFIED RESIDUE	GB 5410603
A	127	MSE	MET	MODIFIED RESIDUE	GB 5410603
A	145	MSE	MET	MODIFIED RESIDUE	GB 5410603
A	147	MSE	MET	MODIFIED RESIDUE	GB 5410603
A	218	MSE	MET	MODIFIED RESIDUE	GB 5410603
A	272	MSE	MET	MODIFIED RESIDUE	GB 5410603
A	341	MSE	MET	MODIFIED RESIDUE	GB 5410603
A	400	MSE	MET	MODIFIED RESIDUE	GB 5410603
B	1	MSE	MET	MODIFIED RESIDUE	GB 5410603
B	57	MSE	MET	MODIFIED RESIDUE	GB 5410603
B	124	MSE	MET	MODIFIED RESIDUE	GB 5410603
B	127	MSE	MET	MODIFIED RESIDUE	GB 5410603
B	145	MSE	MET	MODIFIED RESIDUE	GB 5410603
B	147	MSE	MET	MODIFIED RESIDUE	GB 5410603
B	218	MSE	MET	MODIFIED RESIDUE	GB 5410603
B	272	MSE	MET	MODIFIED RESIDUE	GB 5410603
B	341	MSE	MET	MODIFIED RESIDUE	GB 5410603
B	400	MSE	MET	MODIFIED RESIDUE	GB 5410603
C	1	MSE	MET	MODIFIED RESIDUE	GB 5410603

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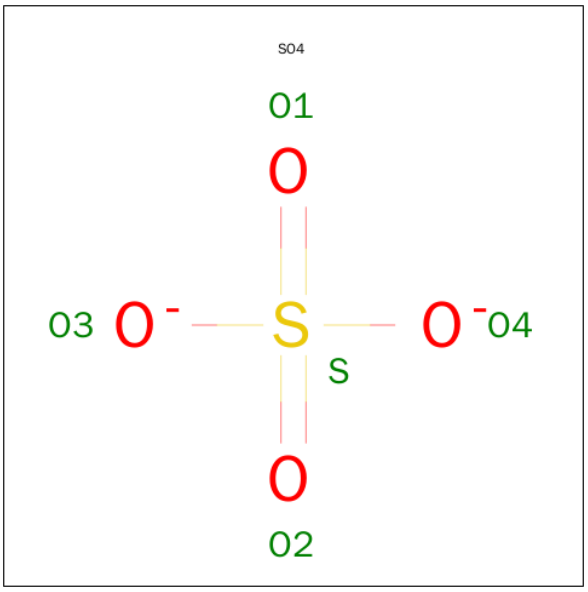
Chain	Residue	Modelled	Actual	Comment	Reference
C	57	MSE	MET	MODIFIED RESIDUE	GB 5410603
C	124	MSE	MET	MODIFIED RESIDUE	GB 5410603
C	127	MSE	MET	MODIFIED RESIDUE	GB 5410603
C	145	MSE	MET	MODIFIED RESIDUE	GB 5410603
C	147	MSE	MET	MODIFIED RESIDUE	GB 5410603
C	218	MSE	MET	MODIFIED RESIDUE	GB 5410603
C	272	MSE	MET	MODIFIED RESIDUE	GB 5410603
C	341	MSE	MET	MODIFIED RESIDUE	GB 5410603
C	400	MSE	MET	MODIFIED RESIDUE	GB 5410603
D	1	MSE	MET	MODIFIED RESIDUE	GB 5410603
D	57	MSE	MET	MODIFIED RESIDUE	GB 5410603
D	124	MSE	MET	MODIFIED RESIDUE	GB 5410603
D	127	MSE	MET	MODIFIED RESIDUE	GB 5410603
D	145	MSE	MET	MODIFIED RESIDUE	GB 5410603
D	147	MSE	MET	MODIFIED RESIDUE	GB 5410603
D	218	MSE	MET	MODIFIED RESIDUE	GB 5410603
D	272	MSE	MET	MODIFIED RESIDUE	GB 5410603
D	341	MSE	MET	MODIFIED RESIDUE	GB 5410603
D	400	MSE	MET	MODIFIED RESIDUE	GB 5410603

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

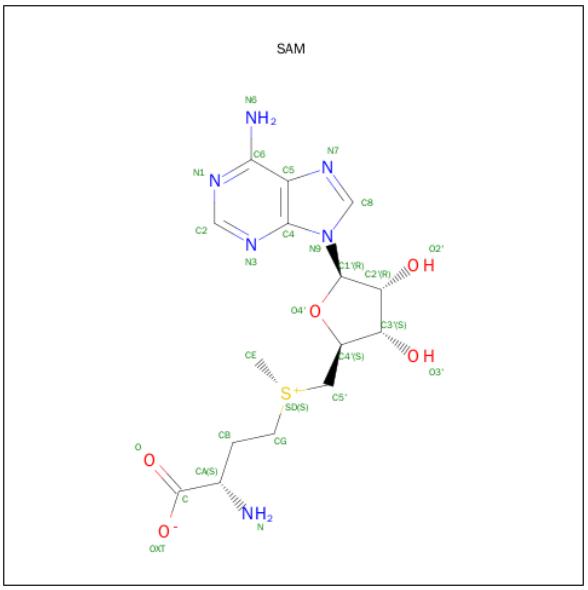
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



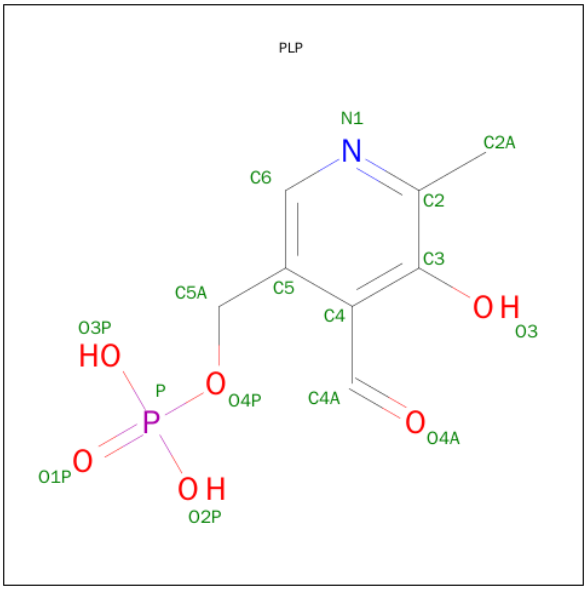
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



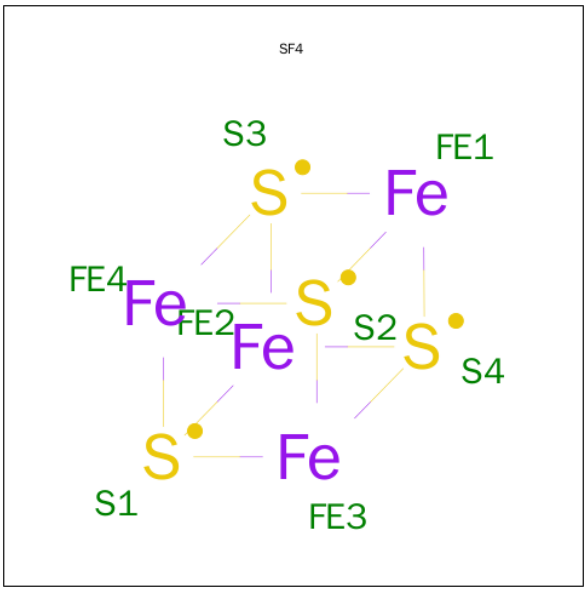
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	D	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 5 is LYSINE (three-letter code: PLP, LYS) (formula: $C_8H_{10}NO_6P$, $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	2	Total	C	N	O	P	0	1
			28	17	3	7	1		
5	B	2	Total	C	N	O	P	0	1
			28	17	3	7	1		
5	C	2	Total	C	N	O	P	0	1
			28	17	3	7	1		
5	D	2	Total	C	N	O	P	0	1
			28	17	3	7	1		

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Fe S 8 4 4	0	0
6	B	1	Total Fe S 8 4 4	0	0
6	C	1	Total Fe S 8 4 4	0	0
6	D	1	Total Fe S 8 4 4	0	0

- Molecule 7 is water.

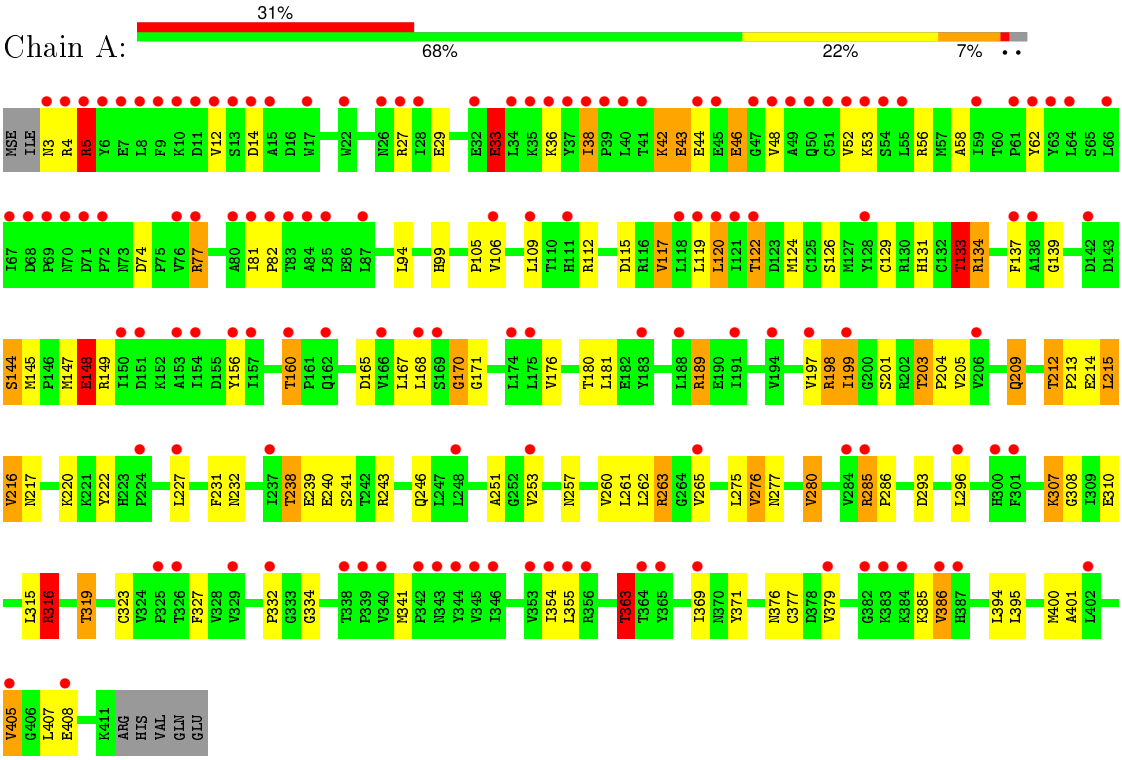
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	135	Total O 135 135	0	0
7	B	116	Total O 116 116	0	0
7	C	183	Total O 183 183	0	0
7	D	174	Total O 174 174	0	0

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.

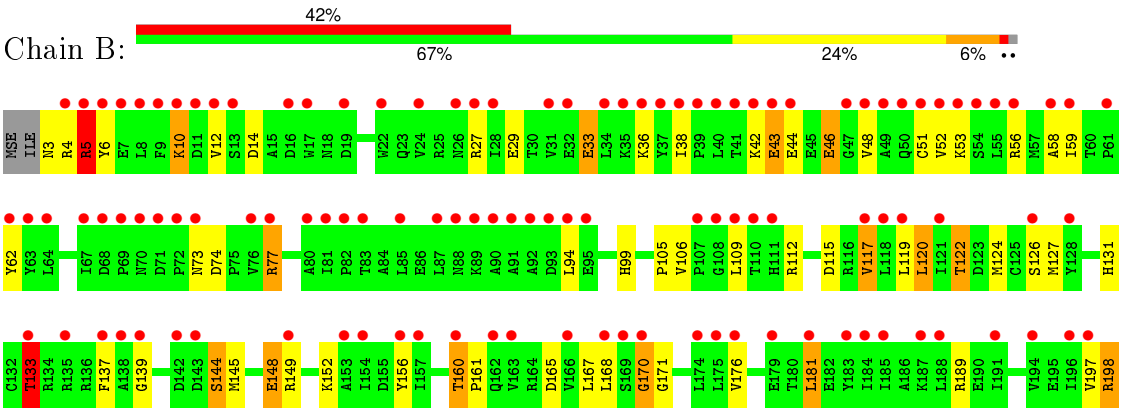
- Molecule 1: L-lysine 2,3-aminomutase

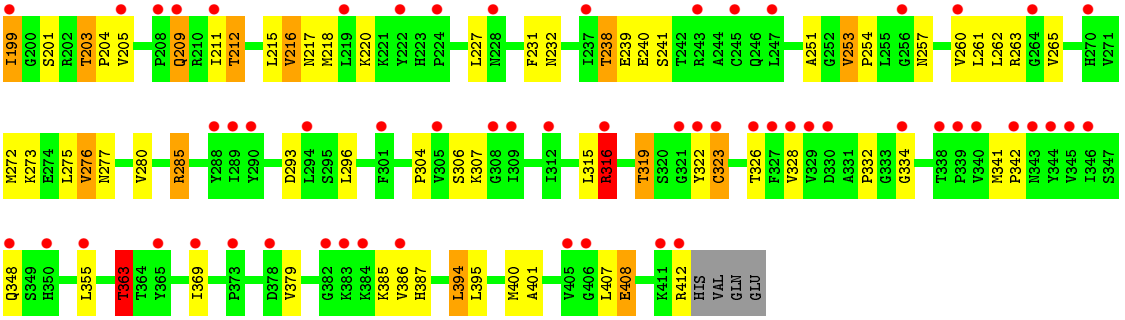
Chain A:



- Molecule 1: L-lysine 2,3-aminomutase

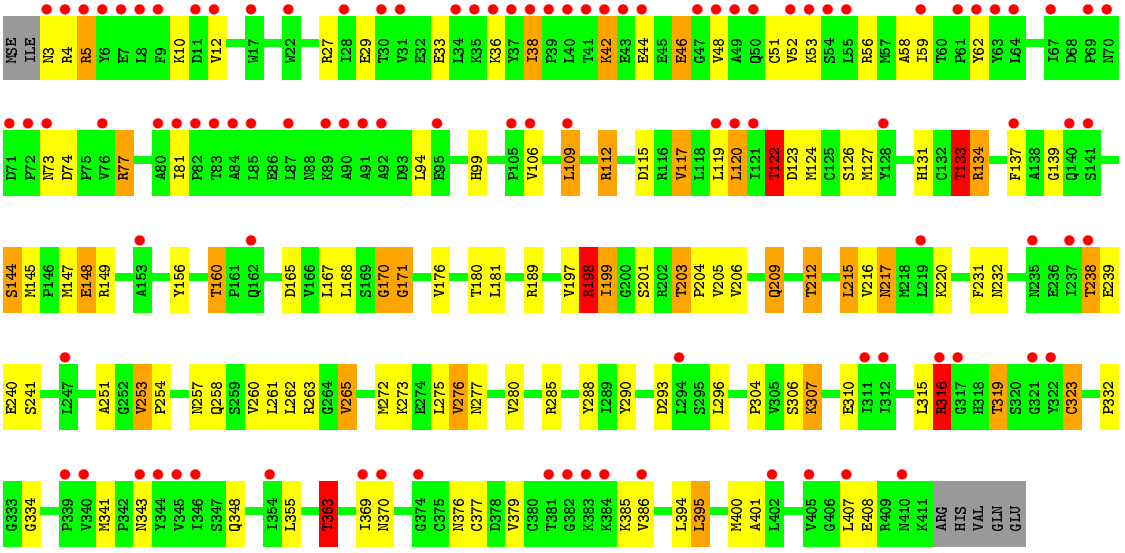
Chain B:





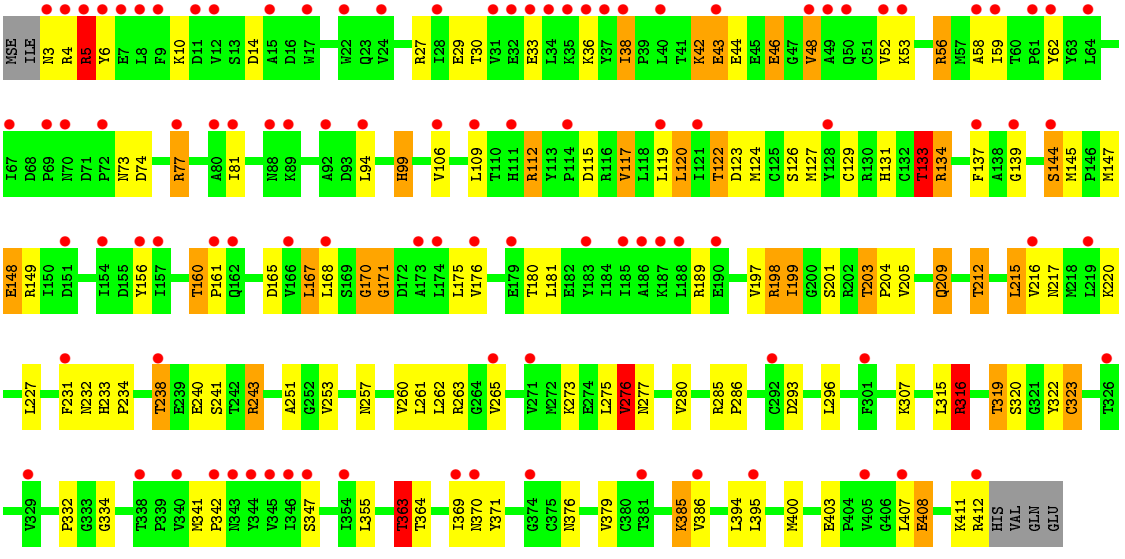
• Molecule 1: L-lysine 2,3-aminomutase

Chain C:



• Molecule 1: L-lysine 2,3-aminomutase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	118.89Å 92.93Å 177.74Å 90.00° 96.74° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 46.61 – 3.00	Depositor EDS
% Data completeness (in resolution range)	81.5 (50.00-2.10) 96.8 (46.61-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	5.65 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.184 , 0.225 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å^2)	50.2	Xtriage
Anisotropy	1.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 48.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	2 of 76379 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14034	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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: SO4, ZN, SF4, SAM, PLP

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	1.47	7/3391 (0.2%)	1.17	35/4590 (0.8%)
1	B	1.50	8/3388 (0.2%)	1.14	25/4586 (0.5%)
1	C	1.05	6/3380 (0.2%)	1.18	34/4576 (0.7%)
1	D	1.19	7/3402 (0.2%)	1.15	35/4604 (0.8%)
All	All	1.32	28/13561 (0.2%)	1.16	129/18356 (0.7%)

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	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	408	GLU	CD-OE2	51.67	1.82	1.25
1	A	148	GLU	CG-CD	48.53	2.24	1.51
1	B	408	GLU	CD-OE1	-44.21	0.77	1.25
1	A	33	GLU	CG-CD	-38.65	0.94	1.51
1	A	46	GLU	CG-CD	-32.43	1.03	1.51

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	408	GLU	CG-CD-OE2	-25.33	67.64	118.30
1	A	33	GLU	CB-CG-CD	19.16	165.93	114.20
1	D	408	GLU	CG-CD-OE1	-16.68	84.94	118.30
1	B	408	GLU	CG-CD-OE1	15.71	149.73	118.30
1	B	263	ARG	NE-CZ-NH2	15.03	127.81	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	GLU	Sidechain
1	A	170	GLY	Peptide
1	B	170	GLY	Peptide
1	B	408	GLU	Sidechain
1	C	170	GLY	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	3285	0	3300	99	0
1	B	3288	0	3306	91	0
1	C	3280	0	3295	112	0
1	D	3297	0	3313	121	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	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	27	0	21	0	0
4	B	27	0	21	0	0
4	C	27	0	21	0	0
4	D	27	0	21	0	0
5	A	28	0	28	0	0
5	B	28	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	28	0	28	0	0
5	D	28	0	28	0	0
6	A	8	0	0	0	0
6	B	8	0	0	0	0
6	C	8	0	0	1	0
6	D	8	0	0	1	0
7	A	135	0	0	7	0
7	B	116	0	0	3	0
7	C	183	0	0	10	1
7	D	174	0	0	8	0
All	All	14034	0	13410	376	1

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 14.

The worst 5 of 376 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:285[B]:ARG:CD	1:D:285[B]:ARG:HD2	1.54	1.37
1:C:285[B]:ARG:CD	1:D:285[B]:ARG:CD	2.09	1.31
1:C:285[B]:ARG:HD2	1:D:285[B]:ARG:CD	1.65	1.23
1:C:285[B]:ARG:HD2	1:D:285[B]:ARG:NE	1.62	1.14
1:D:243[A]:ARG:HD2	7:D:578:HOH:O	1.48	1.11

All (1) 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)
7:C:764:HOH:O	7:C:764:HOH:O[2_454]	1.88	0.32

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	416/416 (100%)	400 (96%)	13 (3%)	3 (1%)	26	21
1	B	416/416 (100%)	398 (96%)	15 (4%)	3 (1%)	26	21
1	C	415/416 (100%)	397 (96%)	15 (4%)	3 (1%)	26	21
1	D	417/416 (100%)	397 (95%)	17 (4%)	3 (1%)	26	21
All	All	1664/1664 (100%)	1592 (96%)	60 (4%)	12 (1%)	26	21

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	GLY
1	B	52	VAL
1	B	171	GLY
1	C	171	GLY
1	D	52	VAL

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	374/362 (103%)	316 (84%)	58 (16%)	3	1
1	B	374/362 (103%)	315 (84%)	59 (16%)	3	1
1	C	373/362 (103%)	320 (86%)	53 (14%)	4	2
1	D	375/362 (104%)	318 (85%)	57 (15%)	3	1
All	All	1496/1448 (103%)	1269 (85%)	227 (15%)	4	1

5 of 227 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	296	LEU
1	C	119	LEU
1	D	276	VAL
1	B	316[A]	ARG
1	B	407	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	343	ASN
1	C	159	ASN
1	D	257	ASN
1	B	370	ASN
1	C	3	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 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	$\#\|Z\| > 2$
4	SAM	A	417	6	21,29,29	2.20	4 (19%)	17,42,42	2.22	7 (41%)
6	SF4	A	418	1,4	0,12,12	0.00	-	0,24,24	0.00	-
5	PLP	A	419	5	15,15,16	2.67	2 (13%)	21,22,23	1.24	3 (14%)
5	LYS	A	420[A]	-	6,9,9	0.39	0	4,10,10	0.68	0
5	LYS	A	420[B]	-	6,9,9	0.38	0	4,10,10	0.70	0
3	SO4	A	592	-	4,4,4	0.19	0	6,6,6	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SAM	B	417	6	21,29,29	2.15	5 (23%)	17,42,42	2.38	6 (35%)
6	SF4	B	418	1,4	0,12,12	0.00	-	0,24,24	0.00	-
5	PLP	B	419	5	15,15,16	2.69	2 (13%)	21,22,23	0.92	0
5	LYS	B	420[A]	-	6,9,9	0.40	0	4,10,10	1.17	0
5	LYS	B	420[B]	-	6,9,9	0.40	0	4,10,10	1.10	0
3	SO4	B	495	-	4,4,4	0.26	0	6,6,6	0.27	0
4	SAM	C	417	6	21,29,29	2.29	5 (23%)	17,42,42	2.21	5 (29%)
6	SF4	C	418	1,4	0,12,12	0.00	-	0,24,24	0.00	-
5	PLP	C	419	5	15,15,16	2.74	3 (20%)	21,22,23	0.97	1 (4%)
5	LYS	C	420[A]	-	6,9,9	0.45	0	4,10,10	1.20	0
5	LYS	C	420[B]	-	6,9,9	0.44	0	4,10,10	1.11	0
3	SO4	C	593	-	4,4,4	0.21	0	6,6,6	0.39	0
4	SAM	D	417	6	21,29,29	2.20	3 (14%)	17,42,42	2.30	5 (29%)
6	SF4	D	418	1,4	0,12,12	0.00	-	0,24,24	0.00	-
5	PLP	D	419	5	15,15,16	2.84	3 (20%)	21,22,23	1.21	2 (9%)
5	LYS	D	420[A]	-	6,9,9	0.34	0	4,10,10	1.04	0
5	LYS	D	420[B]	-	6,9,9	0.36	0	4,10,10	0.93	0
3	SO4	D	494	-	4,4,4	0.24	0	6,6,6	0.43	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
4	SAM	A	417	6	-	0/8/33/33	0/3/3/3
6	SF4	A	418	1,4	-	0/0/48/48	0/6/5/5
5	PLP	A	419	5	-	0/6/6/8	0/1/1/1
5	LYS	A	420[A]	-	-	0/5/9/9	0/0/0/0
5	LYS	A	420[B]	-	-	0/5/9/9	0/0/0/0
3	SO4	A	592	-	-	0/0/0/0	0/0/0/0
4	SAM	B	417	6	-	0/8/33/33	0/3/3/3
6	SF4	B	418	1,4	-	0/0/48/48	0/6/5/5
5	PLP	B	419	5	-	0/6/6/8	0/1/1/1
5	LYS	B	420[A]	-	-	0/5/9/9	0/0/0/0
5	LYS	B	420[B]	-	-	0/5/9/9	0/0/0/0
3	SO4	B	495	-	-	0/0/0/0	0/0/0/0
4	SAM	C	417	6	-	0/8/33/33	0/3/3/3
6	SF4	C	418	1,4	-	0/0/48/48	0/6/5/5
5	PLP	C	419	5	-	0/6/6/8	0/1/1/1
5	LYS	C	420[A]	-	-	0/5/9/9	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LYS	C	420[B]	-	-	0/5/9/9	0/0/0/0
3	SO4	C	593	-	-	0/0/0/0	0/0/0/0
4	SAM	D	417	6	-	0/8/33/33	0/3/3/3
6	SF4	D	418	1,4	-	0/0/48/48	0/6/5/5
5	PLP	D	419	5	-	0/6/6/8	0/1/1/1
5	LYS	D	420[A]	-	-	0/5/9/9	0/0/0/0
5	LYS	D	420[B]	-	-	0/5/9/9	0/0/0/0
3	SO4	D	494	-	-	0/0/0/0	0/0/0/0

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	419	PLP	C4A-C4	-9.72	1.31	1.51
5	C	419	PLP	C4A-C4	-9.45	1.32	1.51
5	B	419	PLP	C4A-C4	-9.28	1.32	1.51
5	A	419	PLP	C4A-C4	-8.92	1.33	1.51
5	D	419	PLP	P-O2P	-3.16	1.43	1.54

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	417	SAM	N3-C2-N1	-6.20	124.15	128.89
4	D	417	SAM	N3-C2-N1	-5.88	124.39	128.89
4	A	417	SAM	N3-C2-N1	-5.36	124.79	128.89
4	C	417	SAM	N3-C2-N1	-4.86	125.17	128.89
4	B	417	SAM	C2'-C1'-N9	-4.39	107.59	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	418	SF4	1	0
6	D	418	SF4	1	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	400/416 (96%)	1.71	130 (32%)	1	1	18, 39, 61, 72	9 (2%)
1	B	401/416 (96%)	1.99	173 (43%)	0	0	20, 43, 79, 98	7 (1%)
1	C	400/416 (96%)	1.50	100 (25%)	1	1	16, 32, 59, 73	7 (1%)
1	D	401/416 (96%)	1.45	101 (25%)	1	1	15, 32, 55, 69	6 (1%)
All	All	1602/1664 (96%)	1.66	504 (31%)	1	1	15, 36, 65, 98	29 (1%)

The worst 5 of 504 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	48	VAL	11.1
1	B	22	TRP	8.4
1	C	64	LEU	7.6
1	B	38	ILE	7.5
1	B	54	SER	6.9

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	SO4	C	593	5/5	0.89	0.59	8.81	79,80,81,81	0
3	SO4	B	495	5/5	0.87	0.44	4.05	101,101,101,101	0
3	SO4	A	592	5/5	0.86	0.40	3.96	98,98,99,99	0
3	SO4	D	494	5/5	0.79	0.54	3.50	88,88,88,89	0
4	SAM	C	417	27/27	0.91	0.20	2.15	21,23,25,31	1
4	SAM	B	417	27/27	0.85	0.26	1.31	32,34,39,43	1
5	LYS	D	420[B]	10/10	0.91	0.22	1.13	24,25,28,29	3
5	LYS	D	420[A]	10/10	0.91	0.22	1.13	24,25,28,29	3
5	LYS	C	420[A]	10/10	0.92	0.16	0.97	22,24,27,27	3
5	LYS	C	420[B]	10/10	0.92	0.16	0.97	22,24,27,27	3
4	SAM	A	417	27/27	0.91	0.19	0.86	25,27,31,36	1
4	SAM	D	417	27/27	0.91	0.19	0.83	21,23,26,33	1
5	LYS	B	420[B]	10/10	0.85	0.25	0.43	32,34,39,39	3
5	LYS	B	420[A]	10/10	0.85	0.25	0.43	32,34,39,39	3
5	PLP	C	419	15/16	0.95	0.16	0.24	18,24,25,26	0
5	PLP	D	419	15/16	0.95	0.19	0.14	20,27,29,30	0
5	LYS	A	420[B]	10/10	0.94	0.18	0.12	27,29,32,33	3
5	LYS	A	420[A]	10/10	0.94	0.18	-0.10	27,29,32,33	3
5	PLP	B	419	15/16	0.95	0.19	-0.72	27,34,36,37	0
5	PLP	A	419	15/16	0.95	0.18	-0.87	24,31,32,33	0
2	ZN	D	421	1/1	0.84	0.11	-1.38	31,31,31,31	0
2	ZN	B	421	1/1	0.97	0.09	-1.60	45,45,45,45	0
6	SF4	B	418	8/8	0.93	0.09	-1.74	35,38,40,40	0
2	ZN	C	421	1/1	0.81	0.09	-1.76	36,36,36,36	0
2	ZN	A	421	1/1	0.98	0.09	-1.79	36,36,36,36	0
6	SF4	C	418	8/8	0.98	0.06	-2.15	22,24,25,26	0
6	SF4	A	418	8/8	0.97	0.07	-2.82	24,27,29,29	0
6	SF4	D	418	8/8	0.96	0.08	-3.06	21,22,25,26	0

6.5 Other polymers (i)

There are no such residues in this entry.