



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2025 – 09:24 PM EDT

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

<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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

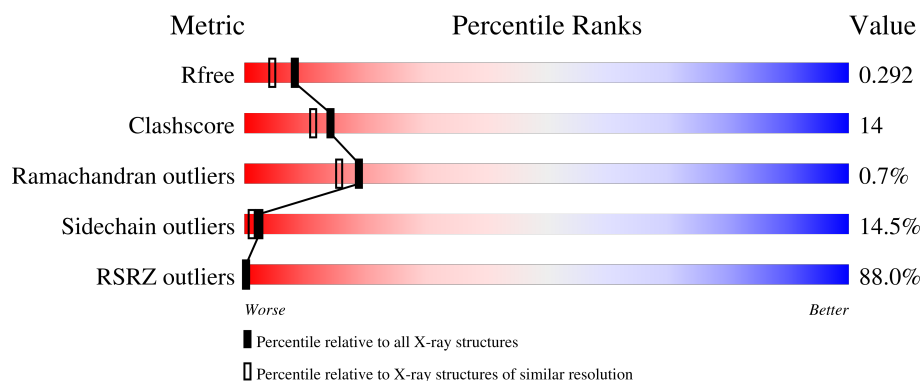
1 Overall quality at a glance ⓘ

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}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (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	<div> <div>86%</div> <div> <div>68%</div> <div>22%</div> <div>7%</div> <div>..</div> </div> </div>
1	B	416	<div> <div>90%</div> <div> <div>67%</div> <div>24%</div> <div>6%</div> <div>..</div> </div> </div>
1	C	416	<div> <div>82%</div> <div> <div>67%</div> <div>23%</div> <div>7%</div> <div>..</div> </div> </div>
1	D	416	<div> <div>80%</div> <div> <div>66%</div> <div>24%</div> <div>7%</div> <div>..</div> </div> </div>

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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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).

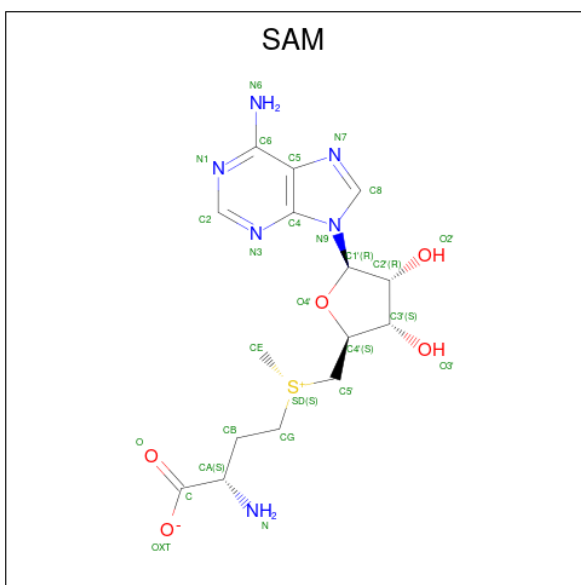
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



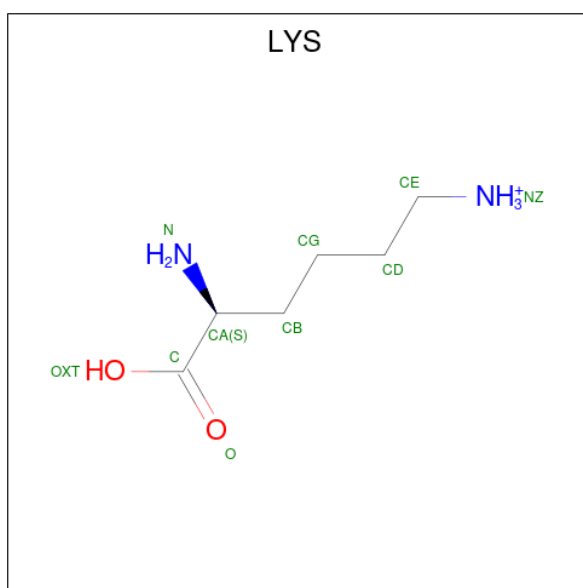
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

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



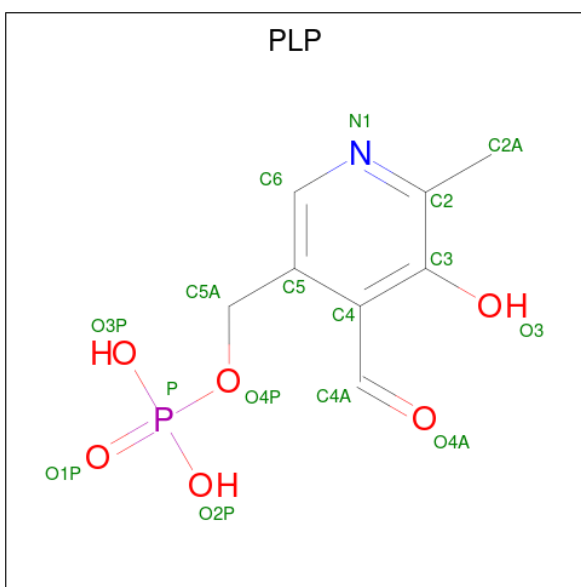
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	D	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

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



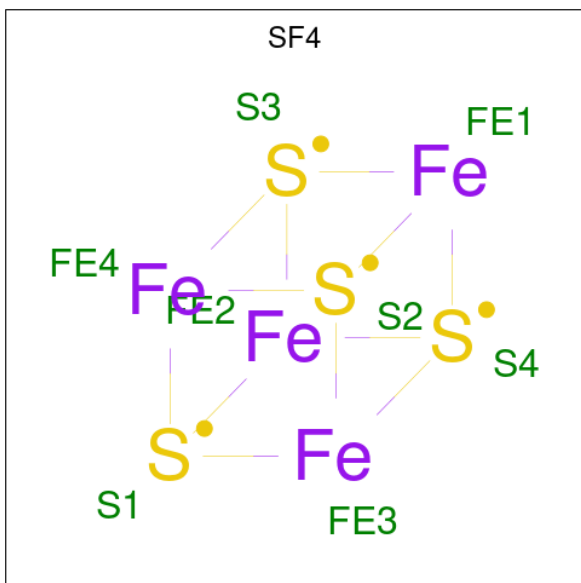
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			13	9	2	2		
5	B	1	Total	C	N	O	0	1
			13	9	2	2		
5	C	1	Total	C	N	O	0	1
			13	9	2	2		
5	D	1	Total	C	N	O	0	1
			13	9	2	2		

- Molecule 6 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: 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 (three-letter code: SF4) (formula: Fe₄S₄).



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

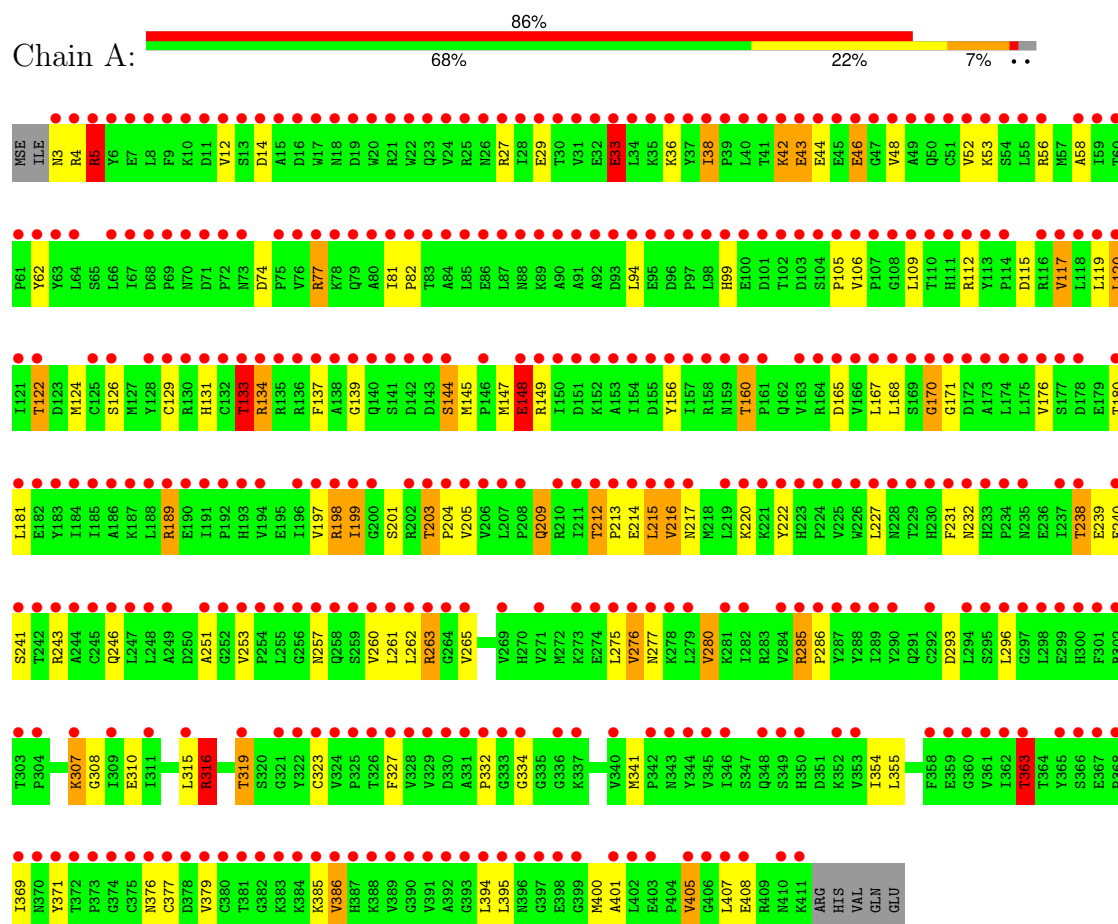
- Molecule 8 is water.

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

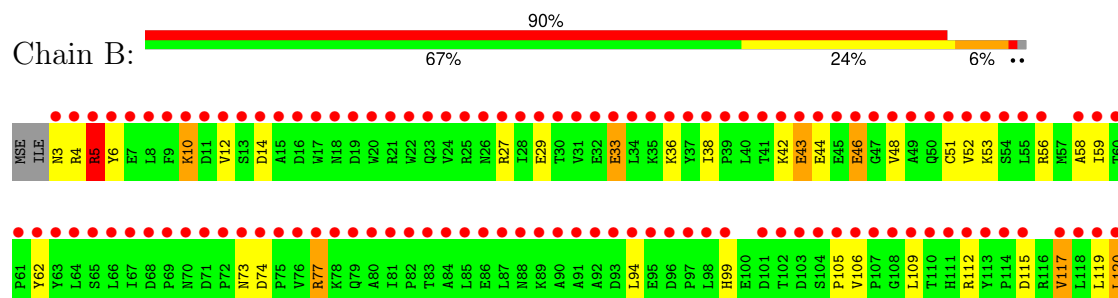
3 Residue-property plots

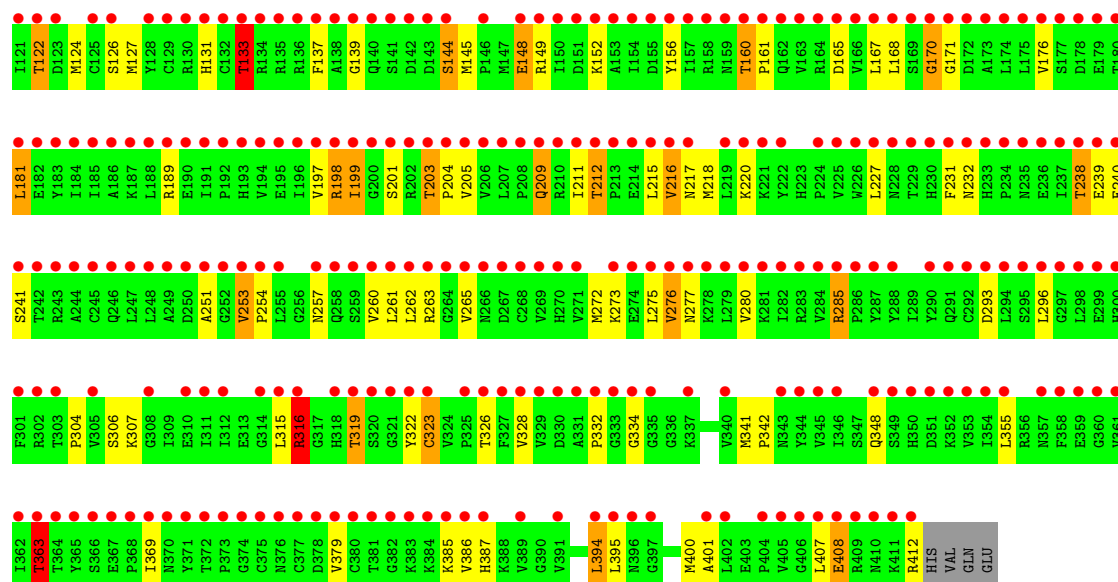
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

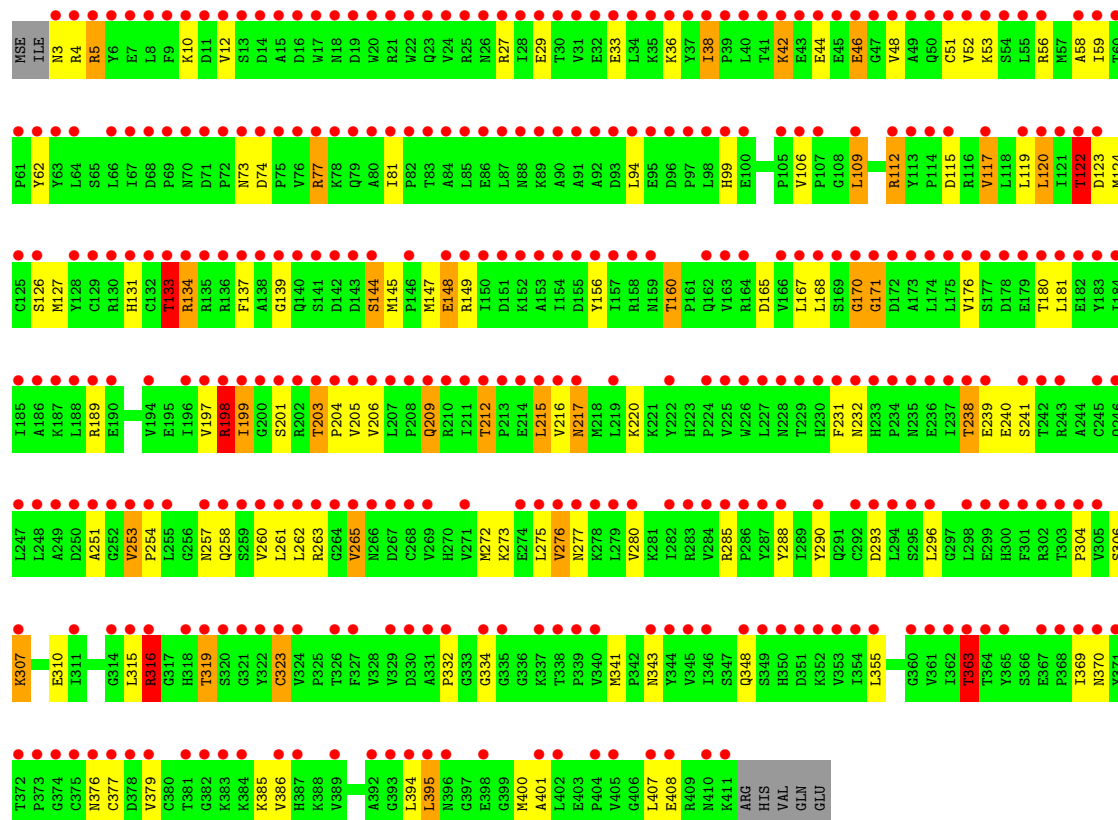
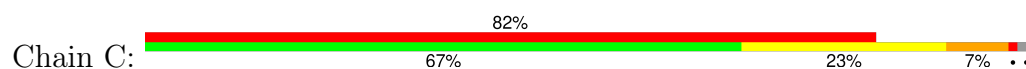


• Molecule 1: L-lysine 2,3-aminomutase

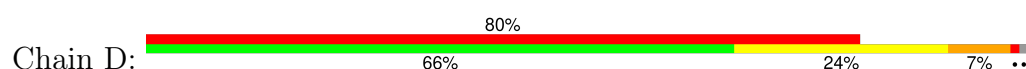




• Molecule 1: L-lysine 2,3-aminomutase



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



P368	I369	Y370	Y371	T372	P373	G374	C375	N376	C377	D378	V379	C380	T381	G382	K383	K384	K385	V386	H387	K388	V389	G390	V391	A392	C393	L394	L395	N396	G397	E398	G399	M400	A401	L402	E403	P404	V405	G406	L407	E408	R409	M410	K411	R412	HIS	VAL	GLN	GLU											
V305	S306	K307	G308	I309	E310	I311	I312	E313	G314	L315	R316	T319	S320	G321	G322	C323	V324	P325	T326	F327	G328	V329	D330	A331	P332	G333	G334	G335	G336	K337	V340	M341	P342	N343	Y344	V345	I346	Q347	Q348	S349	H350	D351	K352	V353	I354	L355	F356	E359	G360	V361	I362	T363	T364	Y365	S366	E367			
T242	R243	A244	C245	Q246	L247	L248	A249	D250	A251	G252	V253	P254	L255	G256	N257	Q258	S259	V260	L261	L262	R263	G264	V265	V266	H270	V271	N272	K273	E274	L275	V276	N277	L278	L279	V280	K281	L282	R285	P286	V287	V288	L289	Y290	Q291	C292	D293	L294	S295	L296	Q297	L298	E299	H300	F301	R302	T303	P304		
E182	Y183	I184	I185	A186	K187	L188	R189	E190	I191	P192	H193	V194	E195	I196	V197	R198	I199	G200	S201	R202	T203	P204	V205	V206	L207	Q209	R210	I211	T212	P213	E214	L215	V216	N217	K218	L219	K220	K221	Y222	H223	P224	V225	V226	L227	N228	T229	H230	F231	N232	H233	P234	N235	E236	L237	T238	E239	E240	S241	
P61	Y62	Y63	L64	S65	L66	I67	D68	P69	N70	D71	P72	N73	D74	P75	V76	R77	K78	Q79	A80	I81	P82	T83	A84	R85	E86	L87	N88	K89	A90	A91	A92	D93	L94	E95	D96	P97	L98	H99	E100	D101	S104	P105	V106	P107	G108	L109	T110	H111	R112	Y113	P114	D115	S116	V117	L118	L119	I120	I121	
T122	D123	M124	C125	S126	M127	Y128	C129	A130	H131	C132	T133	R134	R135	A136	F137	A138	G139	Q140	S141	D142	D143	S144	M145	P146	M147	E148	L149	I150	D151	K152	A153	I154	D155	I156	I157	R158	N159	T160	P161	Q162	V163	R164	D165	V166	L167	L168	S169	G170	G171	D172	A173	L174	L175	V176	S177	D178	E179	T180	L181
MSE	ILE	N3	R4	R5	Y6	E7	L8	F9	K10	D11	V12	S13	D14	A15	D16	W17	N18	D19	W20	R21	W22	Q23	V24	R25	N26	R27	I28	E29	T30	V31	E32	E33	L34	K35	Y37	K36	I38	P39	L40	T41	K42	E43	E44	E45	E46	G47	V48	A49	Q50	C51	V52	K53	S54	R55	R56	M57	A58	I59	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	10427 reflections (8.58%)	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: SAM, ZN, SF4, PLP, SO4

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(°)	Ideal(°)
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

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	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	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	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%)	19	16
1	B	416/416 (100%)	398 (96%)	15 (4%)	3 (1%)	19	16
1	C	415/416 (100%)	397 (96%)	15 (4%)	3 (1%)	19	16
1	D	417/416 (100%)	397 (95%)	17 (4%)	3 (1%)	19	16
All	All	1664/1664 (100%)	1592 (96%)	60 (4%)	12 (1%)	19	16

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

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

Mol	Chain	Res	Type
1	B	407	LEU
1	D	379	VAL
1	C	209	GLN
1	D	363	THR
1	D	215	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	209	GLN
1	D	232	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
5	LYS	D	420[A]	-	8,9,9	0.94	1 (12%)	7,10,10	1.17	1 (14%)
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
5	LYS	C	420[B]	-	8,9,9	1.02	0	7,10,10	0.90	0
6	PLP	A	419	5	15,15,16	2.72	2 (13%)	21,22,23	1.18	2 (9%)
4	SAM	B	417	7	23,29,29	1.64	3 (13%)	20,42,42	1.68	6 (30%)
5	LYS	B	420[A]	-	8,9,9	0.74	0	7,10,10	1.02	1 (14%)
7	SF4	B	418	4,1	0,12,12	-	-	-		
7	SF4	D	418	4,1	0,12,12	-	-	-		
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
5	LYS	C	420[A]	-	8,9,9	1.03	0	7,10,10	0.94	0
4	SAM	D	417	7	23,29,29	1.40	3 (13%)	20,42,42	1.82	5 (25%)
7	SF4	A	418	4,1	0,12,12	-	-	-		
6	PLP	B	419	5	15,15,16	2.76	2 (13%)	21,22,23	0.93	0
4	SAM	C	417	7	23,29,29	1.48	3 (13%)	20,42,42	1.83	5 (25%)
7	SF4	C	418	4,1	0,12,12	-	-	-		
3	SO4	A	592	-	4,4,4	0.30	0	6,6,6	0.22	0
5	LYS	D	420[B]	-	8,9,9	0.94	1 (12%)	7,10,10	1.12	1 (14%)
3	SO4	D	494	-	4,4,4	0.31	0	6,6,6	0.34	0
6	PLP	D	419	5	15,15,16	2.88	2 (13%)	21,22,23	1.16	1 (4%)
3	SO4	C	593	-	4,4,4	0.24	0	6,6,6	0.47	0
4	SAM	A	417	7	23,29,29	1.57	3 (13%)	20,42,42	2.02	5 (25%)
5	LYS	B	420[B]	-	8,9,9	0.75	0	7,10,10	0.99	1 (14%)

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
5	LYS	D	420[A]	-	-	1/9/9/9	-
6	PLP	C	419	5	-	0/6/6/8	0/1/1/1
5	LYS	A	420[B]	-	-	1/9/9/9	-
5	LYS	C	420[B]	-	-	1/9/9/9	-
6	PLP	A	419	5	-	1/6/6/8	0/1/1/1
4	SAM	B	417	7	-	2/13/33/33	0/3/3/3
5	LYS	B	420[A]	-	-	1/9/9/9	-
7	SF4	B	418	4,1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SF4	D	418	4,1	-	-	0/6/5/5
5	LYS	A	420[A]	-	-	1/9/9/9	-
5	LYS	C	420[A]	-	-	1/9/9/9	-
4	SAM	D	417	7	-	2/13/33/33	0/3/3/3
7	SF4	A	418	4,1	-	-	0/6/5/5
6	PLP	B	419	5	-	0/6/6/8	0/1/1/1
4	SAM	C	417	7	-	3/13/33/33	0/3/3/3
7	SF4	C	418	4,1	-	-	0/6/5/5
5	LYS	D	420[B]	-	-	1/9/9/9	-
6	PLP	D	419	5	-	0/6/6/8	0/1/1/1
4	SAM	A	417	7	-	2/13/33/33	0/3/3/3
5	LYS	B	420[B]	-	-	1/9/9/9	-

The worst 5 of 25 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	B	417	SAM	OXT-C	5.04	1.46	1.30

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	417	SAM	C4'-O4'-C1'	-4.99	105.36	109.92
4	D	417	SAM	O4'-C1'-N9	4.69	114.96	108.75
4	A	417	SAM	O4'-C1'-N9	4.49	114.70	108.75
4	A	417	SAM	CG-SD-C5'	-4.00	93.65	103.43
4	C	417	SAM	CG-SD-C5'	-3.92	93.85	103.43

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

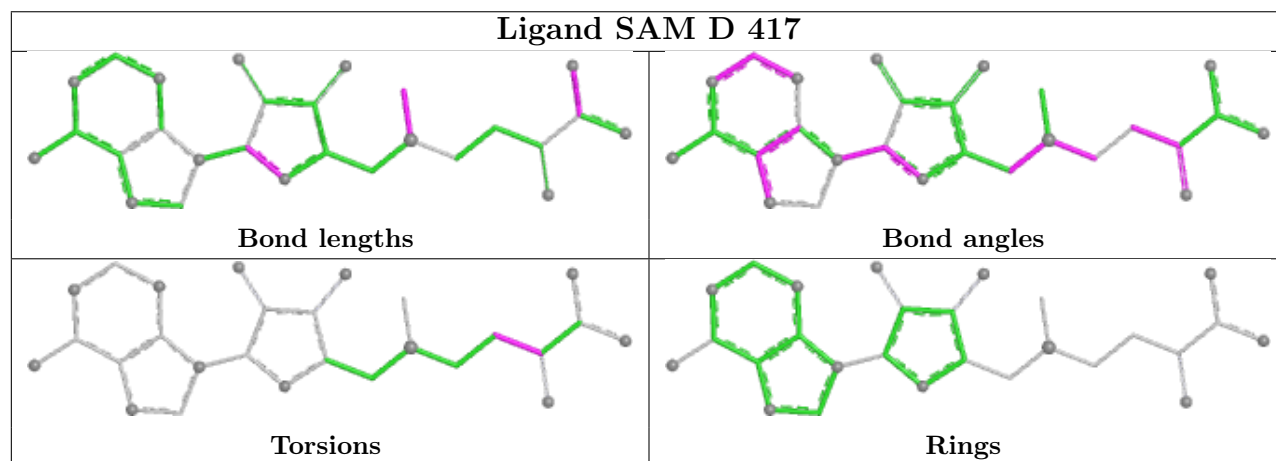
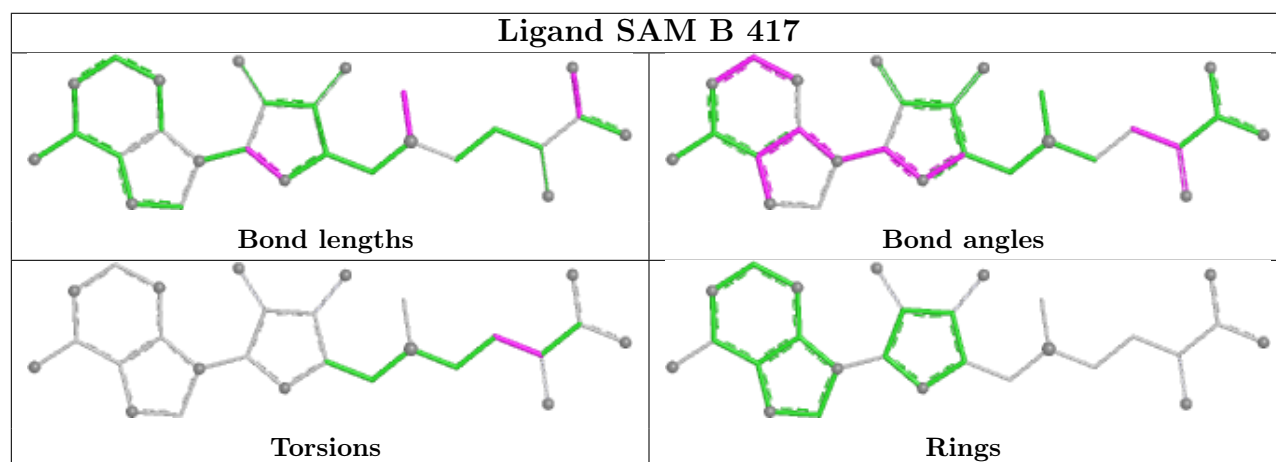
Mol	Chain	Res	Type	Atoms
4	C	417	SAM	N-CA-CB-CG
4	D	417	SAM	N-CA-CB-CG
4	A	417	SAM	C-CA-CB-CG
4	B	417	SAM	C-CA-CB-CG
4	C	417	SAM	C-CA-CB-CG

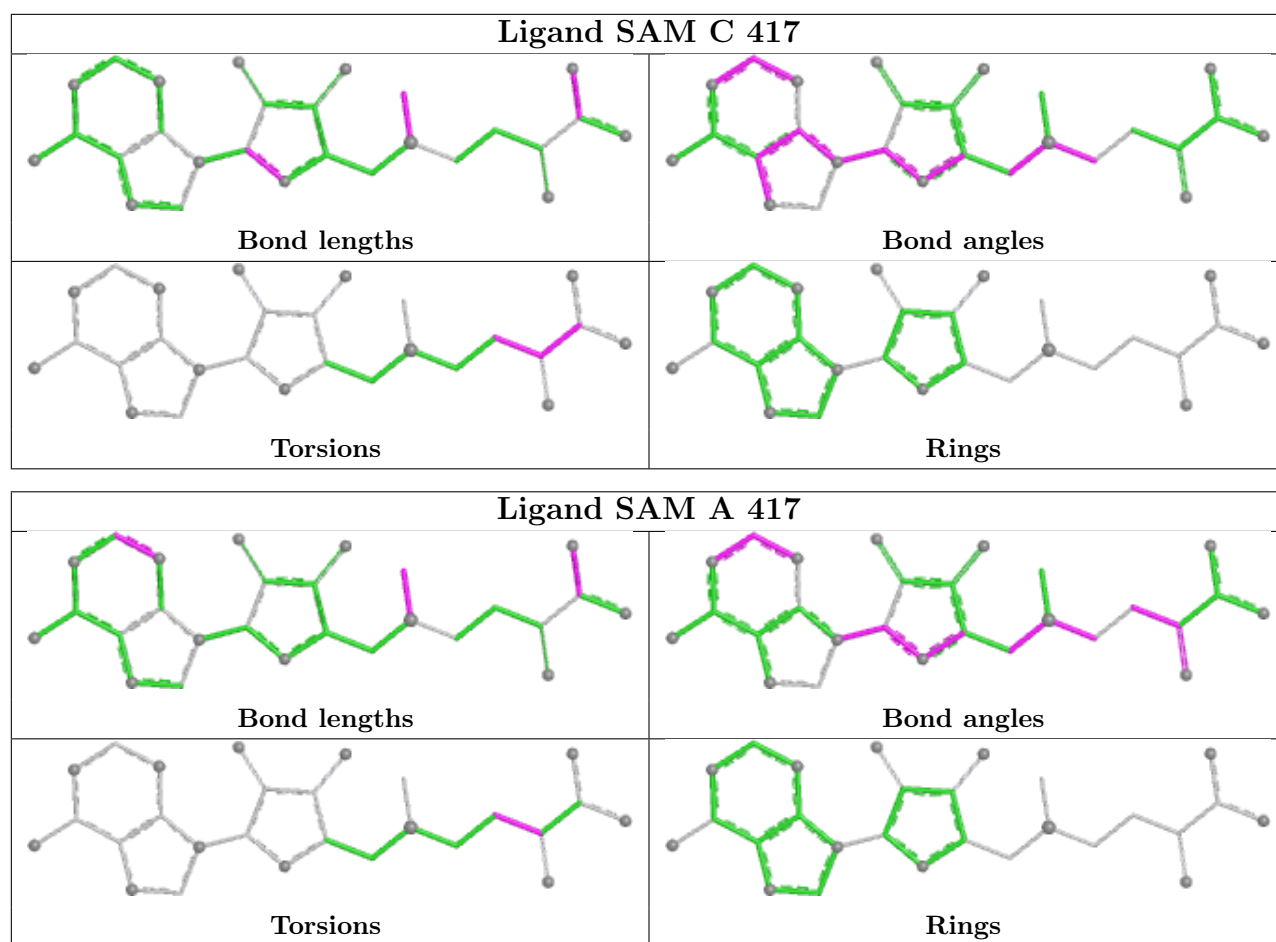
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	418	SF4	1	0
7	C	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%)	3.65	357 (89%) 0 0	12, 38, 60, 72	18 (4%)
1	B	401/416 (96%)	4.14	376 (93%) 0 0	13, 42, 78, 98	15 (3%)
1	C	400/416 (96%)	3.48	343 (85%) 0 0	11, 32, 58, 73	15 (3%)
1	D	401/416 (96%)	3.27	334 (83%) 0 0	9, 32, 54, 69	15 (3%)
All	All	1602/1664 (96%)	3.63	1410 (88%) 0 0	9, 36, 64, 98	63 (3%)

The worst 5 of 1410 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	47	GLY	13.3
1	D	52	VAL	12.2
1	A	48	VAL	12.0
1	B	31	VAL	11.5
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 monosaccharides in this entry.

6.4 Ligands [i](#)

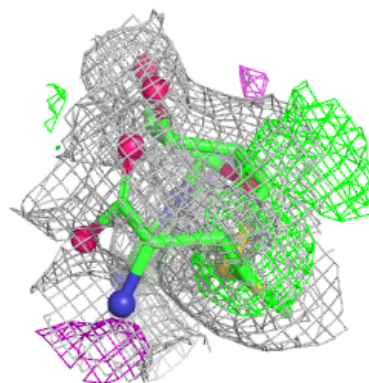
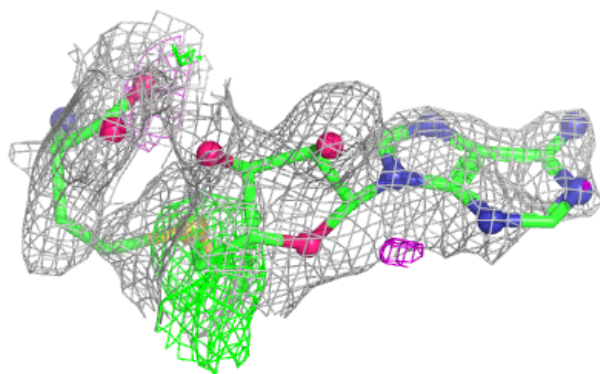
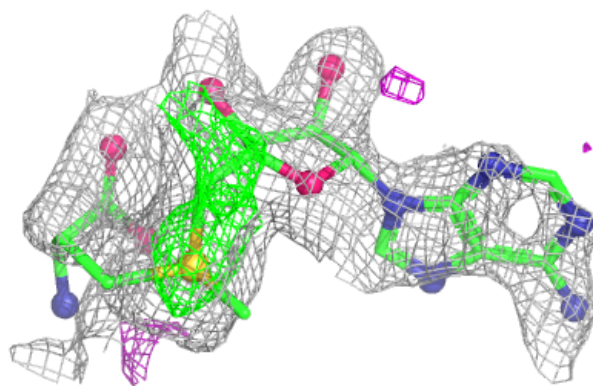
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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	D	419	15/16	0.90	0.14	20,27,29,30	0
6	PLP	C	419	15/16	0.90	0.16	18,24,25,26	0
7	SF4	D	418	8/8	0.90	0.08	21,22,25,26	0
2	ZN	D	421	1/1	0.91	0.08	31,31,31,31	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

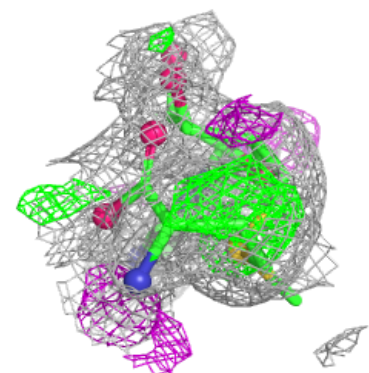
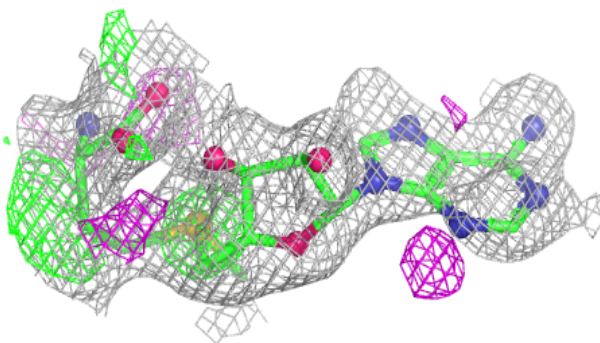
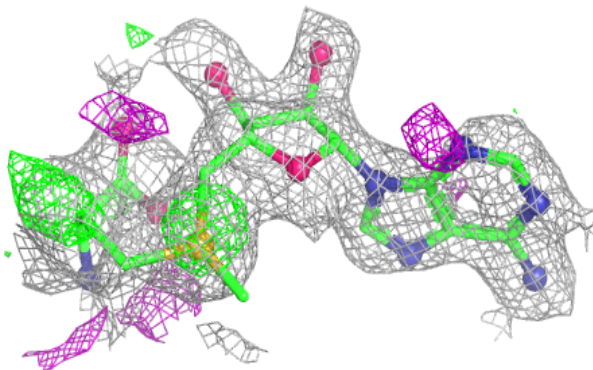
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

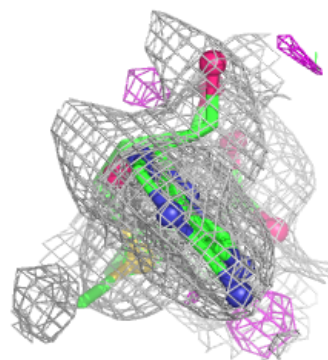
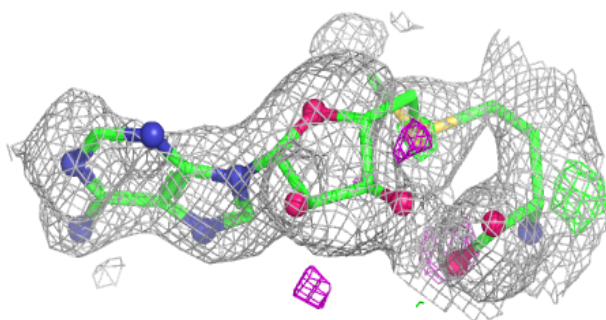
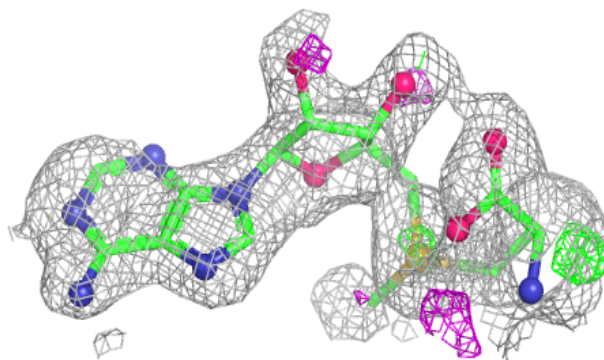
**Electron density around SAM D 417:**

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

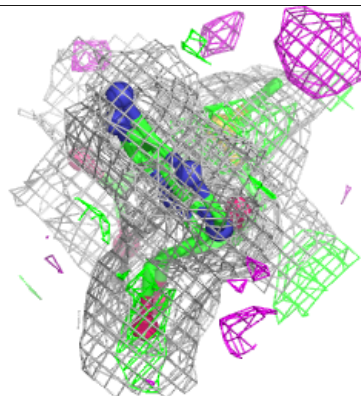
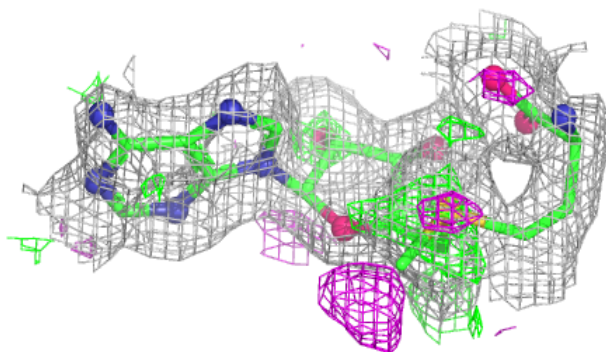
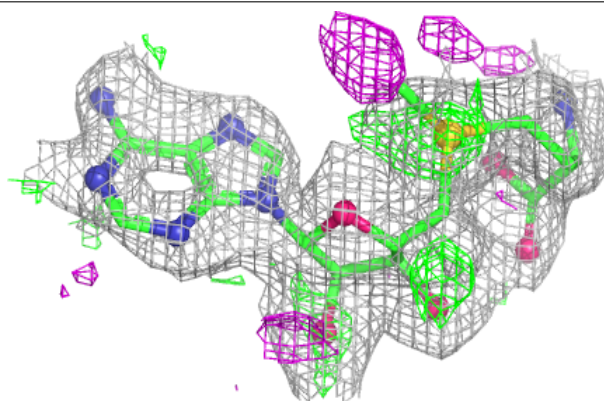


Electron density around SAM A 417:

$2mF_o-DF_c$ (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.