



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:14 PM GMT

PDB ID : 1J0B
Title : Crystal Structure Analysis of the ACC deaminase homologue complexed with inhibitor
Authors : Fujino, A.; Ose, T.; Honma, M.; Yao, M.; Tanaka, I.
Deposited on : 2002-11-12
Resolution : 2.70 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

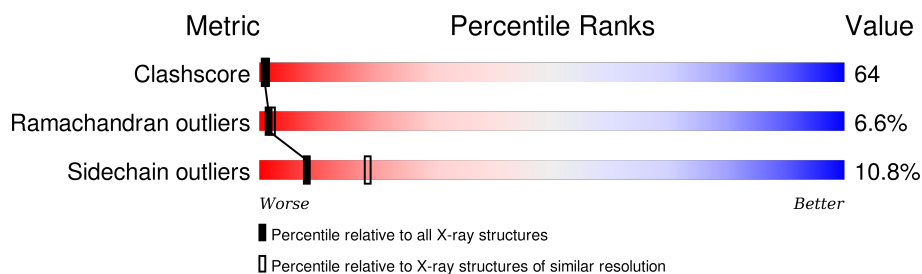
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)


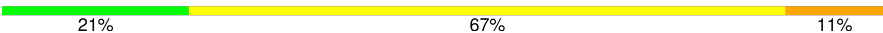
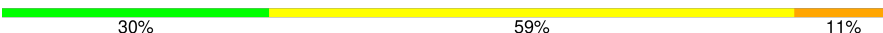


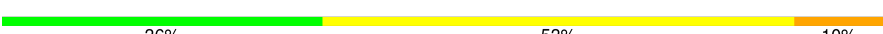
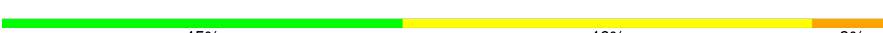




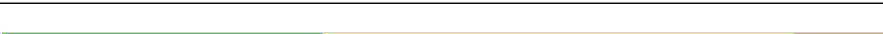





The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	325	
1	B	325	
1	C	325	
1	D	325	
1	E	325	
1	F	325	
1	G	325	

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Mol	Chain	Length	Quality of chain
1	H	325	
1	I	325	
1	J	325	
1	K	325	
1	L	325	
1	M	325	
1	N	325	
1	O	325	
1	P	325	
1	Q	325	
1	R	325	
1	S	325	
1	T	325	
1	U	325	
1	V	325	
1	W	325	
1	X	325	

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
2	5PA	B	1021	-	-	X	-
2	5PA	D	1041	-	-	X	-
2	5PA	E	1051	-	-	X	-
2	5PA	F	1061	-	-	X	-
2	5PA	H	1081	-	-	X	-
2	5PA	I	1091	-	-	X	-
2	5PA	J	1101	-	-	X	-
2	5PA	K	1111	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	5PA	M	1131	-	-	X	-
2	5PA	P	1161	-	-	X	-
2	5PA	Q	1171	-	-	X	-
2	5PA	R	1181	-	-	X	-
2	5PA	S	1191	-	-	X	-
2	5PA	V	1221	-	-	X	-
2	5PA	W	1231	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 60948 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 1-aminocyclopropane-1-carboxylate deaminase.

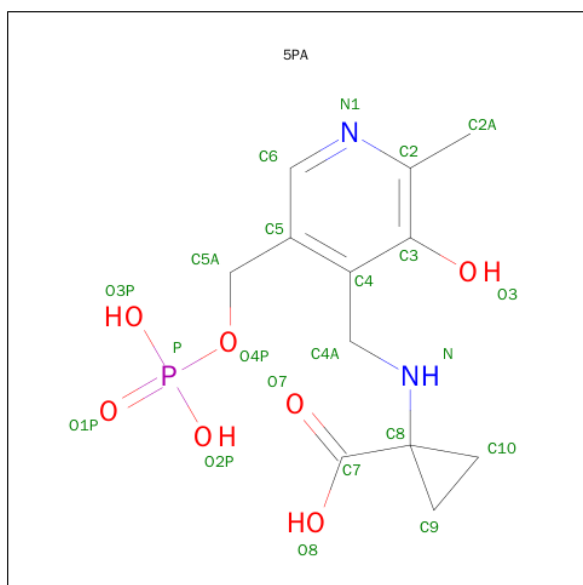
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	B	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	C	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	D	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	E	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	F	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	G	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	H	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	I	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	J	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	K	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	L	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	M	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	N	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	O	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	P	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	R	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	S	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	T	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	U	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	V	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	W	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	X	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			

- Molecule 2 is N-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-Y-LMETHYL]-1-AMINO-CYCLOPROPANECARBOXYLIC ACID (three-letter code: 5PA) (formula: C₁₂H₁₇N₂O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	12	2	7	1		
2	B	1	Total	C	N	O	P	0	0
			22	12	2	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	D	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	E	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	F	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	G	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	H	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	I	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	J	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	K	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	L	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	M	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	N	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	O	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	P	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	Q	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	R	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	S	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	T	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	U	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	V	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	W	1	Total 22	C 12	N 2	O 7	P 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	X	1	Total	C	N	O	P	0	0
			22	12	2	7	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total	O	0	0
			47	47		
3	B	34	Total	O	0	0
			34	34		
3	C	26	Total	O	0	0
			26	26		
3	D	38	Total	O	0	0
			38	38		
3	E	35	Total	O	0	0
			35	35		
3	F	40	Total	O	0	0
			40	40		
3	G	34	Total	O	0	0
			34	34		
3	H	38	Total	O	0	0
			38	38		
3	I	29	Total	O	0	0
			29	29		
3	J	30	Total	O	0	0
			30	30		
3	K	33	Total	O	0	0
			33	33		
3	L	29	Total	O	0	0
			29	29		
3	M	29	Total	O	0	0
			29	29		
3	N	38	Total	O	0	0
			38	38		
3	O	28	Total	O	0	0
			28	28		
3	P	20	Total	O	0	0
			20	20		
3	Q	25	Total	O	0	0
			25	25		
3	R	21	Total	O	0	0
			21	21		

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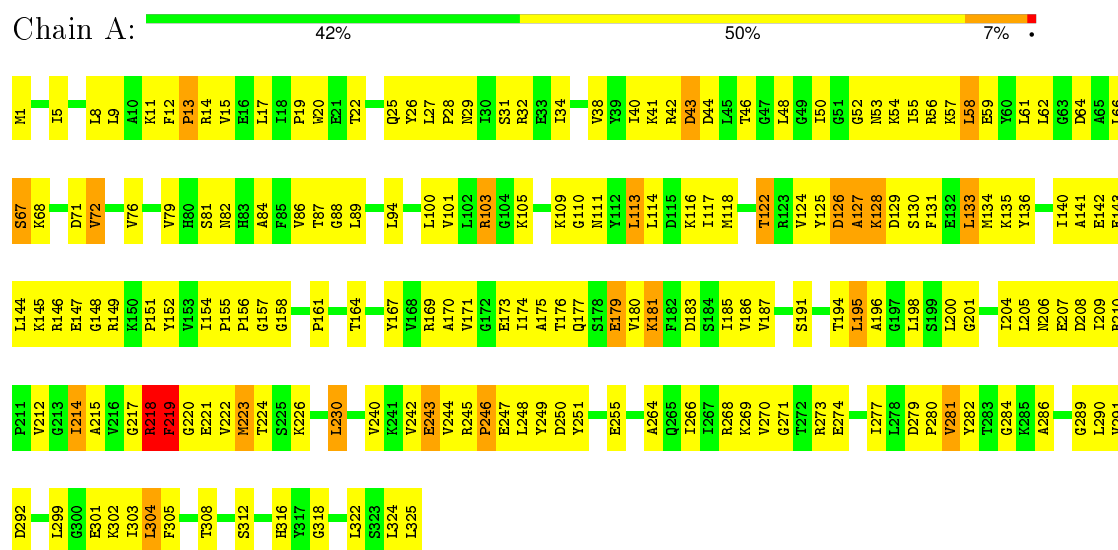
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	S	42	Total 42	O 42	0	0
3	T	40	Total 40	O 40	0	0
3	U	48	Total 48	O 48	0	0
3	V	40	Total 40	O 40	0	0
3	W	34	Total 34	O 34	0	0
3	X	26	Total 26	O 26	0	0

3 Residue-property plots

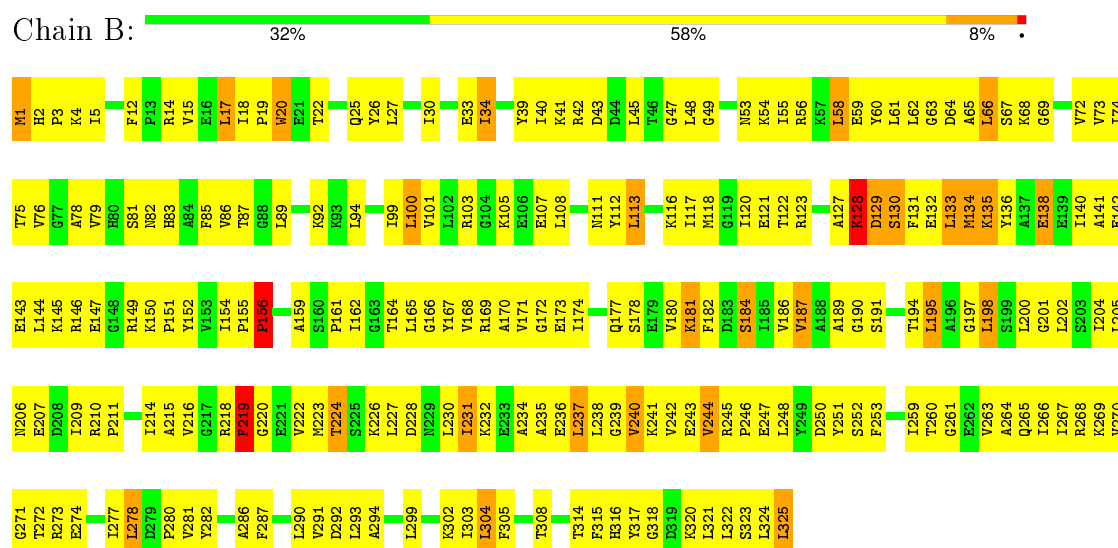
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

Note EDS was not executed.

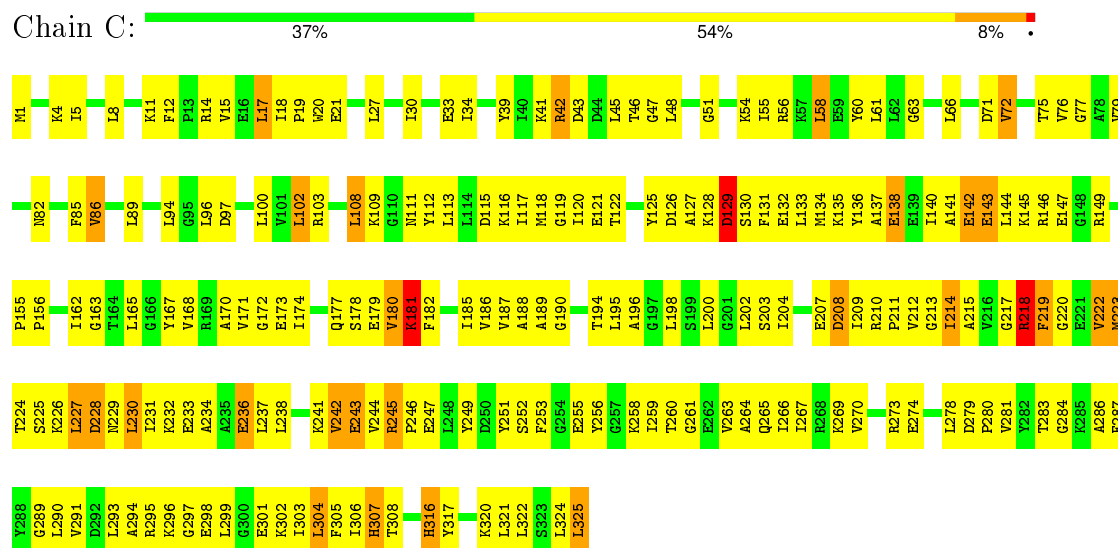
- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase



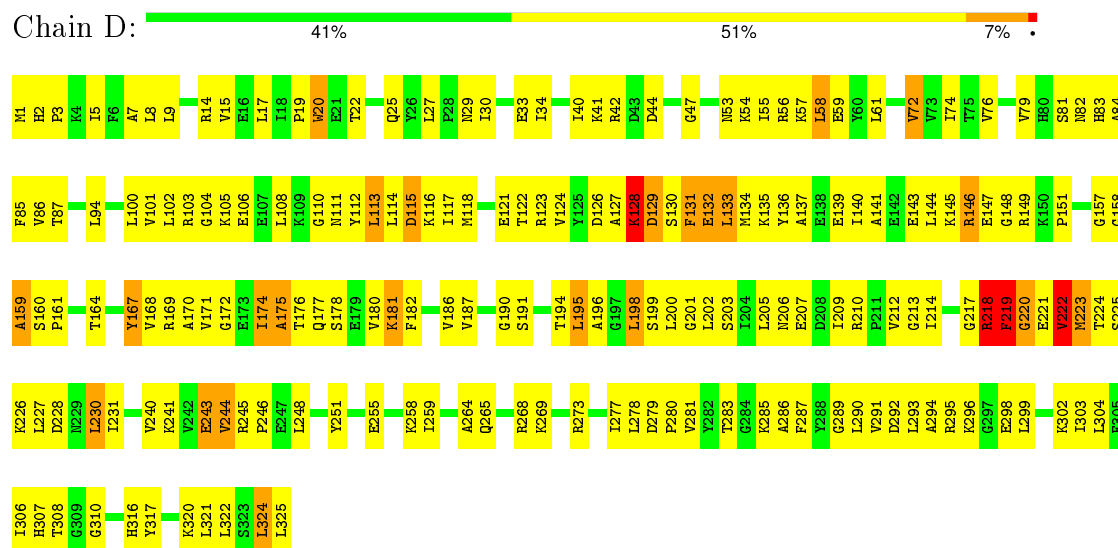
- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase



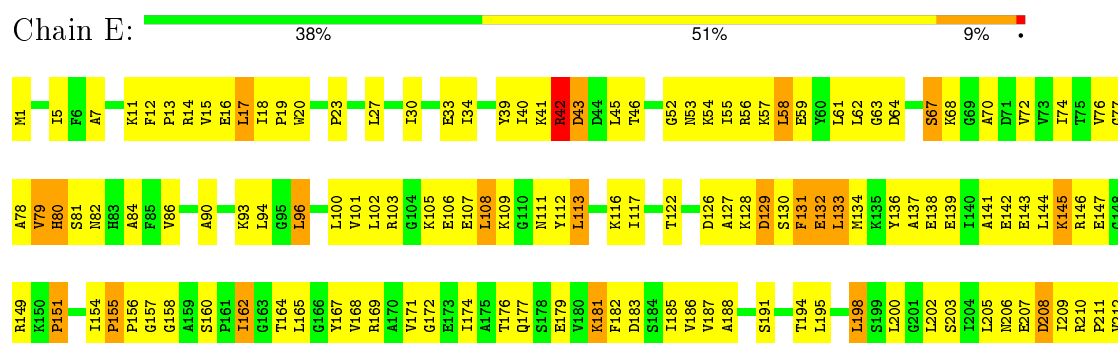
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

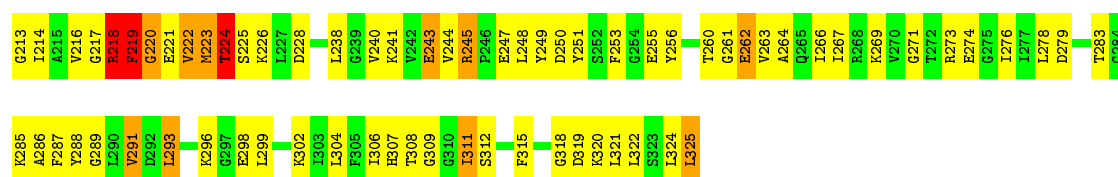


• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase



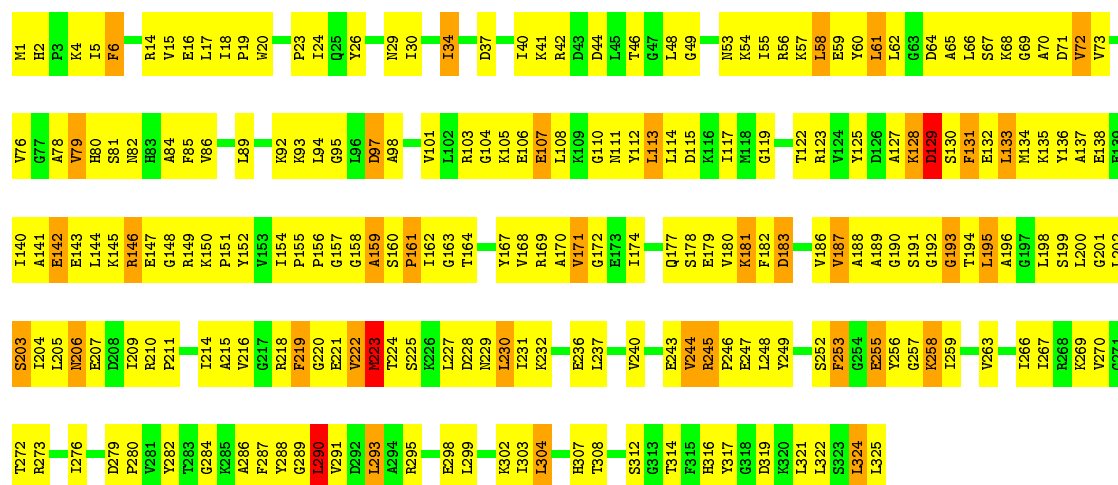
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase





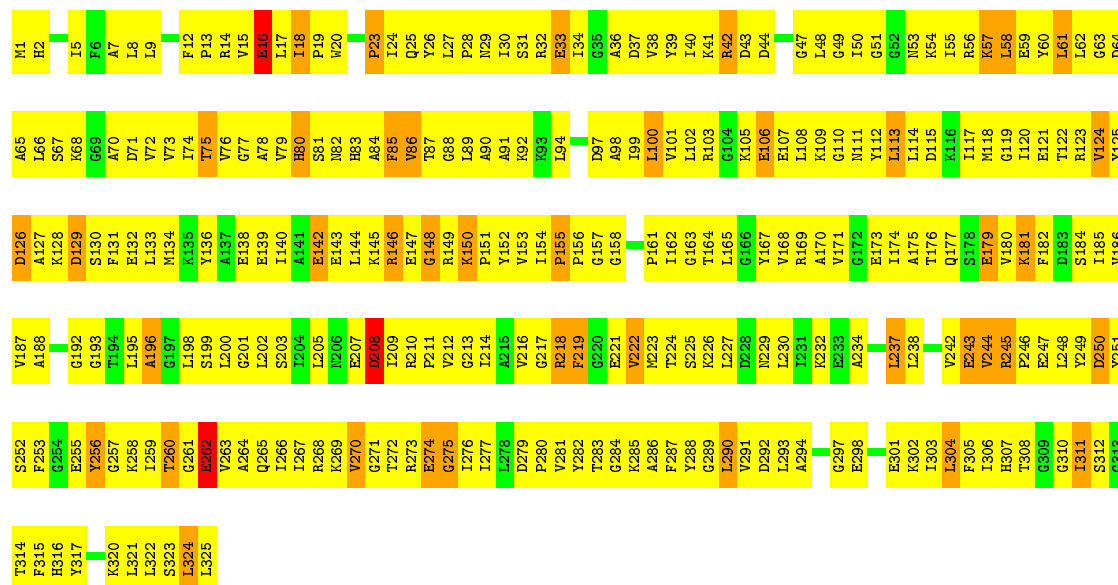
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain F: 31% 57% 11%



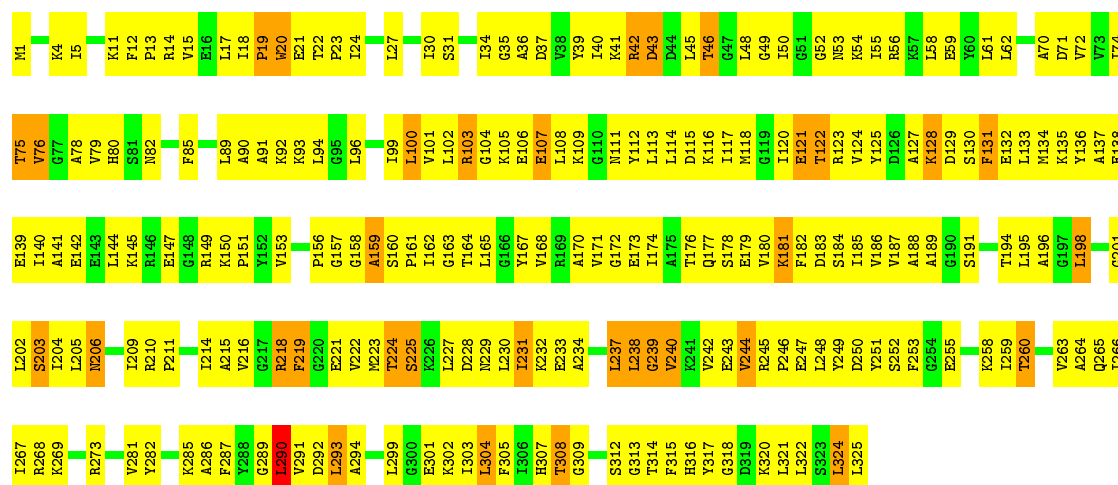
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain G: 16% 70% 13%



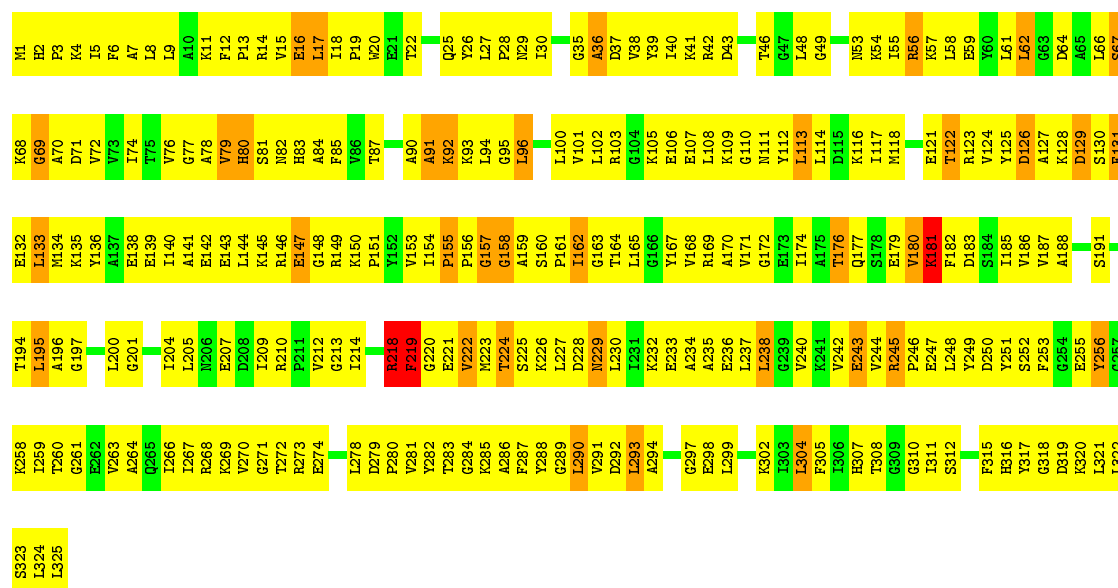
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain H: 29% 60% 10%



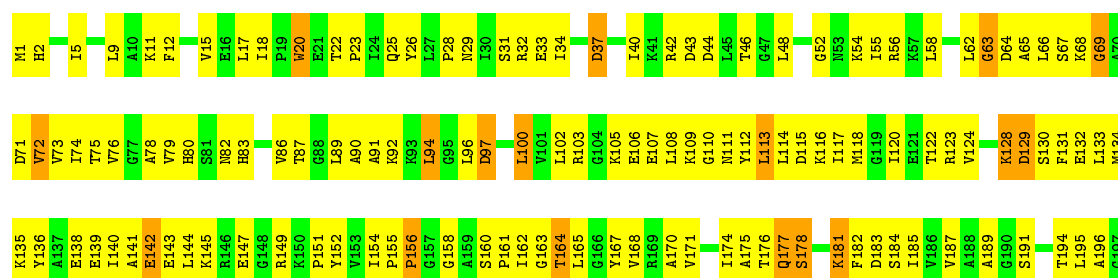
- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

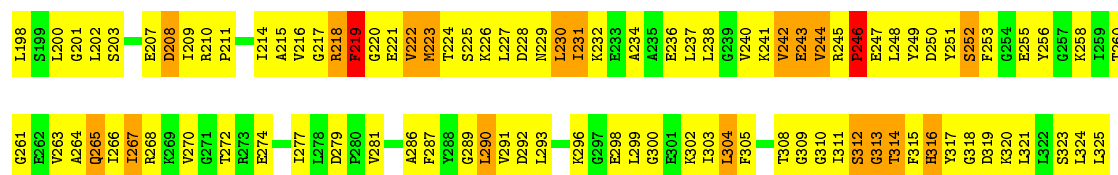
Chain I: 21% 67% 11%



- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

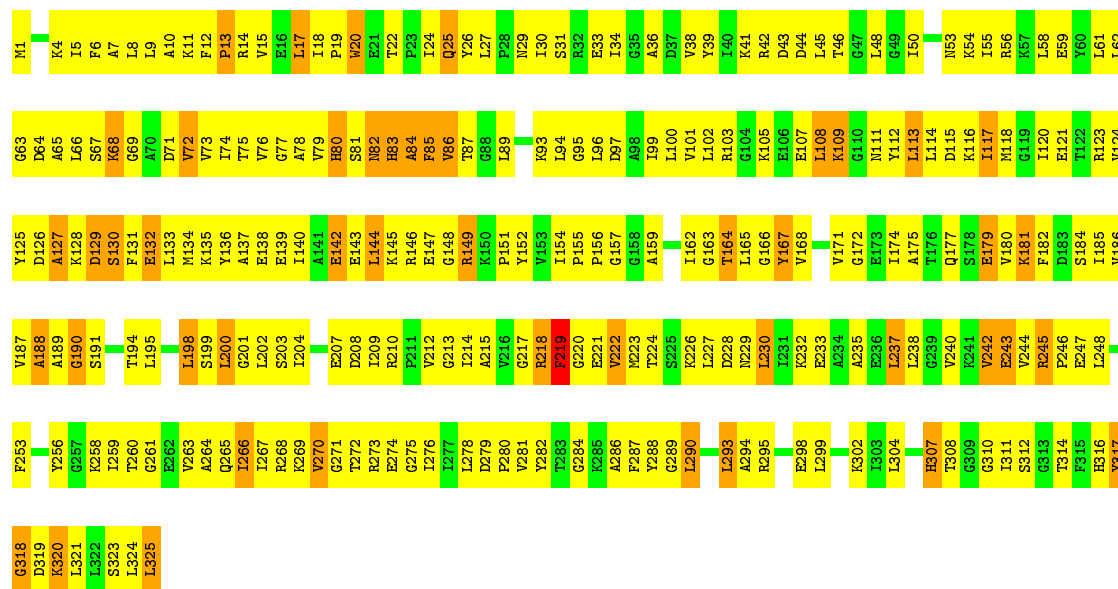
Chain J: 30% 59% 11%





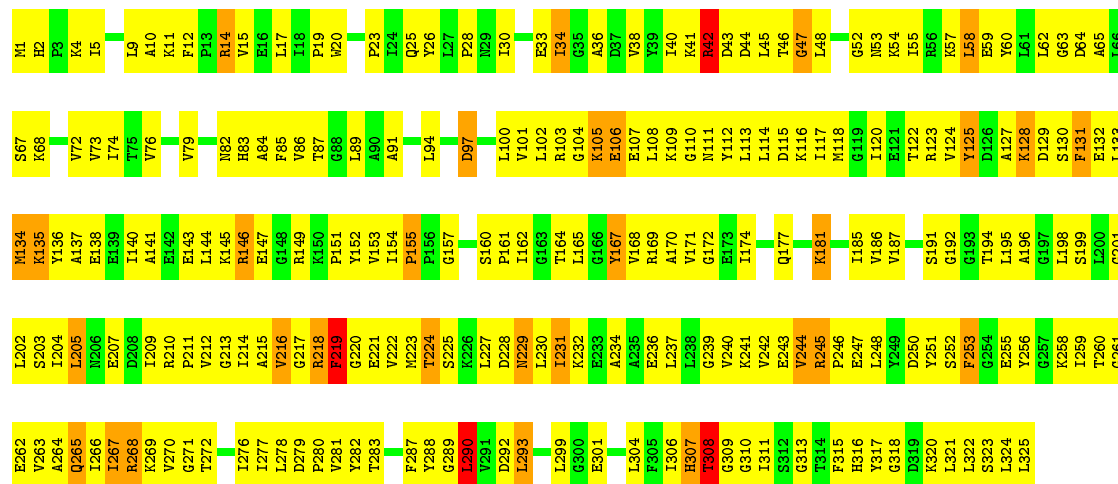
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain K: 24% 62% 14%



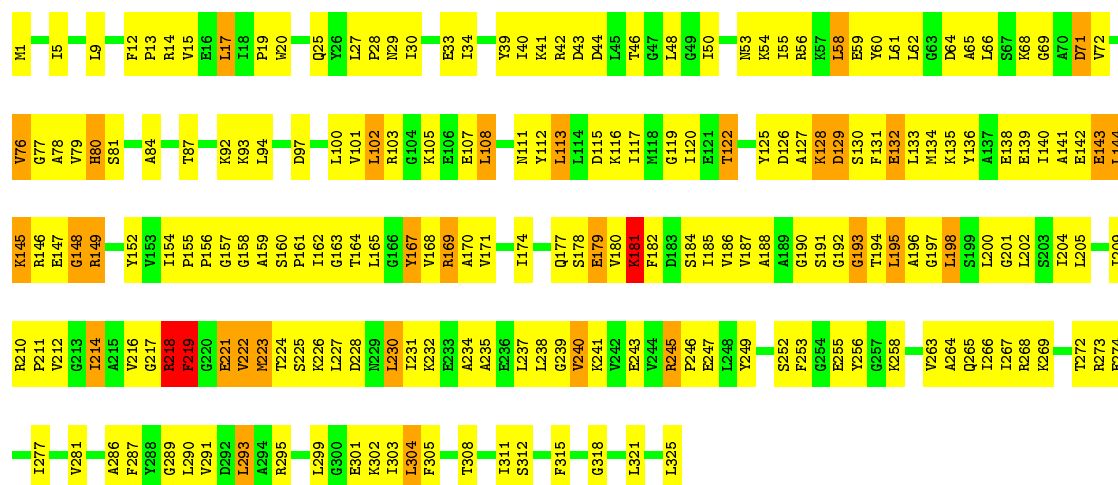
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain L: 29% 61% 9%



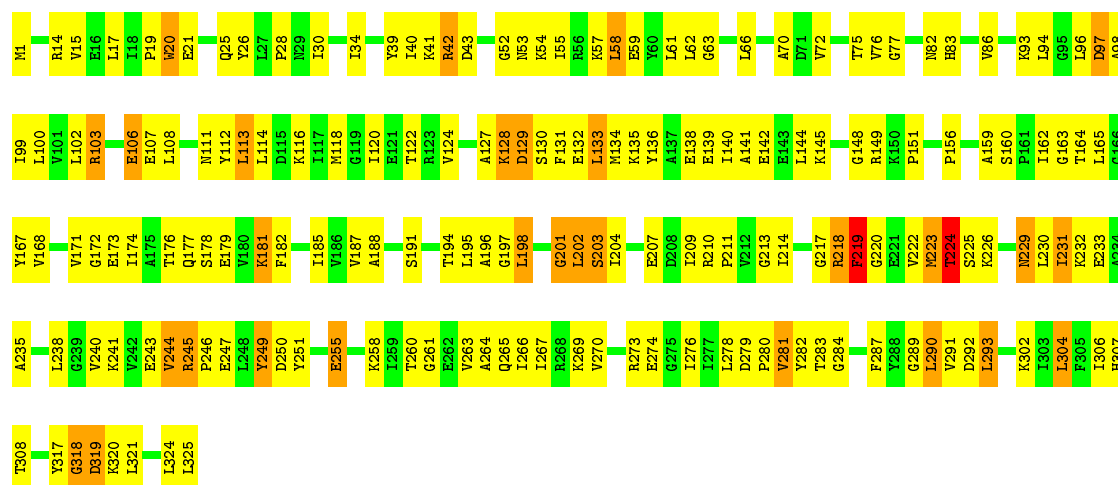
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain M: 36% 53% 10%



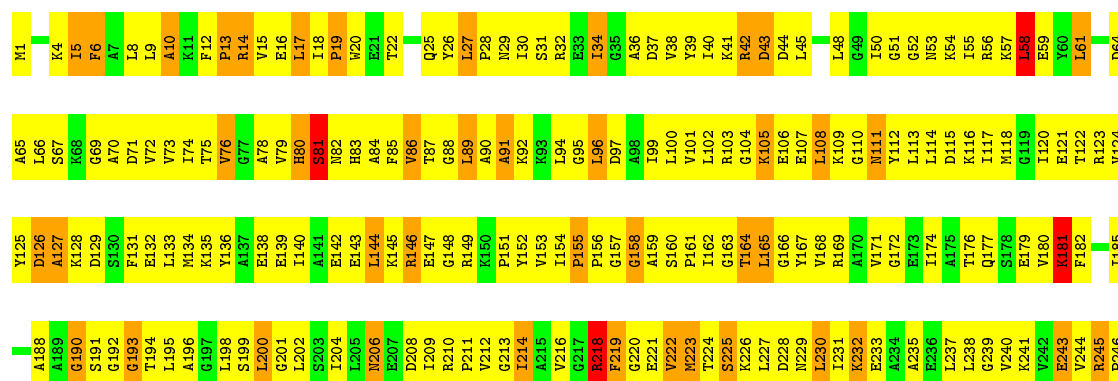
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain N: 45% 46% 9% •

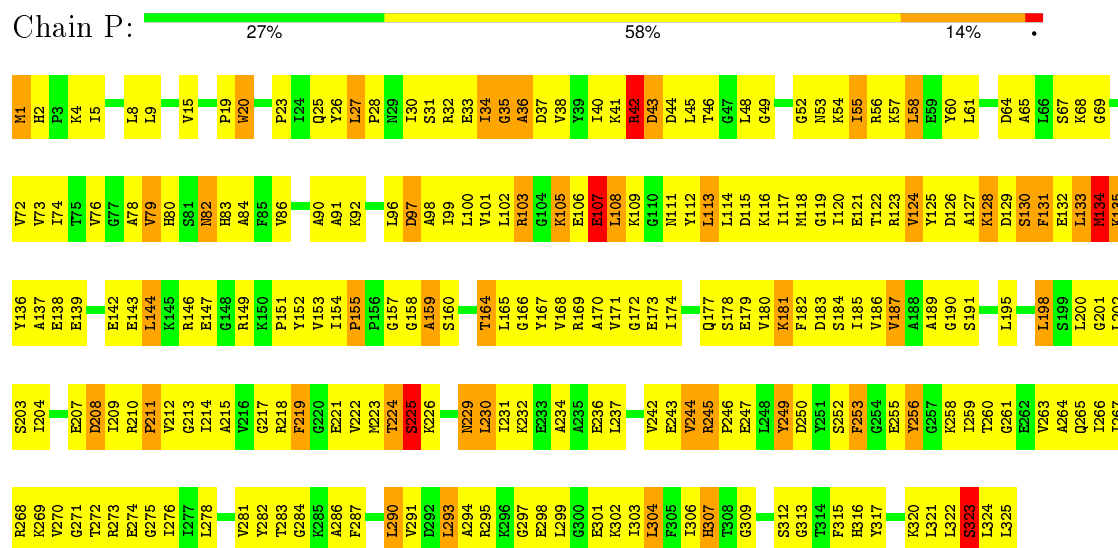


• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

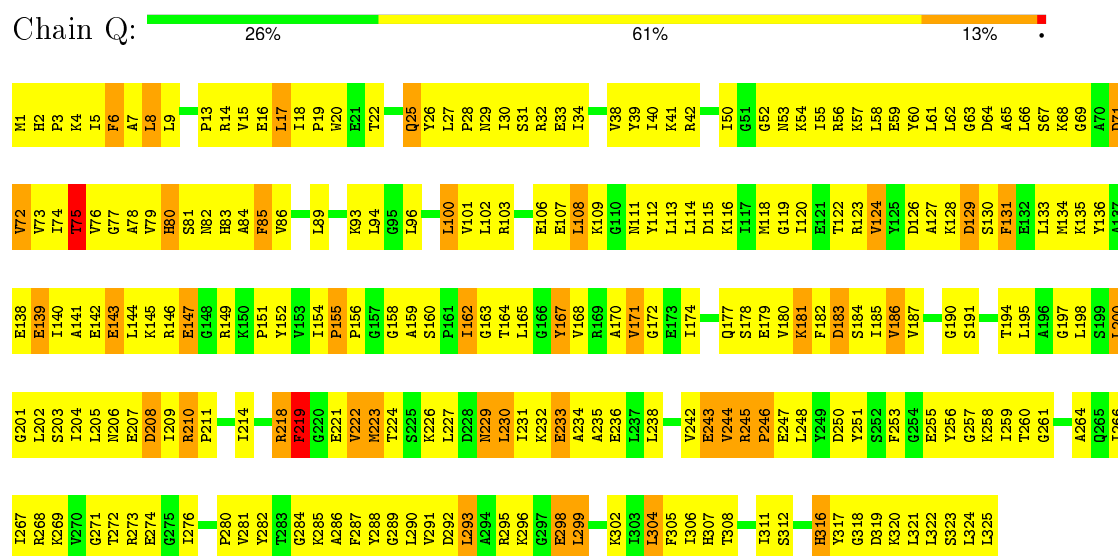
Chain O: 17% 65% 16% •



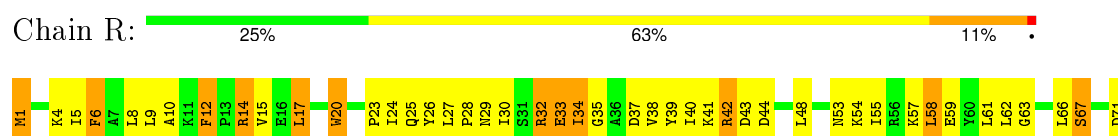
- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

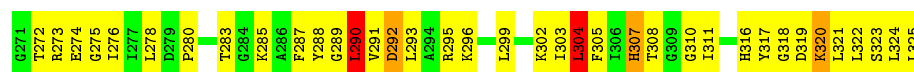


- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase



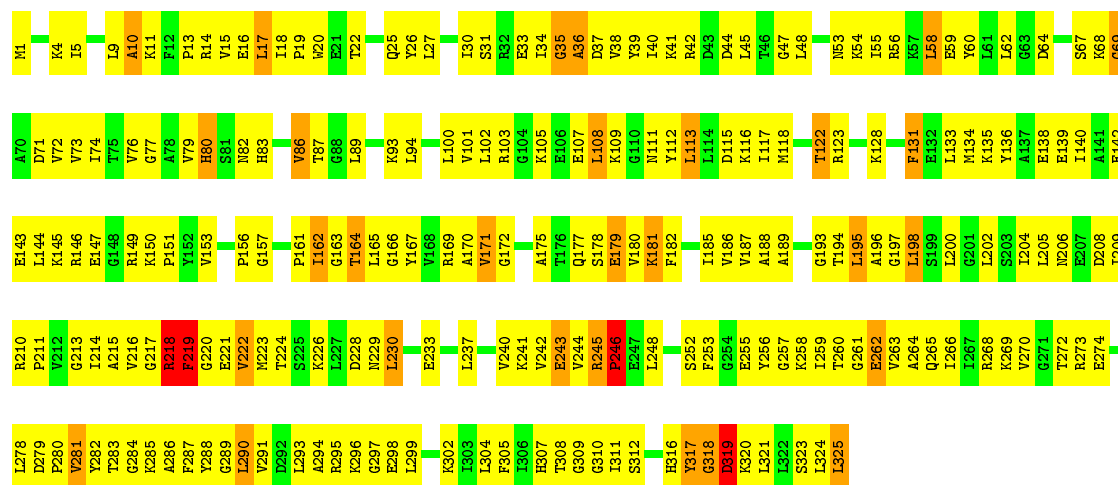
- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase





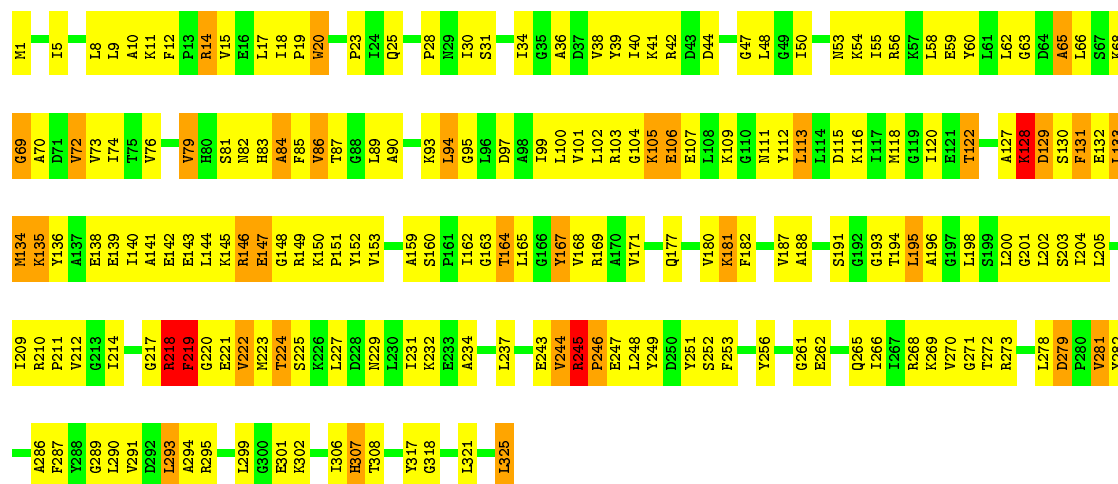
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain U: 32% 58% 9%



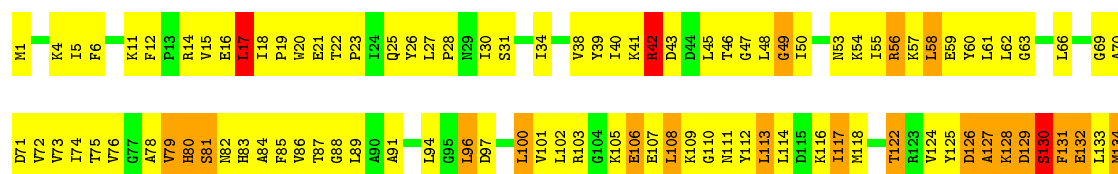
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

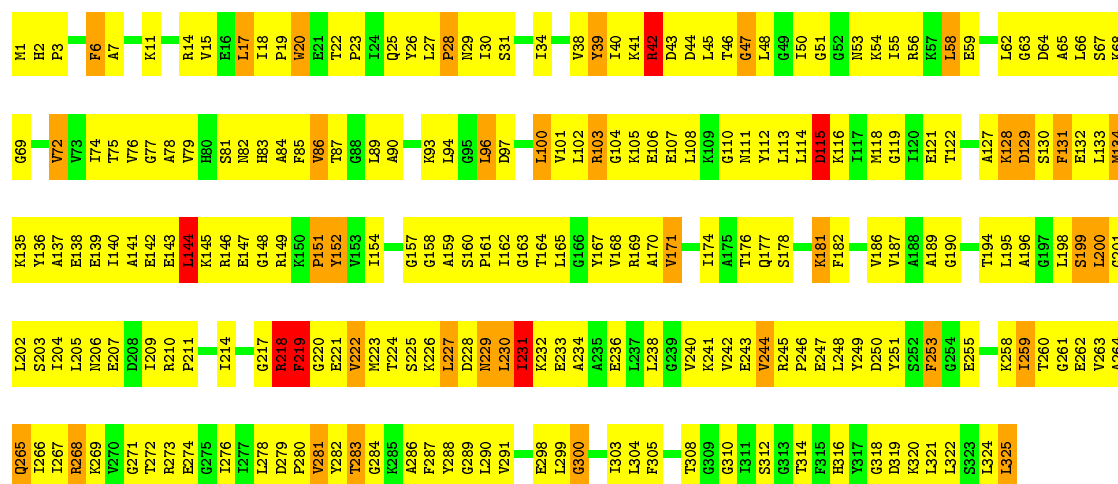
Chain V: 40% 49% 10%



• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain W: 24% 61% 13%





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	105.87Å 147.28Å 149.07Å 73.18° 90.11° 68.49°	Depositor
Resolution (Å)	10.00 – 2.70	Depositor
% Data completeness (in resolution range)	100.0 (10.00-2.70)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.291 , 0.342	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	60948	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5PA

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	0.45	0/2526	0.76	1/3407 (0.0%)
1	B	0.43	0/2526	0.73	0/3407
1	C	0.42	0/2526	0.74	0/3407
1	D	0.45	0/2526	0.74	0/3407
1	E	0.43	0/2526	0.73	1/3407 (0.0%)
1	F	0.46	0/2526	0.73	1/3407 (0.0%)
1	G	0.48	0/2526	0.80	1/3407 (0.0%)
1	H	0.45	0/2526	0.73	1/3407 (0.0%)
1	I	0.49	0/2526	0.77	1/3407 (0.0%)
1	J	0.45	0/2526	0.74	0/3407
1	K	0.47	0/2526	0.76	0/3407
1	L	0.47	0/2526	0.76	2/3407 (0.1%)
1	M	0.45	0/2526	0.75	0/3407
1	N	0.44	0/2526	0.75	2/3407 (0.1%)
1	O	0.48	0/2526	0.80	0/3407
1	P	0.45	0/2526	0.75	3/3407 (0.1%)
1	Q	0.46	0/2526	0.75	0/3407
1	R	0.46	0/2526	0.76	0/3407
1	S	0.45	0/2526	0.74	1/3407 (0.0%)
1	T	0.46	0/2526	0.78	2/3407 (0.1%)
1	U	0.46	0/2526	0.76	0/3407
1	V	0.44	0/2526	0.77	3/3407 (0.1%)
1	W	0.46	0/2526	0.78	3/3407 (0.1%)
1	X	0.45	0/2526	0.77	2/3407 (0.1%)
All	All	0.45	0/60624	0.76	24/81768 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	Q	0	1
1	T	0	1
1	V	0	1
All	All	0	7

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	304	LEU	CA-CB-CG	6.44	130.11	115.30
1	W	17	LEU	CA-CB-CG	6.26	129.70	115.30
1	N	290	LEU	CA-CB-CG	6.01	129.13	115.30
1	T	290	LEU	CA-CB-CG	5.89	128.85	115.30
1	I	17	LEU	CA-CB-CG	5.83	128.72	115.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	167	TYR	Sidechain
1	K	167	TYR	Sidechain
1	L	167	TYR	Sidechain
1	M	167	TYR	Sidechain
1	Q	167	TYR	Sidechain

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	2484	0	2583	236	0
1	B	2484	0	2583	288	0
1	C	2484	0	2583	286	1
1	D	2484	0	2583	264	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2484	0	2583	245	0
1	F	2484	0	2583	278	1
1	G	2484	0	2583	501	0
1	H	2484	0	2583	328	0
1	I	2484	0	2583	413	0
1	J	2484	0	2583	363	0
1	K	2484	0	2583	430	0
1	L	2484	0	2583	341	0
1	M	2484	0	2583	324	0
1	N	2484	0	2583	219	0
1	O	2484	0	2583	457	0
1	P	2484	0	2583	362	0
1	Q	2484	0	2583	392	0
1	R	2484	0	2583	353	0
1	S	2484	0	2583	295	0
1	T	2484	0	2583	326	0
1	U	2484	0	2583	282	0
1	V	2484	0	2583	261	0
1	W	2484	0	2583	409	0
1	X	2484	0	2583	340	0
2	A	22	0	13	5	0
2	B	22	0	13	8	0
2	C	22	0	13	6	0
2	D	22	0	13	7	0
2	E	22	0	13	7	0
2	F	22	0	13	15	0
2	G	22	0	13	3	0
2	H	22	0	13	7	0
2	I	22	0	13	13	0
2	J	22	0	13	9	0
2	K	22	0	13	11	0
2	L	22	0	13	6	0
2	M	22	0	13	10	0
2	N	22	0	13	4	0
2	O	22	0	13	6	0
2	P	22	0	13	10	0
2	Q	22	0	13	15	0
2	R	22	0	13	14	0
2	S	22	0	13	9	0
2	T	22	0	13	6	0
2	U	22	0	13	6	0
2	V	22	0	13	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	W	22	0	13	8	0
2	X	22	0	13	5	0
3	A	47	0	0	10	0
3	B	34	0	0	7	0
3	C	26	0	0	3	0
3	D	38	0	0	9	0
3	E	35	0	0	5	0
3	F	40	0	0	6	0
3	G	34	0	0	12	0
3	H	38	0	0	11	0
3	I	29	0	0	9	0
3	J	30	0	0	8	0
3	K	33	0	0	8	0
3	L	29	0	0	12	0
3	M	29	0	0	8	0
3	N	38	0	0	6	0
3	O	28	0	0	9	0
3	P	20	0	0	11	0
3	Q	25	0	0	13	0
3	R	21	0	0	5	0
3	S	42	0	0	10	0
3	T	40	0	0	12	0
3	U	48	0	0	9	0
3	V	40	0	0	6	0
3	W	34	0	0	10	0
3	X	26	0	0	6	0
All	All	60948	0	62304	7804	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 64.

The worst 5 of 7804 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:X:128:LYS:HD3	1:X:128:LYS:H	1.06	1.19
1:G:147:GLU:CB	1:I:221:GLU:HA	1.75	1.15
1:C:103:ARG:HD3	1:C:133:LEU:HD22	1.21	1.15
1:C:214:ILE:HD13	1:C:286:ALA:HA	1.29	1.14
1:G:147:GLU:HB3	1:I:221:GLU:HA	1.18	1.14

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:PHE:O	1:F:147:GLU:O[1_455]	2.12	0.08

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	323/325 (99%)	268 (83%)	42 (13%)	13 (4%)	4	8
1	B	323/325 (99%)	257 (80%)	50 (16%)	16 (5%)	3	5
1	C	323/325 (99%)	256 (79%)	51 (16%)	16 (5%)	3	5
1	D	323/325 (99%)	273 (84%)	34 (10%)	16 (5%)	3	5
1	E	323/325 (99%)	270 (84%)	36 (11%)	17 (5%)	2	4
1	F	323/325 (99%)	268 (83%)	37 (12%)	18 (6%)	2	3
1	G	323/325 (99%)	232 (72%)	63 (20%)	28 (9%)	1	1
1	H	323/325 (99%)	258 (80%)	51 (16%)	14 (4%)	3	7
1	I	323/325 (99%)	250 (77%)	50 (16%)	23 (7%)	1	2
1	J	323/325 (99%)	242 (75%)	57 (18%)	24 (7%)	1	1
1	K	323/325 (99%)	231 (72%)	61 (19%)	31 (10%)	1	1
1	L	323/325 (99%)	260 (80%)	43 (13%)	20 (6%)	2	2
1	M	323/325 (99%)	263 (81%)	45 (14%)	15 (5%)	3	6
1	N	323/325 (99%)	275 (85%)	37 (12%)	11 (3%)	5	10
1	O	323/325 (99%)	208 (64%)	69 (21%)	46 (14%)	0	0
1	P	323/325 (99%)	241 (75%)	56 (17%)	26 (8%)	1	1
1	Q	323/325 (99%)	241 (75%)	58 (18%)	24 (7%)	1	1
1	R	323/325 (99%)	259 (80%)	43 (13%)	21 (6%)	1	2
1	S	323/325 (99%)	255 (79%)	51 (16%)	17 (5%)	2	4
1	T	323/325 (99%)	259 (80%)	38 (12%)	26 (8%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	323/325 (99%)	264 (82%)	40 (12%)	19 (6%)	2	3
1	V	323/325 (99%)	266 (82%)	41 (13%)	16 (5%)	3	5
1	W	323/325 (99%)	234 (72%)	60 (19%)	29 (9%)	1	1
1	X	323/325 (99%)	235 (73%)	59 (18%)	29 (9%)	1	1
All	All	7752/7800 (99%)	6065 (78%)	1172 (15%)	515 (7%)	1	2

5 of 515 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	PHE
1	A	245	ARG
1	B	33	GLU
1	B	72	VAL
1	B	187	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	259/259 (100%)	230 (89%)	29 (11%)	7	17
1	B	259/259 (100%)	232 (90%)	27 (10%)	9	20
1	C	259/259 (100%)	236 (91%)	23 (9%)	12	27
1	D	259/259 (100%)	238 (92%)	21 (8%)	15	33
1	E	259/259 (100%)	231 (89%)	28 (11%)	8	18
1	F	259/259 (100%)	226 (87%)	33 (13%)	5	13
1	G	259/259 (100%)	231 (89%)	28 (11%)	8	18
1	H	259/259 (100%)	231 (89%)	28 (11%)	8	18
1	I	259/259 (100%)	236 (91%)	23 (9%)	12	27
1	J	259/259 (100%)	236 (91%)	23 (9%)	12	27
1	K	259/259 (100%)	234 (90%)	25 (10%)	10	23
1	L	259/259 (100%)	237 (92%)	22 (8%)	13	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	259/259 (100%)	232 (90%)	27 (10%)	9	20
1	N	259/259 (100%)	230 (89%)	29 (11%)	7	17
1	O	259/259 (100%)	228 (88%)	31 (12%)	6	14
1	P	259/259 (100%)	224 (86%)	35 (14%)	5	11
1	Q	259/259 (100%)	232 (90%)	27 (10%)	9	20
1	R	259/259 (100%)	223 (86%)	36 (14%)	4	10
1	S	259/259 (100%)	230 (89%)	29 (11%)	7	17
1	T	259/259 (100%)	230 (89%)	29 (11%)	7	17
1	U	259/259 (100%)	232 (90%)	27 (10%)	9	20
1	V	259/259 (100%)	228 (88%)	31 (12%)	6	14
1	W	259/259 (100%)	227 (88%)	32 (12%)	6	13
1	X	259/259 (100%)	229 (88%)	30 (12%)	7	16
All	All	6216/6216 (100%)	5543 (89%)	673 (11%)	8	18

5 of 673 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	230	LEU
1	O	111	ASN
1	W	122	THR
1	M	76	VAL
1	N	75	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 124 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	25	GLN
1	N	177	GLN
1	W	177	GLN
1	L	82	ASN
1	M	82	ASN

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 ⓘ

24 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	5PA	A	1011	-	19,23,23	2.94	4 (21%)	28,35,35	2.28	7 (25%)
2	5PA	B	1021	1	19,23,23	2.92	4 (21%)	28,35,35	2.21	7 (25%)
2	5PA	C	1031	-	19,23,23	2.91	4 (21%)	28,35,35	2.34	8 (28%)
2	5PA	D	1041	1	19,23,23	2.93	4 (21%)	28,35,35	2.11	7 (25%)
2	5PA	E	1051	-	19,23,23	2.95	4 (21%)	28,35,35	2.19	6 (21%)
2	5PA	F	1061	-	19,23,23	2.94	4 (21%)	28,35,35	2.11	7 (25%)
2	5PA	G	1071	-	19,23,23	2.89	4 (21%)	28,35,35	2.34	7 (25%)
2	5PA	H	1081	-	19,23,23	3.02	5 (26%)	28,35,35	2.10	7 (25%)
2	5PA	I	1091	-	19,23,23	2.89	4 (21%)	28,35,35	2.13	5 (17%)
2	5PA	J	1101	-	19,23,23	2.91	5 (26%)	28,35,35	2.09	6 (21%)
2	5PA	K	1111	-	19,23,23	2.89	4 (21%)	28,35,35	2.56	6 (21%)
2	5PA	L	1121	-	19,23,23	2.94	4 (21%)	28,35,35	2.12	8 (28%)
2	5PA	M	1131	1	19,23,23	2.95	4 (21%)	28,35,35	2.12	7 (25%)
2	5PA	N	1141	-	19,23,23	2.90	4 (21%)	28,35,35	2.28	7 (25%)
2	5PA	O	1151	-	19,23,23	2.98	5 (26%)	28,35,35	1.91	6 (21%)
2	5PA	P	1161	-	19,23,23	2.92	4 (21%)	28,35,35	2.09	6 (21%)
2	5PA	Q	1171	-	19,23,23	2.93	4 (21%)	28,35,35	2.26	7 (25%)
2	5PA	R	1181	-	19,23,23	2.93	4 (21%)	28,35,35	2.13	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	5PA	S	1191	-	19,23,23	2.89	4 (21%)	28,35,35	2.43	8 (28%)
2	5PA	T	1201	1	19,23,23	2.90	4 (21%)	28,35,35	2.15	7 (25%)
2	5PA	U	1211	-	19,23,23	2.91	4 (21%)	28,35,35	2.32	6 (21%)
2	5PA	V	1221	-	19,23,23	2.96	4 (21%)	28,35,35	2.17	7 (25%)
2	5PA	W	1231	-	19,23,23	2.92	4 (21%)	28,35,35	2.08	5 (17%)
2	5PA	X	1241	1	19,23,23	2.91	4 (21%)	28,35,35	2.15	8 (28%)

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	5PA	A	1011	-	-	0/9/22/22	0/1/2/2
2	5PA	B	1021	1	-	0/9/22/22	0/1/2/2
2	5PA	C	1031	-	-	0/9/22/22	0/1/2/2
2	5PA	D	1041	1	-	0/9/22/22	0/1/2/2
2	5PA	E	1051	-	-	0/9/22/22	0/1/2/2
2	5PA	F	1061	-	-	0/9/22/22	0/1/2/2
2	5PA	G	1071	-	-	0/9/22/22	0/1/2/2
2	5PA	H	1081	-	-	0/9/22/22	0/1/2/2
2	5PA	I	1091	-	-	0/9/22/22	0/1/2/2
2	5PA	J	1101	-	-	0/9/22/22	0/1/2/2
2	5PA	K	1111	-	-	0/9/22/22	0/1/2/2
2	5PA	L	1121	-	-	0/9/22/22	0/1/2/2
2	5PA	M	1131	1	-	0/9/22/22	0/1/2/2
2	5PA	N	1141	-	-	0/9/22/22	0/1/2/2
2	5PA	O	1151	-	-	0/9/22/22	0/1/2/2
2	5PA	P	1161	-	-	0/9/22/22	0/1/2/2
2	5PA	Q	1171	-	-	0/9/22/22	0/1/2/2
2	5PA	R	1181	-	-	0/9/22/22	0/1/2/2
2	5PA	S	1191	-	-	0/9/22/22	0/1/2/2
2	5PA	T	1201	1	-	0/9/22/22	0/1/2/2
2	5PA	U	1211	-	-	0/9/22/22	0/1/2/2
2	5PA	V	1221	-	-	0/9/22/22	0/1/2/2
2	5PA	W	1231	-	-	0/9/22/22	0/1/2/2
2	5PA	X	1241	1	-	0/9/22/22	0/1/2/2

The worst 5 of 99 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1051	5PA	C4A-C4	-10.74	1.39	1.51
2	H	1081	5PA	C4A-C4	-10.73	1.39	1.51
2	V	1221	5PA	C4A-C4	-10.71	1.39	1.51
2	A	1011	5PA	C4A-C4	-10.68	1.39	1.51
2	M	1131	5PA	C4A-C4	-10.66	1.39	1.51

The worst 5 of 162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	1181	5PA	C9-C8-N	-4.47	112.70	117.36
2	U	1211	5PA	C9-C8-N	-4.22	112.96	117.36
2	T	1201	5PA	C9-C8-N	-3.71	113.49	117.36
2	L	1121	5PA	C9-C8-N	-3.33	113.89	117.36
2	M	1131	5PA	C9-C8-N	-3.25	113.97	117.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

24 monomers are involved in 197 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1011	5PA	5	0
2	B	1021	5PA	8	0
2	C	1031	5PA	6	0
2	D	1041	5PA	7	0
2	E	1051	5PA	7	0
2	F	1061	5PA	15	0
2	G	1071	5PA	3	0
2	H	1081	5PA	7	0
2	I	1091	5PA	13	0
2	J	1101	5PA	9	0
2	K	1111	5PA	11	0
2	L	1121	5PA	6	0
2	M	1131	5PA	10	0
2	N	1141	5PA	4	0
2	O	1151	5PA	6	0
2	P	1161	5PA	10	0
2	Q	1171	5PA	15	0
2	R	1181	5PA	14	0
2	S	1191	5PA	9	0
2	T	1201	5PA	6	0
2	U	1211	5PA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	V	1221	5PA	7	0
2	W	1231	5PA	8	0
2	X	1241	5PA	5	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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.