



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 27, 2026 – 05:44 PM EDT

PDB ID : 2A5H / pdb_00002a5h
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

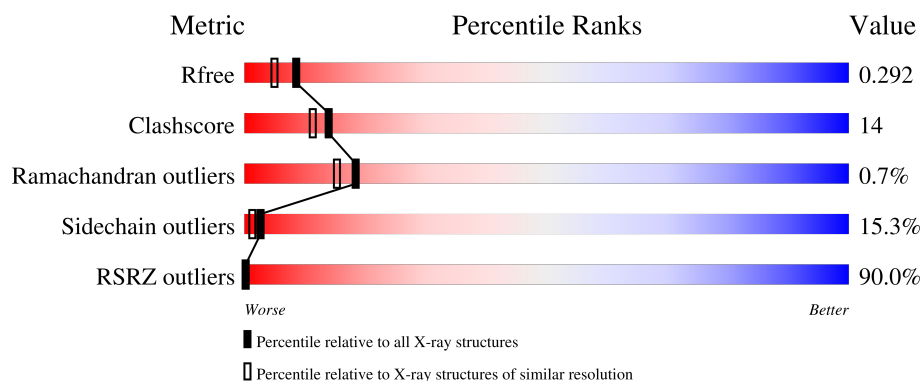
1 Overall quality at a glance

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))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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 $\leq 5\%$. 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	416	88% 66% 24% 7% ..
1	B	416	92% 66% 25% 6% ..
1	C	416	84% 66% 23% 7% ..
1	D	416	83% 65% 25% 7% ..

2 Entry composition

There are 8 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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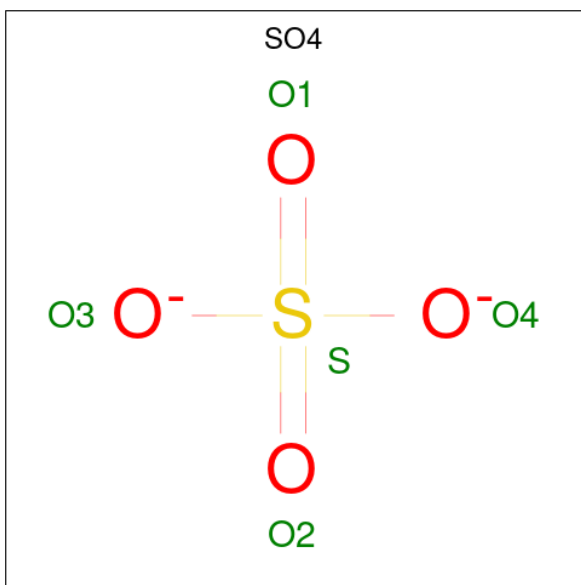
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Chain	Residue	Modelled	Actual	Comment	Reference
C	57	MSE	MET	modified residue	GB 5410603
C	124	MSE	MET	modified residue	GB 5410603
C	127	MSE	MET	modified residue	GB 5410603
C	145	MSE	MET	modified residue	GB 5410603
C	147	MSE	MET	modified residue	GB 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 (CCD ID: ZN) (formula: Zn).

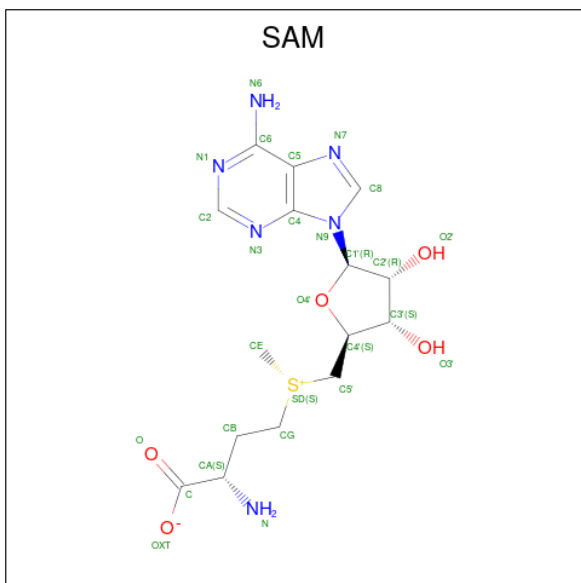
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



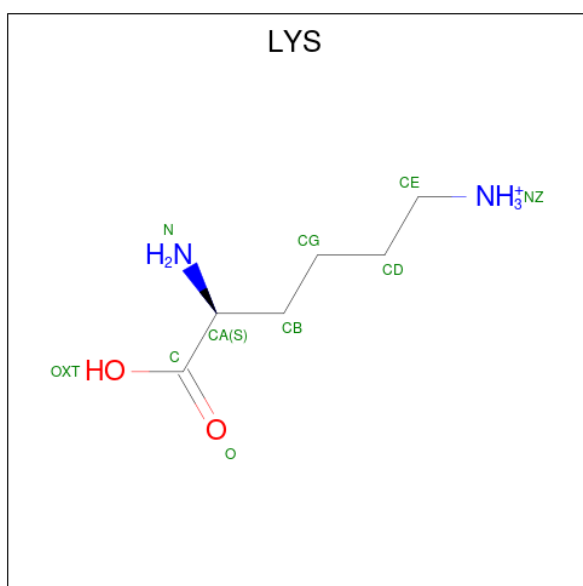
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

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



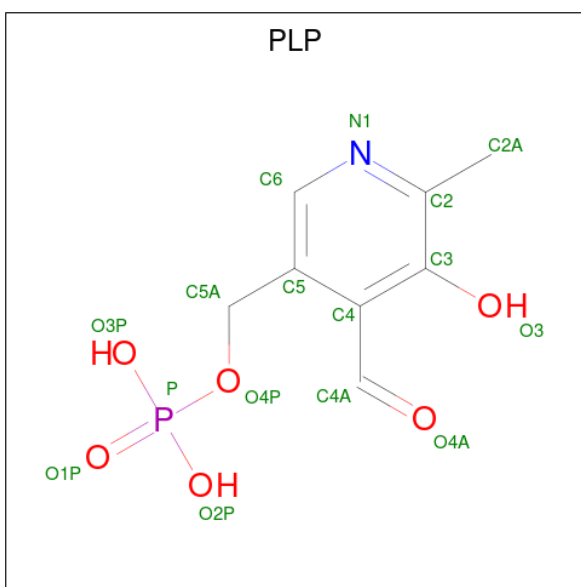
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	D	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 5 is LYSINE (CCD ID: LYS) (formula: $C_6H_{15}N_2O_2$).



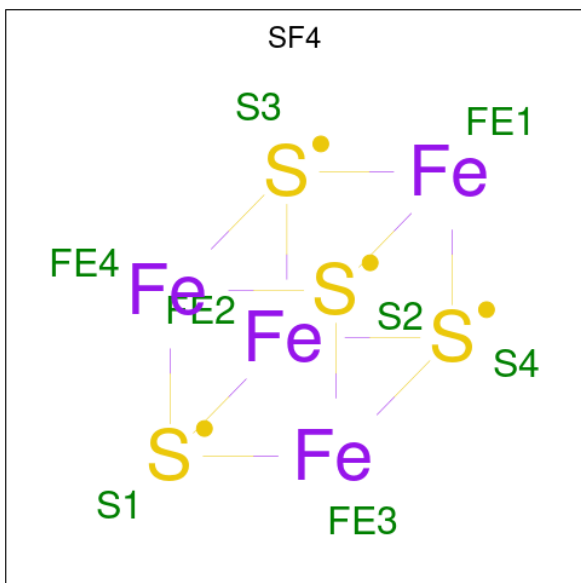
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			13	9	2	2		
5	B	1	Total	C	N	O	0	1
			13	9	2	2		
5	C	1	Total	C	N	O	0	1
			13	9	2	2		
5	D	1	Total	C	N	O	0	1
			13	9	2	2		

- Molecule 6 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
6	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
6	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
6	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

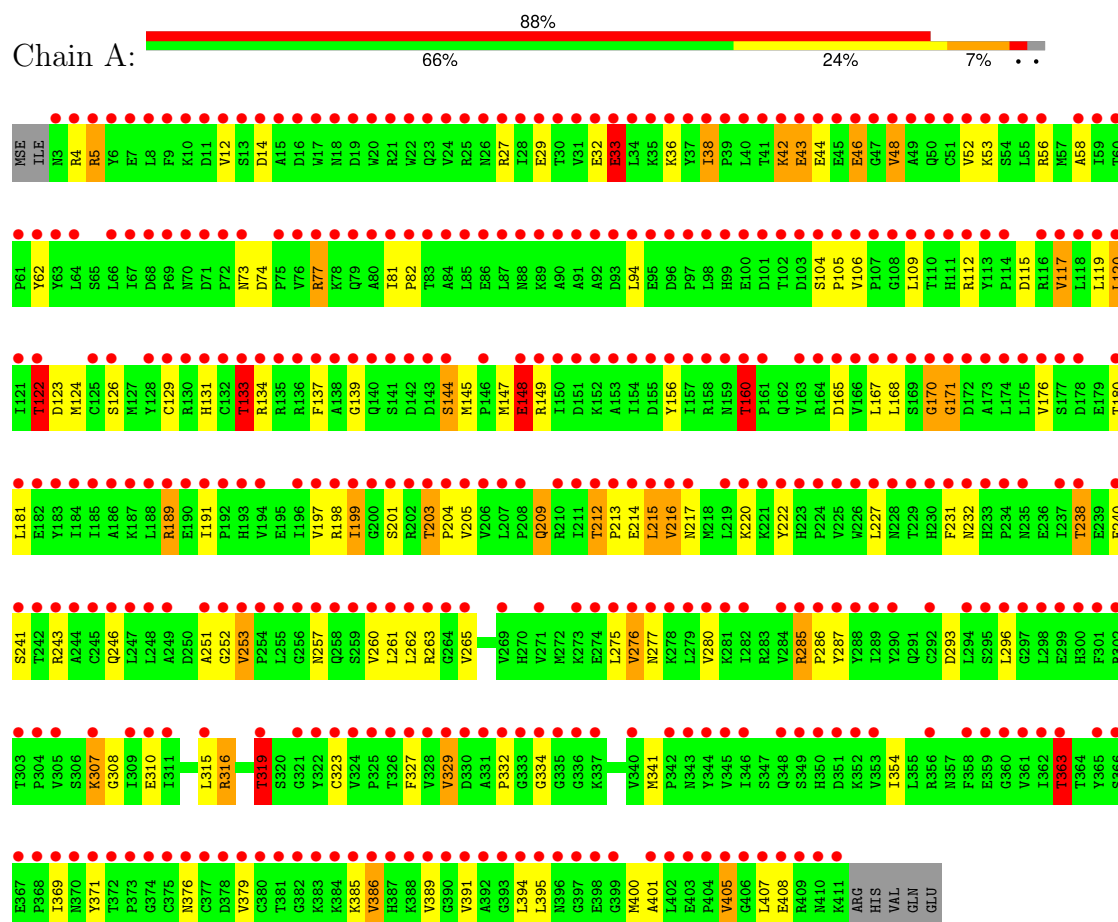
- Molecule 8 is water.

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

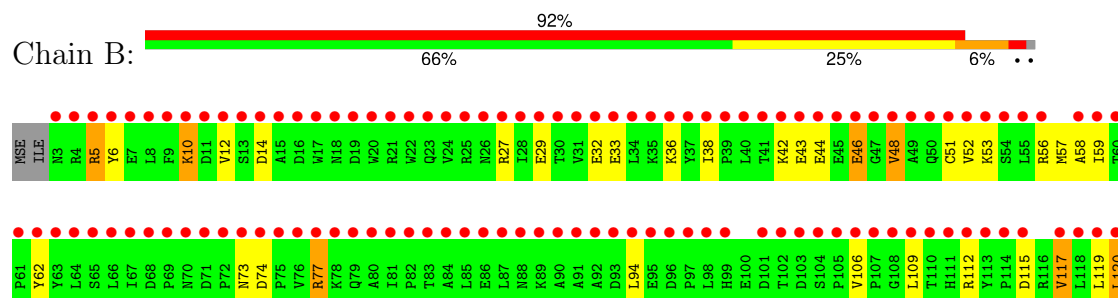
3 Residue-property plots

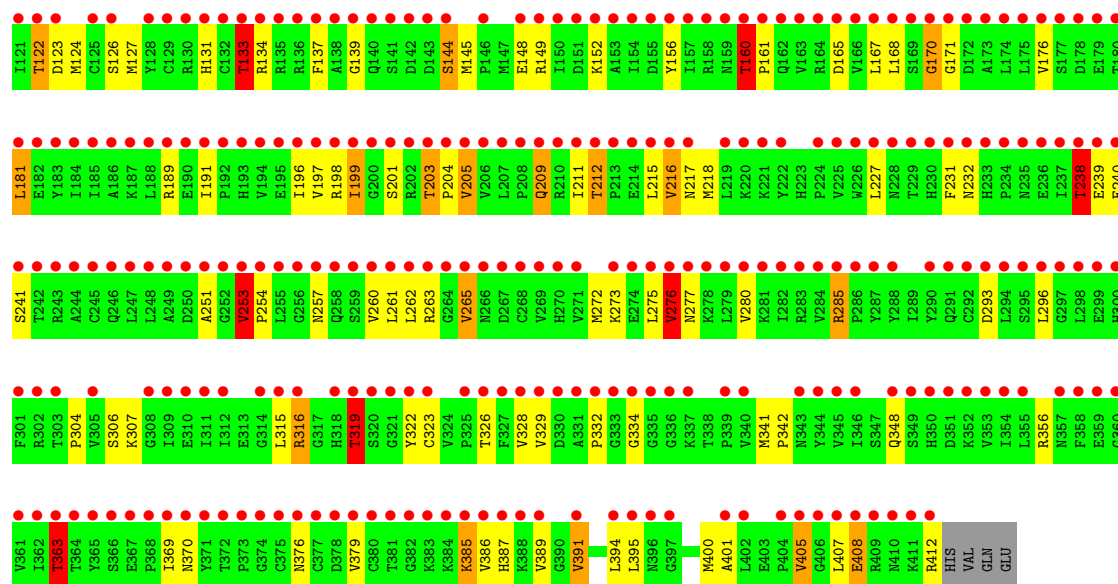
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: L-lysine 2,3-aminomutase

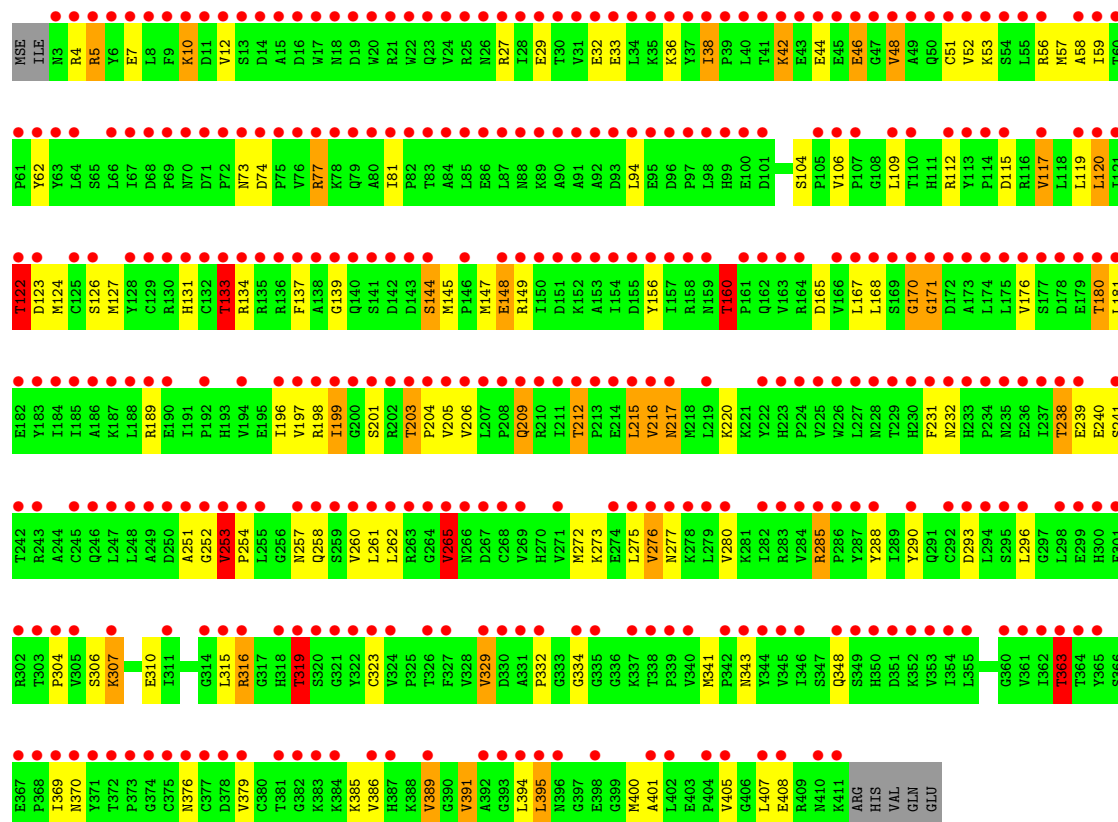
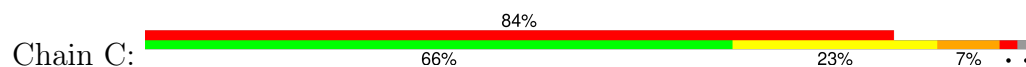


- Molecule 1: L-lysine 2,3-aminomutase

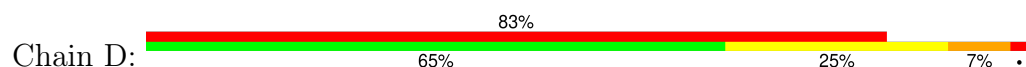




• Molecule 1: L-lysine 2,3-aminomutase



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



Y365	T303	T242	E182	R122	P61	MSE
S366	P304	R243	Y183	D123	Y62	ILE
E367	V305	A244	I184	M124	Y63	N3
P368	S306	C245	I185	C125	L64	R4
I369	K307	Q246	A186	S126	S65	R5
N370	G308	L247	K187	M127	L66	Y6
Y371	I309	L248	I188	Y128	I67	E7
T372	E310	A249	R189	C129	D68	L8
P373	I311	D250	E190	A130	P69	F9
G374	I312	A251	I191	H131	N70	K10
C375	E313	G252	P192	C132	D71	D11
N376	G314	V253	H193	T133	P72	V12
C377	L315	P254	V194	R134	N73	S13
D378	R316	L255	E195	R135	D74	D14
V379	T319	G256	I196	F137	P75	A15
C380	S320	N257	V197	A138	P76	D16
T381	G321	Q258	R198	R77	R77	W17
G382	S321	S259	I199	G139	K78	N18
K383	Y322	V260	G200	Q140	Q79	D19
K384	C323	L261	S201	S141	A80	W20
K385	V324	L262	R202	D142	T81	R21
V386	P325	R263	T203	D143	P82	W22
H387	T326	G264	P204	S144	T83	Q23
K388	F327	V265	V205	M145	A84	V24
V389	V328	N266	V206	P146	L85	R25
G390	V329	D267	L207	M147	E86	N26
V391	D330	C268	P208	E148	L87	R27
A392	A331	V269	Q209	R149	N88	I28
G393	P332	H270	R210	I150	K89	E29
L394	G333	V271	I211	D151	A90	T30
L395	G334	N272	T212	K152	A91	V31
K396	G335	K273	P213	A153	A92	E32
G397	G336	E274	E214	I154	D93	E33
E398	K337	L275	L215	D155	L94	K34
G399	T340	V276	V216	Y156	E95	K35
M400	N277	N277	N217	I157	D96	K36
A401	K278	K278	N218	R158	P97	Y37
L402	L279	L279	L219	N159	L98	I38
E403	V280	V280	K220	T160	H99	P39
V405	K281	K281	K221	P161	E100	L40
G406	I346	I346	H223	Q162	D101	T41
L407	S347	S347	P224	V163	K42	K42
E408	Q348	P286	V225	R164	E43	O43
R409	S349	T287	V226	D165	E44	E44
N410	H350	Y288	L227	V166	E45	E45
K411	D351	L289	N228	L167	E46	E46
R412	K352	V290	T229	L168	G47	G47
VAL	V353	Q291	H230	S169	V48	V48
GLN	I354	C292	F231	G170	T110	A49
GLU	L355	D293	N231	G171	H111	Q50
	R356	L294	N232	D172	R112	C51
	N357	S295	H233	A173	Y113	V52
	F358	L296	P234	L174	P114	K53
	E359	G297	N235	L175	D115	S54
	G360	L298	E236	V176	R116	L55
	V361	T299	L237	S177	R117	R56
	I362	H300	T238	D178	V117	R56
	T363	F301	E239	L118	L118	H57
	T364	R302	E240	L119	L119	A58
				T120	L120	I59
				L181	I121	T60

4 Data and refinement statistics

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 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	81.5 (50.00-2.10) 82.8 (50.00-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.19 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.184 , 0.225 0.266 , 0.292	Depositor DCC
R_{free} test set	27582 reflections (9.17%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	1.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: PLP, SO4, SF4, ZN, SAM

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	1.22	7/3391 (0.2%)	1.37	31/4590 (0.7%)
1	B	1.23	7/3388 (0.2%)	1.27	23/4586 (0.5%)
1	C	1.13	10/3380 (0.3%)	1.28	30/4576 (0.7%)
1	D	1.23	9/3402 (0.3%)	1.29	24/4604 (0.5%)
All	All	1.20	33/13561 (0.2%)	1.30	108/18356 (0.6%)

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 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	408	GLU	CD-OE2	30.07	1.82	1.25
1	A	148	GLU	CG-CD	29.07	2.24	1.52
1	B	408	GLU	CD-OE1	-25.44	0.77	1.25
1	A	33	GLU	CG-CD	-23.23	0.94	1.52
1	D	42	LYS	CG-CD	20.91	2.15	1.52

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	GLU	CB-CG-CD	31.37	165.93	112.60
1	B	408	GLU	CG-CD-OE2	-22.07	67.64	118.40
1	A	46	GLU	CB-CG-CD	17.54	142.41	112.60
1	B	46	GLU	CB-CG-CD	15.27	138.56	112.60
1	D	408	GLU	CG-CD-OE1	-14.55	84.94	118.40

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

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	101	0
1	B	3288	0	3306	97	0
1	C	3280	0	3295	114	0
1	D	3297	0	3313	123	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	2	0
4	C	27	0	21	0	0
4	D	27	0	21	0	0
5	A	13	0	22	0	0
5	B	13	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	13	0	22	0	0
5	D	13	0	22	0	0
6	A	15	0	6	0	0
6	B	15	0	6	0	0
6	C	15	0	6	0	0
6	D	15	0	6	0	0
7	A	8	0	0	0	0
7	B	8	0	0	0	0
7	C	8	0	0	1	0
7	D	8	0	0	1	0
8	A	135	0	0	7	0
8	B	116	0	0	3	0
8	C	183	0	0	10	1
8	D	174	0	0	8	0
All	All	14034	0	13410	386	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 386 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	8: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)
8:C:764:HOH:O	8:C:764:HOH:O[2_454]	1.88	0.32

5.3 Torsion angles

5.3.1 Protein backbone

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%)	18	15
1	B	416/416 (100%)	398 (96%)	15 (4%)	3 (1%)	18	15
1	C	415/416 (100%)	397 (96%)	15 (4%)	3 (1%)	18	15
1	D	417/416 (100%)	397 (95%)	17 (4%)	3 (1%)	18	15
All	All	1664/1664 (100%)	1592 (96%)	60 (4%)	12 (1%)	18	15

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

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%)	314 (84%)	60 (16%)	2	1
1	B	374/362 (103%)	313 (84%)	61 (16%)	2	1
1	C	373/362 (103%)	316 (85%)	57 (15%)	3	1
1	D	375/362 (104%)	314 (84%)	61 (16%)	2	1
All	All	1496/1448 (103%)	1257 (84%)	239 (16%)	3	1

5 of 239 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	391	VAL
1	D	296	LEU
1	C	197	VAL
1	D	276	VAL
1	D	395	LEU

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

Mol	Chain	Res	Type
1	D	232	ASN
1	D	257	ASN
1	D	370	ASN
1	B	232	ASN
1	B	209	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 oligosaccharides 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
7	SF4	C	418	1,4	0,12,12	-	-	-		
5	LYS	C	420[A]	-	8,9,9	1.03	0	7,10,10	0.94	0
7	SF4	A	418	1,4	0,12,12	-	-	-		
5	LYS	D	420[A]	-	8,9,9	0.94	1 (12%)	7,10,10	1.17	1 (14%)
4	SAM	A	417	7	27,29,29	1.87	8 (29%)	34,42,42	2.09	9 (26%)
5	LYS	B	420[B]	-	8,9,9	0.75	0	7,10,10	0.99	1 (14%)
7	SF4	B	418	1,4	0,12,12	-	-	-		
4	SAM	B	417	7	27,29,29	1.86	6 (22%)	34,42,42	2.01	12 (35%)
6	PLP	A	419	5	15,15,16	2.72	2 (13%)	21,22,23	1.18	2 (9%)
5	LYS	B	420[A]	-	8,9,9	0.74	0	7,10,10	1.02	1 (14%)
4	SAM	C	417	7	27,29,29	1.87	6 (22%)	34,42,42	1.99	11 (32%)
6	PLP	C	419	5	15,15,16	2.80	3 (20%)	21,22,23	0.97	0
5	LYS	A	420[B]	-	8,9,9	0.85	1 (12%)	7,10,10	1.05	0
3	SO4	C	593	-	4,4,4	0.24	0	6,6,6	0.47	0
3	SO4	D	494	-	4,4,4	0.31	0	6,6,6	0.34	0
4	SAM	D	417	7	27,29,29	1.74	6 (22%)	34,42,42	2.25	14 (41%)
5	LYS	A	420[A]	-	8,9,9	0.85	1 (12%)	7,10,10	1.04	0
3	SO4	B	495	-	4,4,4	0.25	0	6,6,6	0.31	0
6	PLP	B	419	5	15,15,16	2.76	2 (13%)	21,22,23	0.93	0
3	SO4	A	592	-	4,4,4	0.30	0	6,6,6	0.22	0
5	LYS	C	420[B]	-	8,9,9	1.02	0	7,10,10	0.90	0
5	LYS	D	420[B]	-	8,9,9	0.94	1 (12%)	7,10,10	1.12	1 (14%)
7	SF4	D	418	1,4	0,12,12	-	-	-		
6	PLP	D	419	5	15,15,16	2.88	2 (13%)	21,22,23	1.16	1 (4%)

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
7	SF4	C	418	1,4	-	-	0/6/5/5
5	LYS	C	420[A]	-	-	1/9/9/9	-
7	SF4	A	418	1,4	-	-	0/6/5/5
5	LYS	D	420[A]	-	-	1/9/9/9	-
4	SAM	A	417	7	-	2/17/33/33	0/3/3/3
5	LYS	B	420[B]	-	-	1/9/9/9	-
7	SF4	B	418	1,4	-	-	0/6/5/5
4	SAM	B	417	7	-	2/17/33/33	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PLP	A	419	5	-	1/6/6/8	0/1/1/1
5	LYS	B	420[A]	-	-	1/9/9/9	-
4	SAM	C	417	7	-	3/17/33/33	0/3/3/3
6	PLP	C	419	5	-	0/6/6/8	0/1/1/1
5	LYS	A	420[B]	-	-	1/9/9/9	-
4	SAM	D	417	7	-	2/17/33/33	0/3/3/3
5	LYS	A	420[A]	-	-	1/9/9/9	-
6	PLP	B	419	5	-	0/6/6/8	0/1/1/1
5	LYS	C	420[B]	-	-	1/9/9/9	-
5	LYS	D	420[B]	-	-	1/9/9/9	-
7	SF4	D	418	1,4	-	-	0/6/5/5
6	PLP	D	419	5	-	0/6/6/8	0/1/1/1

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	419	PLP	C4A-C4	-9.92	1.31	1.51
6	C	419	PLP	C4A-C4	-9.65	1.32	1.51
6	B	419	PLP	C4A-C4	-9.47	1.32	1.51
6	A	419	PLP	C4A-C4	-9.10	1.33	1.51
4	C	417	SAM	C5-C4	5.26	1.48	1.39

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	417	SAM	C5-C4-N3	-5.03	119.79	126.72
4	A	417	SAM	C5-C4-N3	-4.80	120.11	126.72
4	C	417	SAM	C5-C4-N3	-4.72	120.22	126.72
4	D	417	SAM	N3-C4-N9	4.48	134.79	127.17
4	A	417	SAM	N3-C4-N9	4.42	134.69	127.17

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

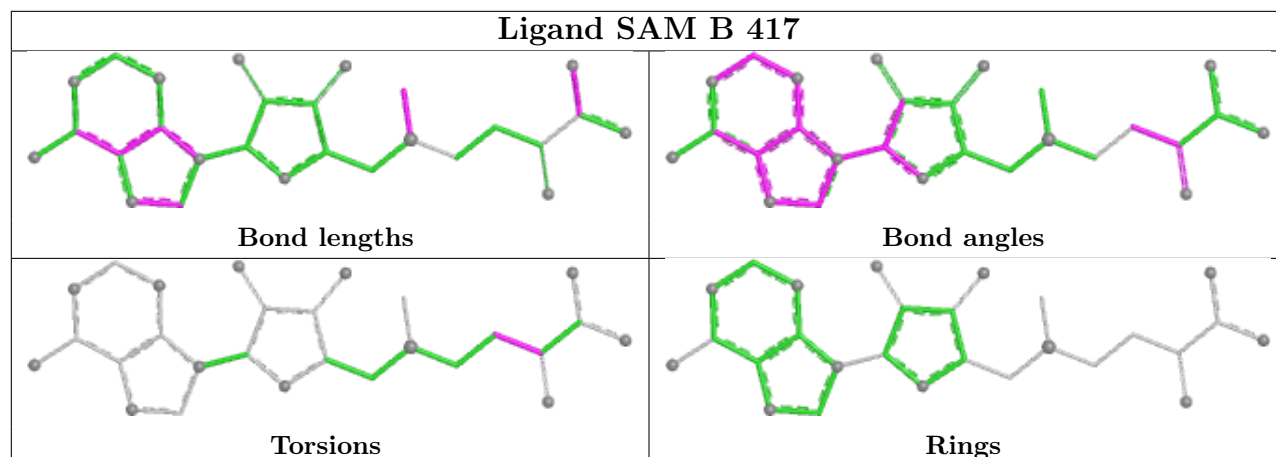
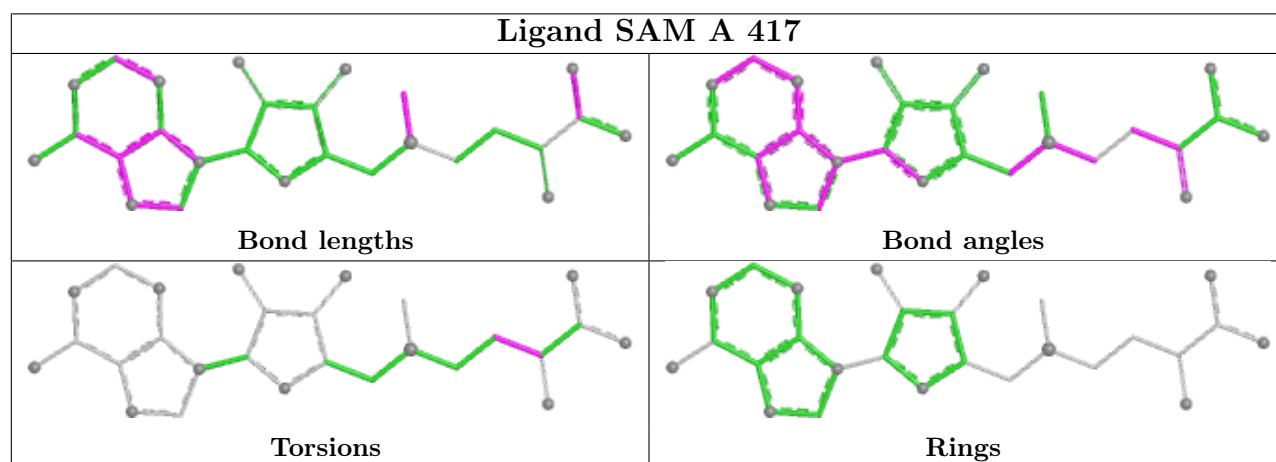
Mol	Chain	Res	Type	Atoms
4	C	417	SAM	N-CA-CB-CG
4	D	417	SAM	N-CA-CB-CG
4	A	417	SAM	C-CA-CB-CG
4	B	417	SAM	C-CA-CB-CG
4	C	417	SAM	C-CA-CB-CG

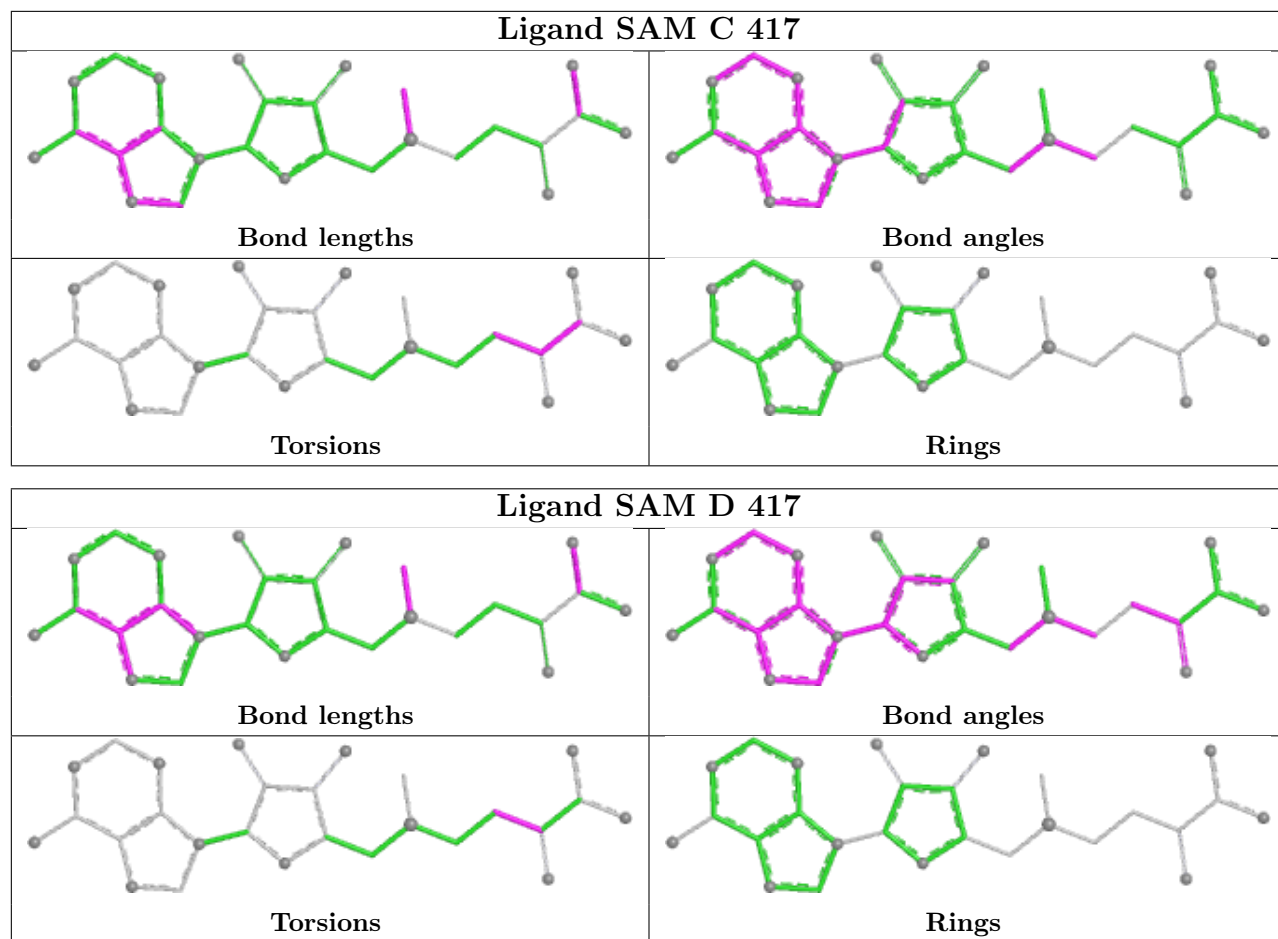
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	418	SF4	1	0
4	B	417	SAM	2	0
7	D	418	SF4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	400/416 (96%)	3.79	366 (91%) 0 0	12, 38, 60, 72	18 (4%)
1	B	401/416 (96%)	4.27	381 (95%) 0 0	13, 42, 78, 98	15 (3%)
1	C	400/416 (96%)	3.61	349 (87%) 0 0	11, 32, 58, 73	15 (3%)
1	D	401/416 (96%)	3.40	345 (86%) 0 0	9, 32, 54, 69	15 (3%)
All	All	1602/1664 (96%)	3.77	1441 (89%) 0 0	9, 36, 64, 98	63 (3%)

The worst 5 of 1441 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	47	GLY	13.6
1	D	52	VAL	12.6
1	A	48	VAL	12.3
1	B	31	VAL	11.8
1	A	46	GLU	10.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

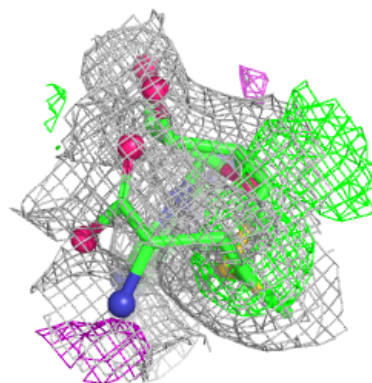
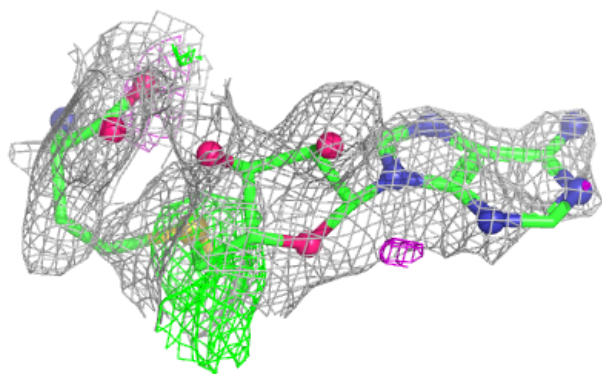
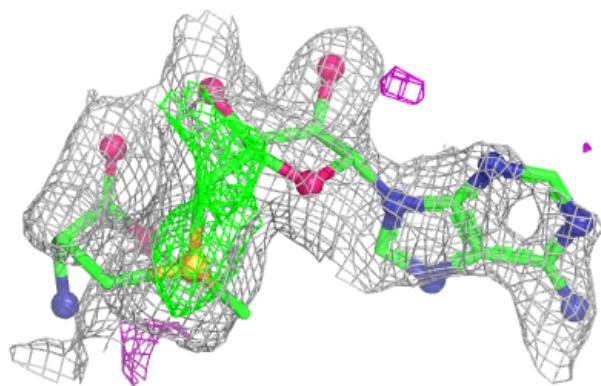
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	C	593	5/5	0.37	0.31	79,80,81,81	0
3	SO4	A	592	5/5	0.48	0.28	98,98,99,99	0
5	LYS	C	420[A]	10/10	0.51	0.28	22,24,27,27	3
5	LYS	C	420[B]	10/10	0.51	0.28	22,24,27,27	3
3	SO4	D	494	5/5	0.55	0.25	88,88,88,89	0
5	LYS	B	420[B]	10/10	0.64	0.30	32,34,39,39	3
4	SAM	B	417	27/27	0.64	0.27	32,34,39,43	1
5	LYS	B	420[A]	10/10	0.64	0.30	32,34,39,39	3
3	SO4	B	495	5/5	0.66	0.27	101,101,101,101	0
4	SAM	D	417	27/27	0.76	0.23	21,23,26,33	1
4	SAM	A	417	27/27	0.77	0.20	25,27,31,36	1
5	LYS	A	420[A]	10/10	0.79	0.20	27,29,32,33	3
5	LYS	A	420[B]	10/10	0.79	0.20	27,29,32,33	3
4	SAM	C	417	27/27	0.79	0.21	21,23,25,31	1
6	PLP	A	419	15/16	0.84	0.20	24,31,32,33	0
5	LYS	D	420[B]	10/10	0.86	0.15	24,25,28,29	3
5	LYS	D	420[A]	10/10	0.86	0.15	24,25,28,29	3
6	PLP	B	419	15/16	0.88	0.17	27,34,36,37	0
7	SF4	B	418	8/8	0.88	0.12	35,38,40,40	0
6	PLP	C	419	15/16	0.90	0.16	18,24,25,26	0
6	PLP	D	419	15/16	0.90	0.14	20,27,29,30	0
2	ZN	D	421	1/1	0.90	0.08	31,31,31,31	0
7	SF4	D	418	8/8	0.90	0.08	21,22,25,26	0
7	SF4	C	418	8/8	0.92	0.08	22,24,25,26	0
7	SF4	A	418	8/8	0.93	0.08	24,27,29,29	0
2	ZN	B	421	1/1	0.94	0.07	45,45,45,45	0
2	ZN	C	421	1/1	0.97	0.04	36,36,36,36	0
2	ZN	A	421	1/1	0.98	0.05	36,36,36,36	0

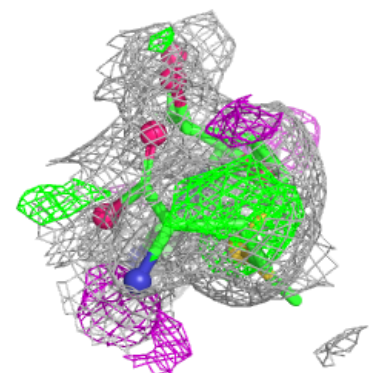
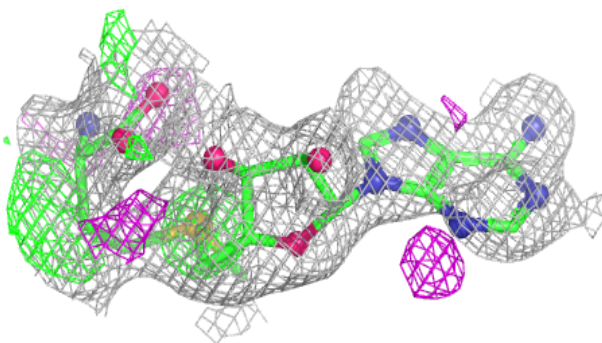
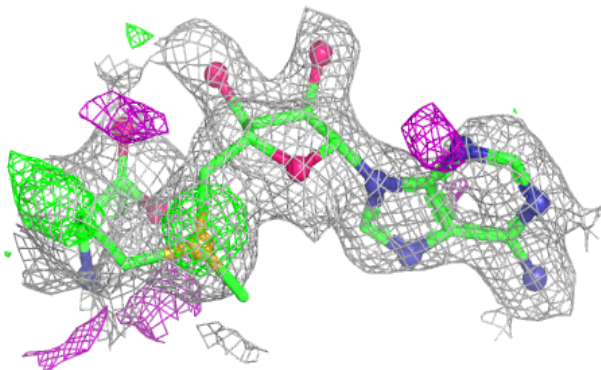
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SAM B 417:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

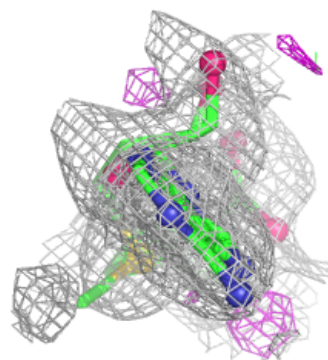
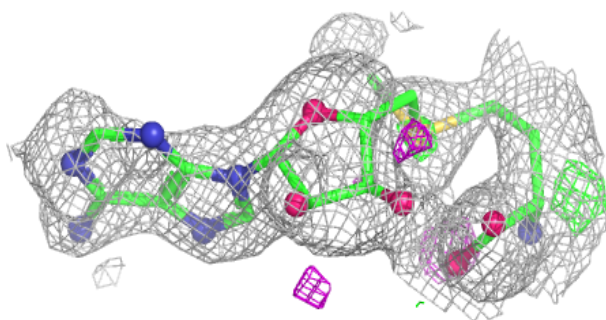
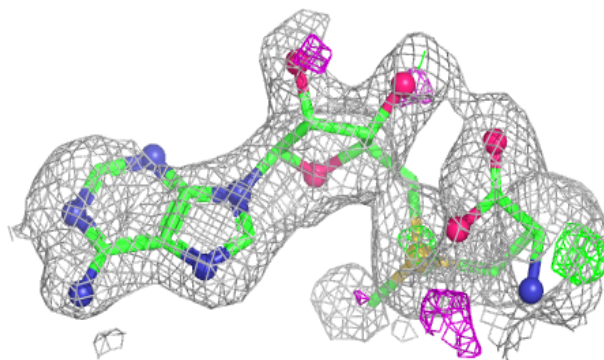
**Electron density around SAM D 417:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

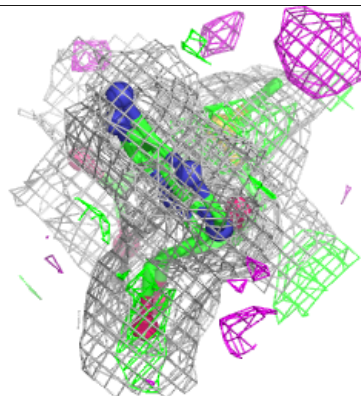
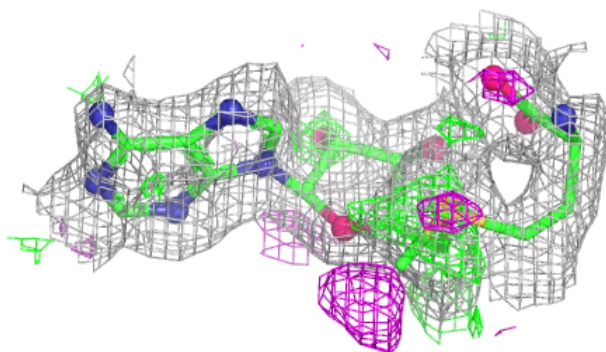
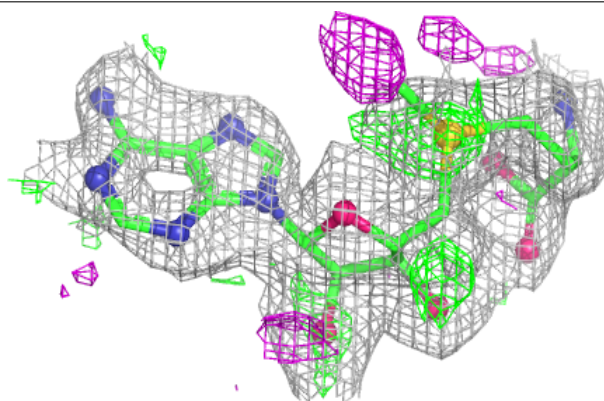


Electron density around SAM A 417:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around SAM C 417:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.