



## wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Feb 8, 2020 – 03:49 AM EST

PDB ID : 6Q7L  
EMDB ID: : EMD-4469  
Title : Spiral structure of E. coli RavA in the RavA-LdcI cage-like complex  
Authors : Arragain, B.; Felix, J.; Malet, H.; Gutsche, I.; Jessop, M.  
Deposited on : 2018-12-13  
Resolution : 7.60 Å(reported)  
Based on PDB ID : 3NBX, 3N75

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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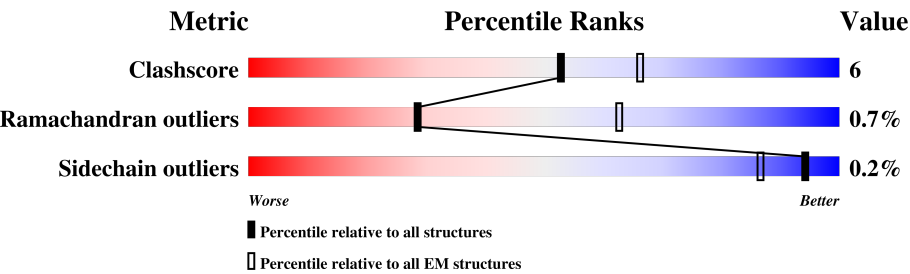
MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.60 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.
















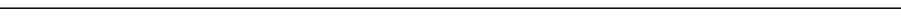



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	715	80% 20% .
1	B	715	82% 17% .
1	C	715	82% 17% .
1	D	715	83% 16% .
1	E	715	83% 16% .
1	F	715	82% 18% .
1	G	715	82% 18% .
1	H	715	80% 19% .
1	I	715	82% 17% .

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Mol	Chain	Length	Quality of chain
1	J	715	 83% 17% .
1	K	715	 83% 16% .
1	L	715	 82% 17% .
1	M	715	 81% 18% .
1	N	715	 82% 18% .
1	O	715	 83% 17% .
1	P	715	 83% 16% .
1	Q	715	 82% 18% .
1	R	715	 81% 18% .
1	S	715	 83% 16% .
1	T	715	 82% 17% .
2	U	498	 82% 14% .
3	V	497	 82% 14% .
3	W	497	 80% 16% . .
3	X	497	 81% 15% .
3	Y	497	 84% 12% . .
3	Z	497	 84% 12% .

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 137337 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Inducible lysine decarboxylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	711	Total	C	N	O	S	1	0
			5690	3642	952	1059	37		
1	B	711	Total	C	N	O	S	1	0
			5690	3642	952	1059	37		
1	C	711	Total	C	N	O	S	2	0
			5696	3646	952	1061	37		
1	D	711	Total	C	N	O	S	2	0
			5696	3646	952	1061	37		
1	E	711	Total	C	N	O	S	1	0
			5690	3642	952	1059	37		
1	F	711	Total	C	N	O	S	1	0
			5690	3642	952	1059	37		
1	G	711	Total	C	N	O	S	2	0
			5696	3646	952	1061	37		
1	H	711	Total	C	N	O	S	1	0
			5690	3642	952	1059	37		
1	I	711	Total	C	N	O	S	2	0
			5696	3646	952	1061	37		
1	J	711	Total	C	N	O	S	1	0
			5690	3642	952	1059	37		
1	K	711	Total	C	N	O	S	1	0
			5690	3642	952	1059	37		
1	L	711	Total	C	N	O	S	2	0
			5696	3646	952	1061	37		
1	M	711	Total	C	N	O	S	1	0
			5690	3642	952	1059	37		
1	N	711	Total	C	N	O	S	2	0
			5696	3646	952	1061	37		
1	O	711	Total	C	N	O	S	1	0
			5690	3642	952	1059	37		
1	P	711	Total	C	N	O	S	1	0
			5690	3642	952	1059	37		
1	Q	711	Total	C	N	O	S	2	0
			5696	3646	952	1061	37		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	711	Total	C	N	O	S	1	0
			5690	3642	952	1059	37		
1	S	711	Total	C	N	O	S	2	0
			5696	3646	952	1061	37		
1	T	711	Total	C	N	O	S	1	0
			5690	3642	952	1059	37		

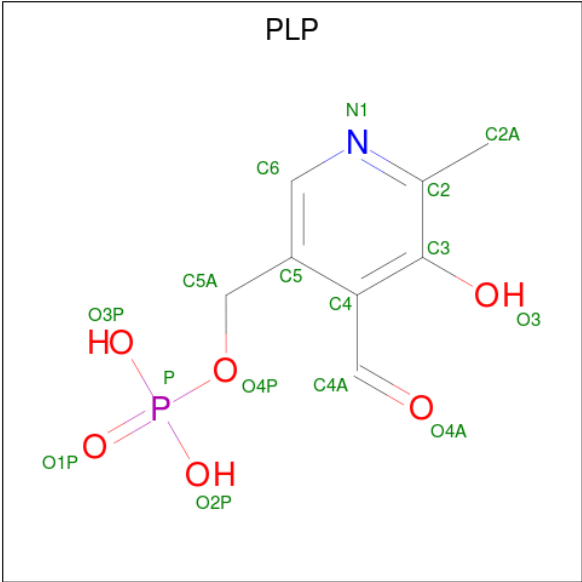
- Molecule 2 is a protein called ATPase RavA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	481	Total	C	N	O	S	0	0
			3847	2446	682	708	11		

- Molecule 3 is a protein called ATPase RavA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	V	481	Total	C	N	O	S	0	0
			3847	2446	682	708	11		
3	W	479	Total	C	N	O	S	0	0
			3833	2439	680	703	11		
3	X	481	Total	C	N	O	S	0	0
			3847	2446	682	708	11		
3	Y	481	Total	C	N	O	S	0	0
			3847	2446	682	708	11		
3	Z	479	Total	C	N	O	S	0	0
			3833	2439	680	703	11		

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



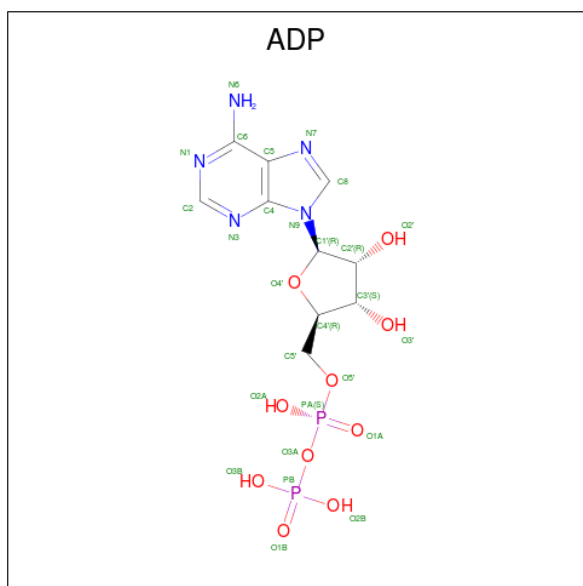
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			15	8	1	5	1	
4	B	1	Total	C	N	O	P	0
			15	8	1	5	1	
4	C	1	Total	C	N	O	P	0
			15	8	1	5	1	
4	D	1	Total	C	N	O	P	0
			15	8	1	5	1	
4	E	1	Total	C	N	O	P	0
			15	8	1	5	1	
4	F	1	Total	C	N	O	P	0
			15	8	1	5	1	
4	G	1	Total	C	N	O	P	0
			15	8	1	5	1	
4	H	1	Total	C	N	O	P	0
			15	8	1	5	1	
4	I	1	Total	C	N	O	P	0
			15	8	1	5	1	
4	J	1	Total	C	N	O	P	0
			15	8	1	5	1	
4	K	1	Total	C	N	O	P	0
			15	8	1	5	1	
4	L	1	Total	C	N	O	P	0
			15	8	1	5	1	
4	M	1	Total	C	N	O	P	0
			15	8	1	5	1	
4	N	1	Total	C	N	O	P	0
			15	8	1	5	1	

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Mol	Chain	Residues	Atoms					AltConf
4	O	1	Total 15	C 8	N 1	O 5	P 1	0
4	P	1	Total 15	C 8	N 1	O 5	P 1	0
4	Q	1	Total 15	C 8	N 1	O 5	P 1	0
4	R	1	Total 15	C 8	N 1	O 5	P 1	0
4	S	1	Total 15	C 8	N 1	O 5	P 1	0
4	T	1	Total 15	C 8	N 1	O 5	P 1	0

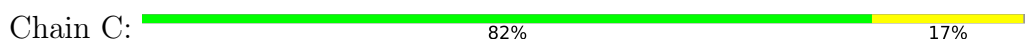
- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).



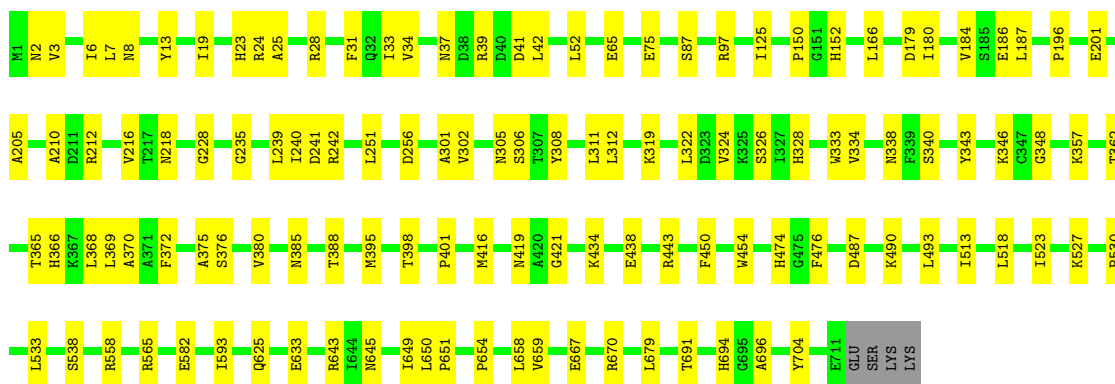
Mol	Chain	Residues	Atoms					AltConf
5	V	1	Total 27	C 10	N 5	O 10	P 2	0
5	W	1	Total 27	C 10	N 5	O 10	P 2	0
5	X	1	Total 27	C 10	N 5	O 10	P 2	0
5	Y	1	Total 27	C 10	N 5	O 10	P 2	0
5	Z	1	Total 27	C 10	N 5	O 10	P 2	0



- Molecule 1: Inducible lysine decarboxylase

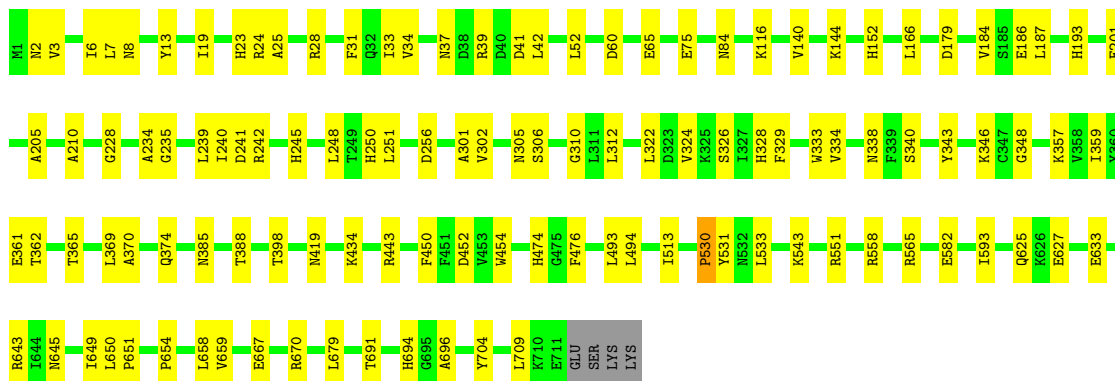






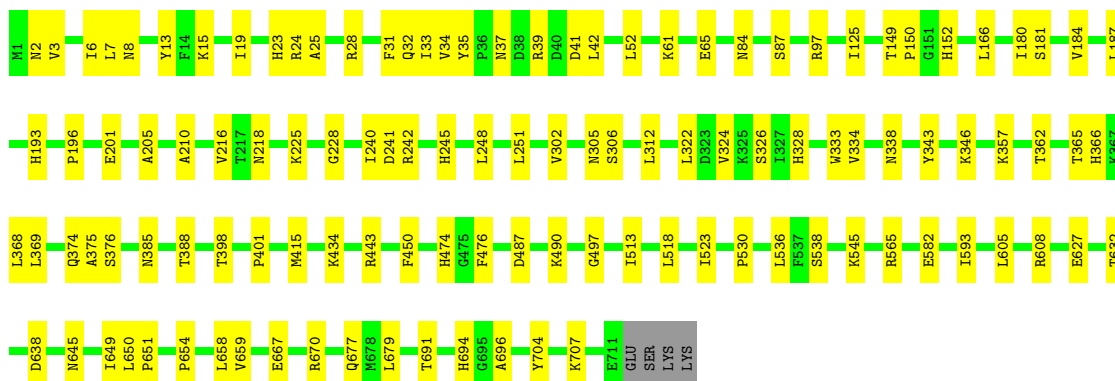
• Molecule 1: Inducible lysine decarboxylase

Chain D: 83% 16% •



• Molecule 1: Inducible lysine decarboxylase

Chain E: 83% 16% •

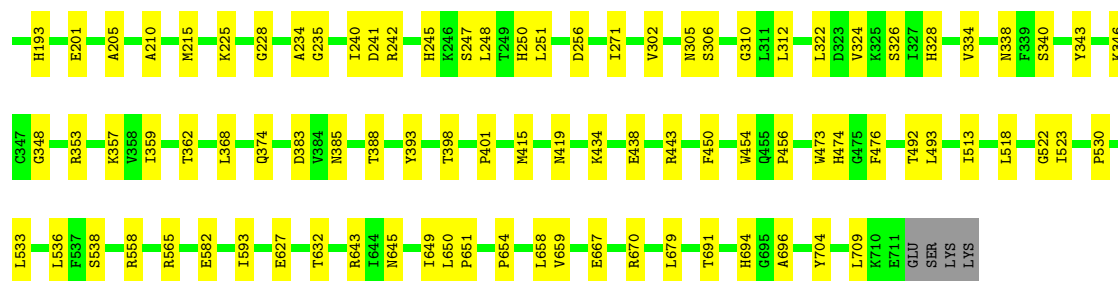


• Molecule 1: Inducible lysine decarboxylase

Chain F: 82% 18% •

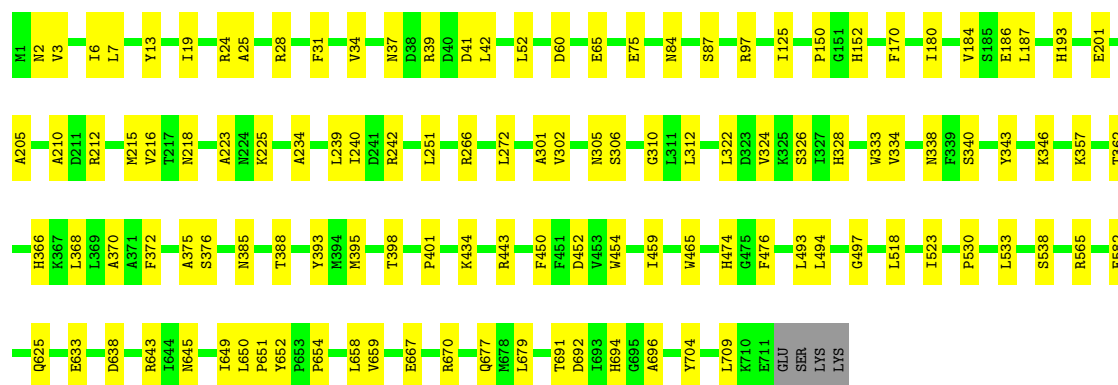






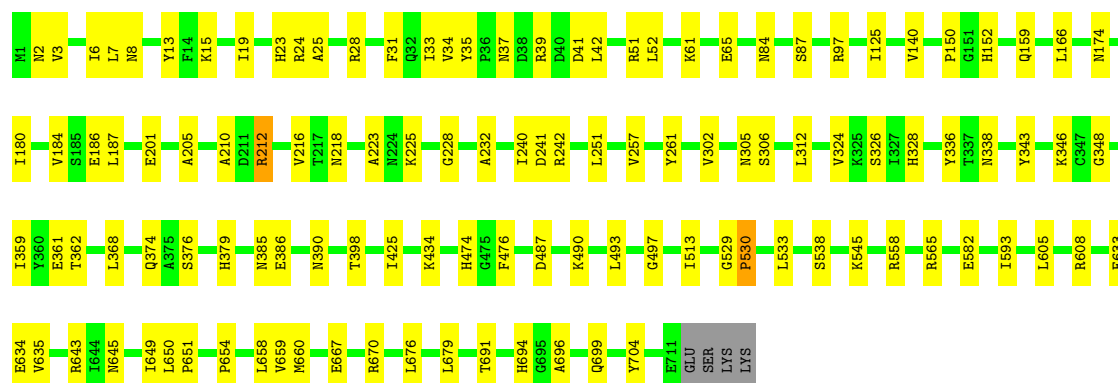
- Molecule 1: Inducible lysine decarboxylase

Chain J: 83% 17% .



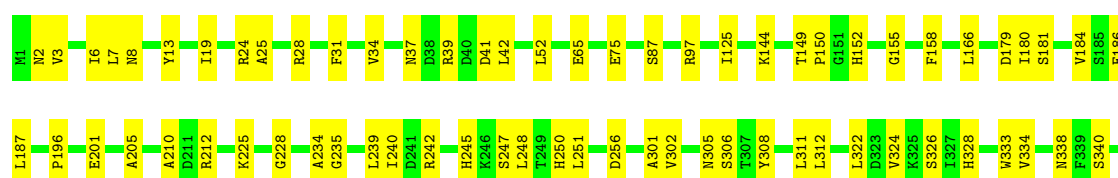
- Molecule 1: Inducible lysine decarboxylase

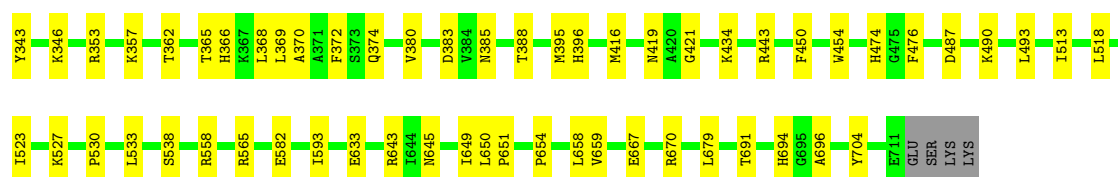
Chain K: 83% 16% .



- Molecule 1: Inducible lysine decarboxylase

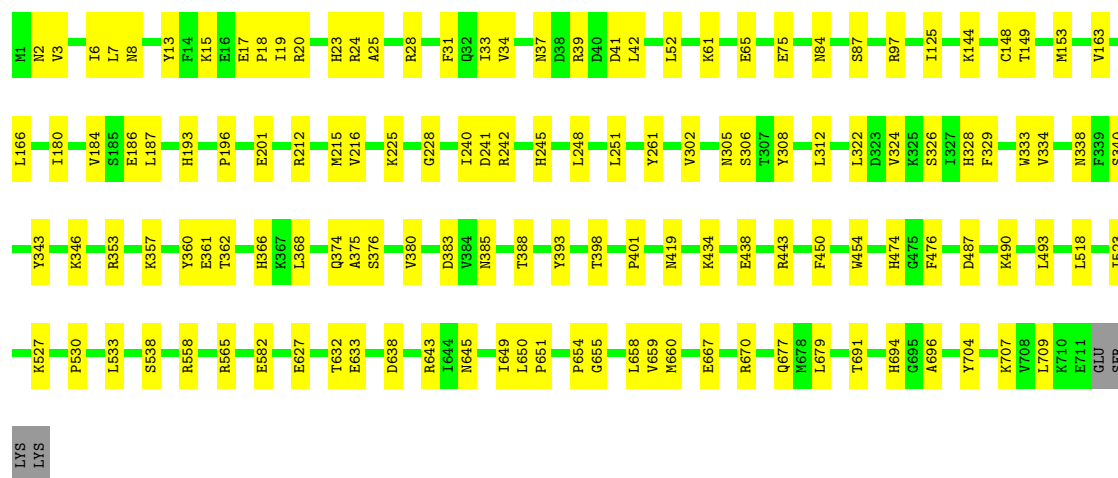
Chain L: 82% 17% .





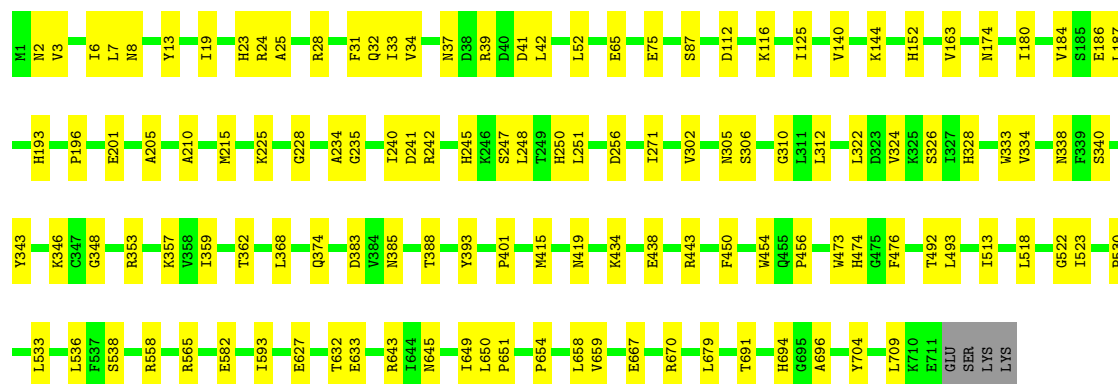
• Molecule 1: Inducible lysine decarboxylase

Chain M: 81% 18%



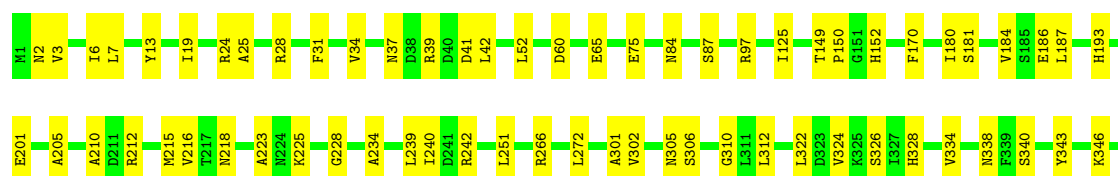
• Molecule 1: Inducible lysine decarboxylase

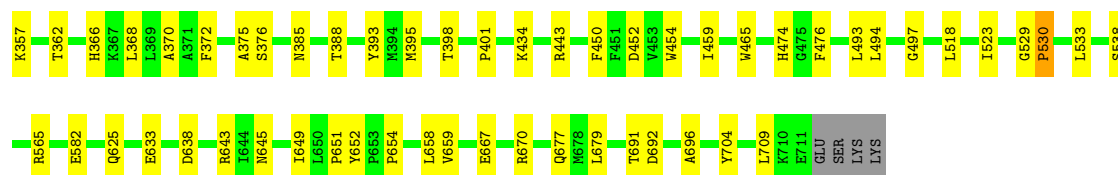
Chain N: 82% 18%



• Molecule 1: Inducible lysine decarboxylase

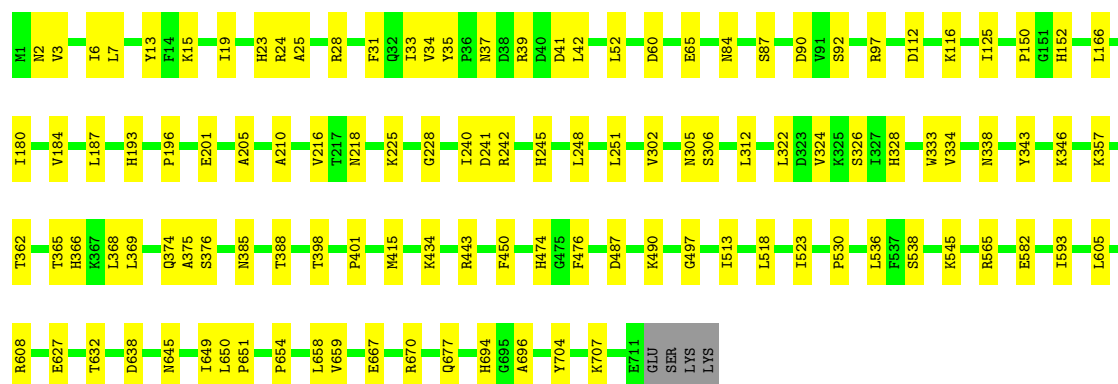
Chain O: 83% 17%





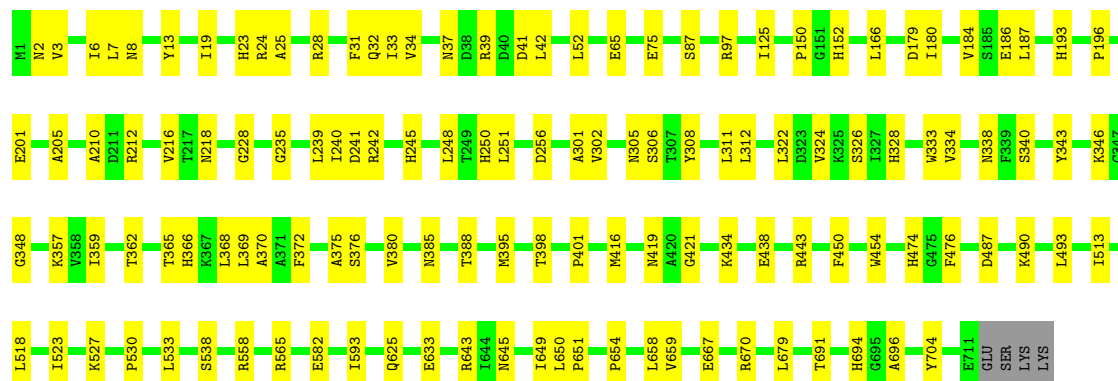
• Molecule 1: Inducible lysine decarboxylase

Chain P: 83% 16%



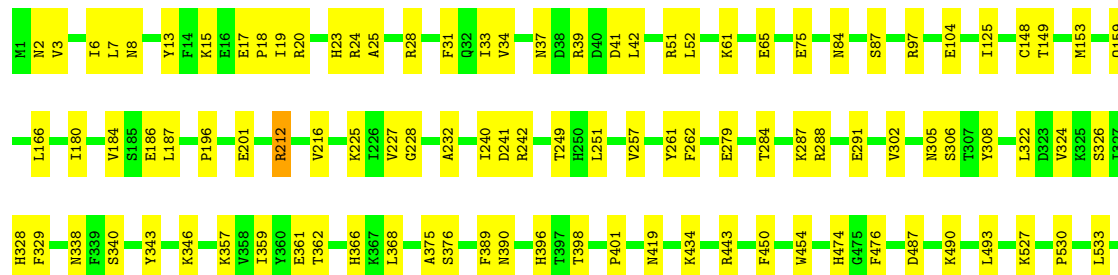
• Molecule 1: Inducible lysine decarboxylase

Chain Q: 82% 18%



• Molecule 1: Inducible lysine decarboxylase

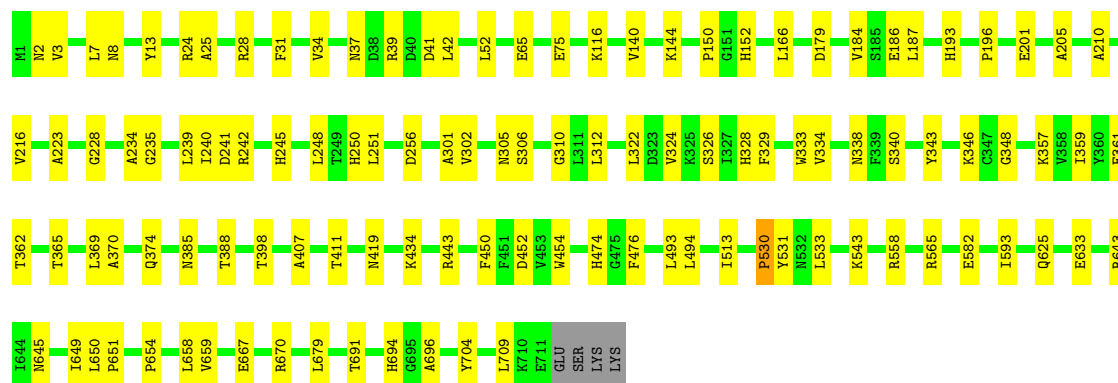
Chain R: 81% 18%





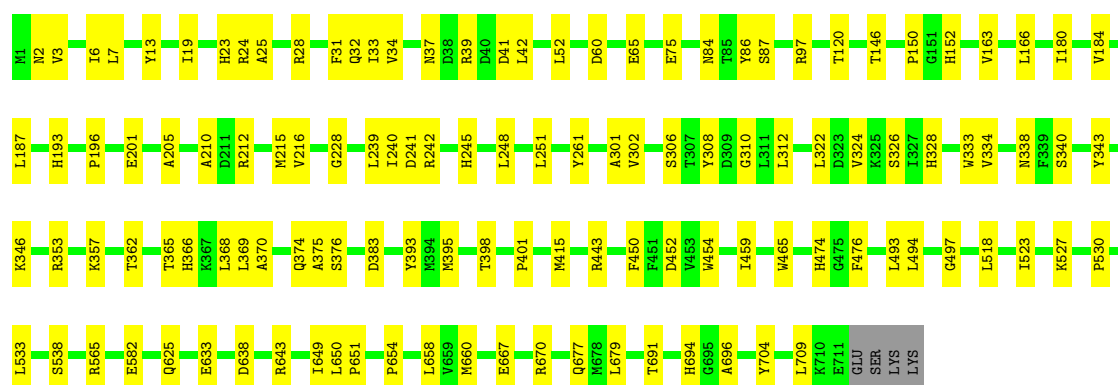
• Molecule 1: Inducible lysine decarboxylase

Chain S: 83% 16%



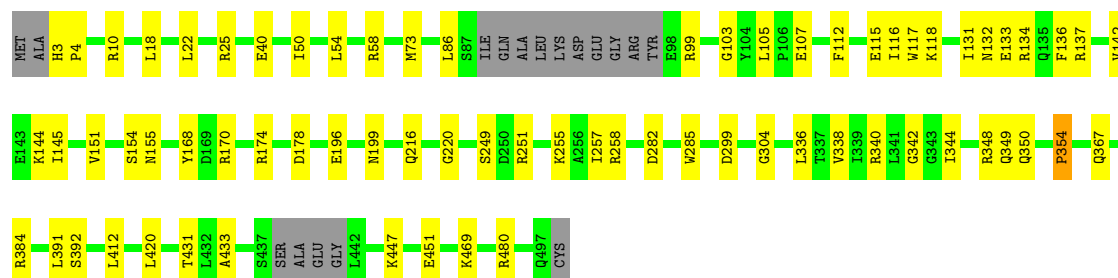
• Molecule 1: Inducible lysine decarboxylase

Chain T: 82% 17%



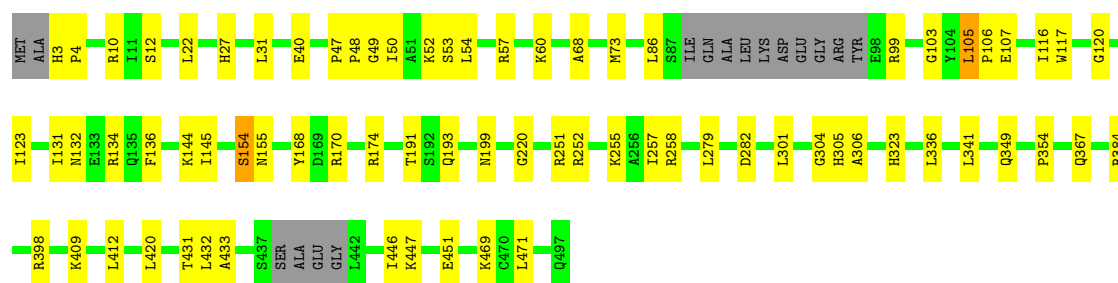
• Molecule 2: ATPase RavA

Chain U: 82% 14%




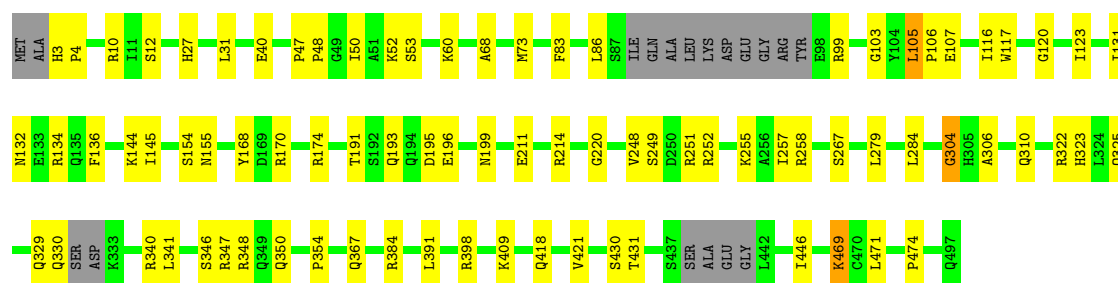
• Molecule 3: ATPase RavA

Chain V: 82% 14%

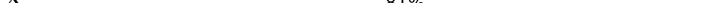


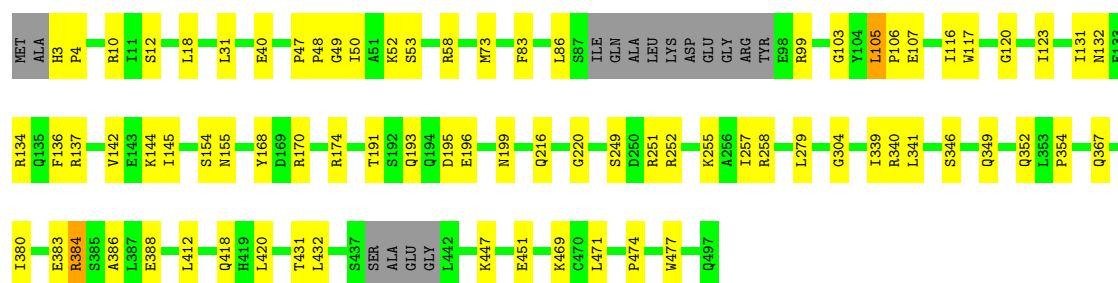
- Molecule 3: ATPase RayA

Chain W:  80% 16% . .

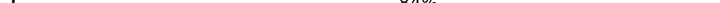


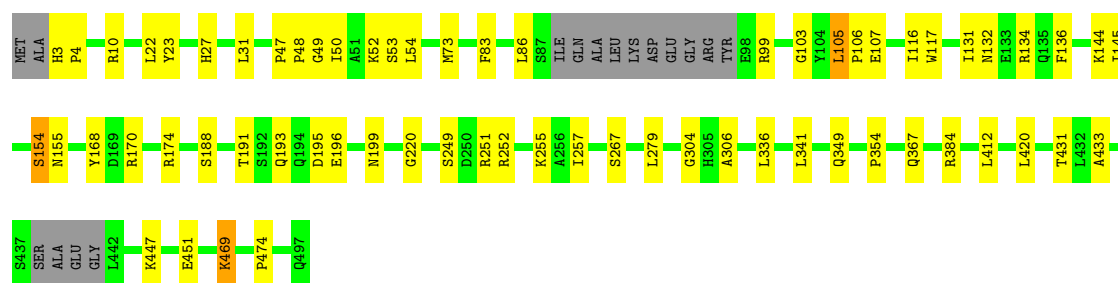
- Molecule 3: ATPase RayA

Chain X:  81% 15% .

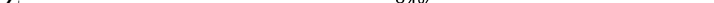


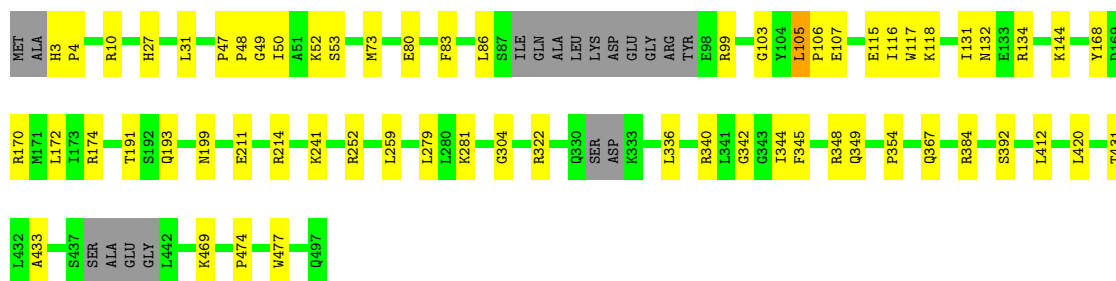
- Molecule 3: ATPase RayA

Chain Y:  84% 12% ..



- Molecule 3: ATPase RayA

Chain Z:  84% 12% .





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	19221	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	41270	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 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: ADP, PLP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.24	0/5834	0.39	0/7907
1	B	0.24	0/5834	0.39	0/7907
1	C	0.24	0/5843	0.39	0/7919
1	D	0.24	0/5843	0.39	0/7919
1	E	0.24	0/5834	0.39	0/7907
1	F	0.24	0/5834	0.39	0/7907
1	G	0.24	0/5843	0.39	0/7919
1	H	0.24	0/5834	0.39	0/7907
1	I	0.24	0/5843	0.39	0/7919
1	J	0.24	0/5834	0.39	0/7907
1	K	0.24	0/5834	0.39	0/7907
1	L	0.24	0/5843	0.39	0/7919
1	M	0.24	0/5834	0.39	0/7907
1	N	0.24	0/5843	0.39	0/7919
1	O	0.24	0/5834	0.39	0/7907
1	P	0.24	0/5834	0.39	0/7907
1	Q	0.24	0/5843	0.39	0/7919
1	R	0.24	0/5834	0.39	0/7907
1	S	0.24	0/5843	0.39	0/7919
1	T	0.24	0/5834	0.39	0/7907
2	U	0.23	0/3919	0.37	0/5300
3	V	0.23	0/3919	0.38	0/5300
3	W	0.23	0/3904	0.38	0/5278
3	X	0.23	0/3919	0.38	0/5300
3	Y	0.23	0/3919	0.37	0/5300
3	Z	0.23	0/3904	0.38	0/5278
All	All	0.24	0/140236	0.39	0/189992

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5690	0	5617	95	0
1	B	5690	0	5617	76	0
1	C	5696	0	5623	79	0
1	D	5696	0	5623	75	0
1	E	5690	0	5617	75	0
1	F	5690	0	5617	86	0
1	G	5696	0	5623	83	0
1	H	5690	0	5617	85	0
1	I	5696	0	5623	79	0
1	J	5690	0	5617	75	0
1	K	5690	0	5617	77	0
1	L	5696	0	5623	82	0
1	M	5690	0	5617	84	0
1	N	5696	0	5623	80	0
1	O	5690	0	5617	76	0
1	P	5690	0	5617	73	0
1	Q	5696	0	5623	82	0
1	R	5690	0	5617	90	0
1	S	5696	0	5623	73	0
1	T	5690	0	5617	76	0
2	U	3847	0	3896	41	0
3	V	3847	0	3896	43	0
3	W	3833	0	3886	59	0
3	X	3847	0	3896	53	0
3	Y	3847	0	3896	38	0
3	Z	3833	0	3886	42	0
4	A	15	0	7	1	0
4	B	15	0	7	2	0
4	C	15	0	7	1	0
4	D	15	0	7	2	0
4	E	15	0	7	2	0
4	F	15	0	7	1	0
4	G	15	0	7	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	15	0	7	2	0
4	I	15	0	7	0	0
4	J	15	0	7	2	0
4	K	15	0	7	1	0
4	L	15	0	7	3	0
4	M	15	0	7	2	0
4	N	15	0	7	2	0
4	O	15	0	7	1	0
4	P	15	0	7	2	0
4	Q	15	0	7	1	0
4	R	15	0	7	1	0
4	S	15	0	7	2	0
4	T	15	0	7	1	0
5	V	27	0	12	2	0
5	W	27	0	12	2	0
5	X	27	0	12	2	0
5	Y	27	0	12	3	0
5	Z	27	0	12	2	0
All	All	137337	0	135944	1672	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 1672 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:R:639:GLU:OE2	3:Z:322:ARG:NH1	1.98	0.97
1:N:667:GLU:OE1	1:N:670:ARG:NH1	2.12	0.82
1:G:667:GLU:OE1	1:G:670:ARG:NH1	2.12	0.82
1:J:667:GLU:OE1	1:J:670:ARG:NH1	2.13	0.82
1:B:667:GLU:OE1	1:B:670:ARG:NH1	2.12	0.82

There are no symmetry-related clashes.

## 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 PDB entries followed by that with respect to all EM entries.

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	710/715 (99%)	612 (86%)	94 (13%)	4 (1%)	27	70
1	B	710/715 (99%)	632 (89%)	73 (10%)	5 (1%)	24	67
1	C	711/715 (99%)	630 (89%)	77 (11%)	4 (1%)	27	70
1	D	711/715 (99%)	638 (90%)	68 (10%)	5 (1%)	24	67
1	E	710/715 (99%)	632 (89%)	74 (10%)	4 (1%)	27	70
1	F	710/715 (99%)	628 (88%)	76 (11%)	6 (1%)	21	65
1	G	711/715 (99%)	635 (89%)	72 (10%)	4 (1%)	27	70
1	H	710/715 (99%)	628 (88%)	78 (11%)	4 (1%)	27	70
1	I	711/715 (99%)	634 (89%)	72 (10%)	5 (1%)	24	67
1	J	710/715 (99%)	638 (90%)	67 (9%)	5 (1%)	24	67
1	K	710/715 (99%)	627 (88%)	79 (11%)	4 (1%)	27	70
1	L	711/715 (99%)	636 (90%)	71 (10%)	4 (1%)	27	70
1	M	710/715 (99%)	628 (88%)	78 (11%)	4 (1%)	27	70
1	N	711/715 (99%)	634 (89%)	72 (10%)	5 (1%)	24	67
1	O	710/715 (99%)	638 (90%)	67 (9%)	5 (1%)	24	67
1	P	710/715 (99%)	632 (89%)	74 (10%)	4 (1%)	27	70
1	Q	711/715 (99%)	629 (88%)	78 (11%)	4 (1%)	27	70
1	R	710/715 (99%)	621 (88%)	86 (12%)	3 (0%)	36	77
1	S	711/715 (99%)	638 (90%)	68 (10%)	5 (1%)	24	67
1	T	710/715 (99%)	634 (89%)	71 (10%)	5 (1%)	24	67
2	U	475/498 (95%)	438 (92%)	34 (7%)	3 (1%)	27	70
3	V	475/497 (96%)	437 (92%)	33 (7%)	5 (1%)	16	58
3	W	471/497 (95%)	434 (92%)	32 (7%)	5 (1%)	16	58
3	X	475/497 (96%)	427 (90%)	45 (10%)	3 (1%)	27	70
3	Y	475/497 (96%)	433 (91%)	37 (8%)	5 (1%)	16	58
3	Z	471/497 (95%)	431 (92%)	37 (8%)	3 (1%)	27	70
All	All	17050/17283 (99%)	15224 (89%)	1713 (10%)	113 (1%)	28	67

5 of 113 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	654	PRO
1	B	530	PRO
1	B	654	PRO
1	C	530	PRO
1	C	654	PRO

### 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 PDB entries followed by that with respect to all EM entries.

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	622/625 (100%)	622 (100%)	0	100	100
1	B	622/625 (100%)	622 (100%)	0	100	100
1	C	623/625 (100%)	623 (100%)	0	100	100
1	D	623/625 (100%)	623 (100%)	0	100	100
1	E	622/625 (100%)	622 (100%)	0	100	100
1	F	622/625 (100%)	622 (100%)	0	100	100
1	G	623/625 (100%)	623 (100%)	0	100	100
1	H	622/625 (100%)	622 (100%)	0	100	100
1	I	623/625 (100%)	623 (100%)	0	100	100
1	J	622/625 (100%)	622 (100%)	0	100	100
1	K	622/625 (100%)	620 (100%)	2 (0%)	93	96
1	L	623/625 (100%)	623 (100%)	0	100	100
1	M	622/625 (100%)	622 (100%)	0	100	100
1	N	623/625 (100%)	623 (100%)	0	100	100
1	O	622/625 (100%)	622 (100%)	0	100	100
1	P	622/625 (100%)	622 (100%)	0	100	100
1	Q	623/625 (100%)	623 (100%)	0	100	100
1	R	622/625 (100%)	620 (100%)	2 (0%)	93	96
1	S	623/625 (100%)	623 (100%)	0	100	100
1	T	622/625 (100%)	622 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	U	416/428 (97%)	411 (99%)	5 (1%)	74	87
3	V	416/427 (97%)	411 (99%)	5 (1%)	74	87
3	W	414/427 (97%)	409 (99%)	5 (1%)	74	87
3	X	416/427 (97%)	411 (99%)	5 (1%)	74	87
3	Y	416/427 (97%)	411 (99%)	5 (1%)	74	87
3	Z	414/427 (97%)	409 (99%)	5 (1%)	74	87
All	All	14940/15063 (99%)	14906 (100%)	34 (0%)	94	96

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	W	144	LYS
3	X	10	ARG
3	Z	199	ASN
3	W	384	ARG
2	U	199	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 183 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	699	GLN
1	N	385	ASN
3	X	132	ASN
1	L	174	ASN
1	M	84	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

25 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
4	PLP	A	801	1	15,15,16	2.38	6 (40%)	20,22,23	0.99	2 (10%)
4	PLP	B	801	1	15,15,16	2.37	6 (40%)	20,22,23	0.98	2 (10%)
4	PLP	C	801	1	15,15,16	2.38	6 (40%)	20,22,23	0.98	2 (10%)
4	PLP	D	801	1	15,15,16	2.38	6 (40%)	20,22,23	0.99	2 (10%)
4	PLP	E	801	1	15,15,16	2.39	6 (40%)	20,22,23	0.99	2 (10%)
4	PLP	F	801	1	15,15,16	2.35	6 (40%)	20,22,23	0.99	2 (10%)
4	PLP	G	801	1	15,15,16	2.33	6 (40%)	20,22,23	0.99	2 (10%)
4	PLP	H	801	1	15,15,16	2.34	6 (40%)	20,22,23	1.00	2 (10%)
4	PLP	I	801	1	15,15,16	2.34	6 (40%)	20,22,23	0.99	2 (10%)
4	PLP	J	801	1	15,15,16	2.34	6 (40%)	20,22,23	0.99	2 (10%)
4	PLP	K	801	1	15,15,16	2.34	6 (40%)	20,22,23	0.99	2 (10%)
4	PLP	L	801	1	15,15,16	2.36	6 (40%)	20,22,23	1.00	2 (10%)
4	PLP	M	801	1	15,15,16	2.34	6 (40%)	20,22,23	0.99	2 (10%)
4	PLP	N	801	1	15,15,16	2.34	6 (40%)	20,22,23	0.98	2 (10%)
4	PLP	O	801	1	15,15,16	2.35	6 (40%)	20,22,23	0.99	2 (10%)
4	PLP	P	801	1	15,15,16	2.38	6 (40%)	20,22,23	0.99	2 (10%)
4	PLP	Q	801	1	15,15,16	2.39	6 (40%)	20,22,23	0.99	2 (10%)
4	PLP	R	801	1	15,15,16	2.36	6 (40%)	20,22,23	0.99	2 (10%)
4	PLP	S	801	1	15,15,16	2.38	6 (40%)	20,22,23	1.00	2 (10%)
4	PLP	T	801	1	15,15,16	2.38	6 (40%)	20,22,23	0.99	2 (10%)
5	ADP	V	800	-	24,29,29	1.02	1 (4%)	25,45,45	1.43	3 (12%)
5	ADP	W	800	-	24,29,29	1.02	1 (4%)	25,45,45	1.44	3 (12%)
5	ADP	X	800	-	24,29,29	1.01	1 (4%)	25,45,45	1.44	3 (12%)
5	ADP	Y	800	-	24,29,29	1.02	1 (4%)	25,45,45	1.44	3 (12%)
5	ADP	Z	800	-	24,29,29	1.02	1 (4%)	25,45,45	1.44	3 (12%)



In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PLP	A	801	1	-	0/6/6/8	0/1/1/1
4	PLP	B	801	1	-	0/6/6/8	0/1/1/1
4	PLP	C	801	1	-	0/6/6/8	0/1/1/1
4	PLP	D	801	1	-	0/6/6/8	0/1/1/1
4	PLP	E	801	1	-	0/6/6/8	0/1/1/1
4	PLP	F	801	1	-	2/6/6/8	0/1/1/1
4	PLP	G	801	1	-	1/6/6/8	0/1/1/1
4	PLP	H	801	1	-	1/6/6/8	0/1/1/1
4	PLP	I	801	1	-	0/6/6/8	0/1/1/1
4	PLP	J	801	1	-	1/6/6/8	0/1/1/1
4	PLP	K	801	1	-	2/6/6/8	0/1/1/1
4	PLP	L	801	1	-	1/6/6/8	0/1/1/1
4	PLP	M	801	1	-	1/6/6/8	0/1/1/1
4	PLP	N	801	1	-	0/6/6/8	0/1/1/1
4	PLP	O	801	1	-	1/6/6/8	0/1/1/1
4	PLP	P	801	1	-	0/6/6/8	0/1/1/1
4	PLP	Q	801	1	-	0/6/6/8	0/1/1/1
4	PLP	R	801	1	-	2/6/6/8	0/1/1/1
4	PLP	S	801	1	-	0/6/6/8	0/1/1/1
4	PLP	T	801	1	-	0/6/6/8	0/1/1/1
5	ADP	V	800	-	-	1/12/32/32	0/3/3/3
5	ADP	W	800	-	-	2/12/32/32	0/3/3/3
5	ADP	X	800	-	-	1/12/32/32	0/3/3/3
5	ADP	Y	800	-	-	0/12/32/32	0/3/3/3
5	ADP	Z	800	-	-	0/12/32/32	0/3/3/3

The worst 5 of 125 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	801	PLP	C4A-C4	5.01	1.62	1.51
4	J	801	PLP	C4A-C4	4.99	1.62	1.51
4	C	801	PLP	C4A-C4	4.99	1.62	1.51
4	Q	801	PLP	C4A-C4	4.99	1.62	1.51
4	S	801	PLP	C4A-C4	4.99	1.62	1.51

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	W	800	ADP	PA-O3A-PB	-3.73	120.72	132.57
5	Z	800	ADP	PA-O3A-PB	-3.72	120.73	132.57
5	Y	800	ADP	PA-O3A-PB	-3.72	120.74	132.57
5	X	800	ADP	PA-O3A-PB	-3.72	120.75	132.57
5	V	800	ADP	PA-O3A-PB	-3.71	120.77	132.57

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	X	800	ADP	C5'-O5'-PA-O1A
5	W	800	ADP	C5'-O5'-PA-O1A
5	V	800	ADP	C5'-O5'-PA-O1A
4	F	801	PLP	C5A-O4P-P-O2P
4	K	801	PLP	C5A-O4P-P-O2P

There are no ring outliers.

24 monomers are involved in 43 short contacts:

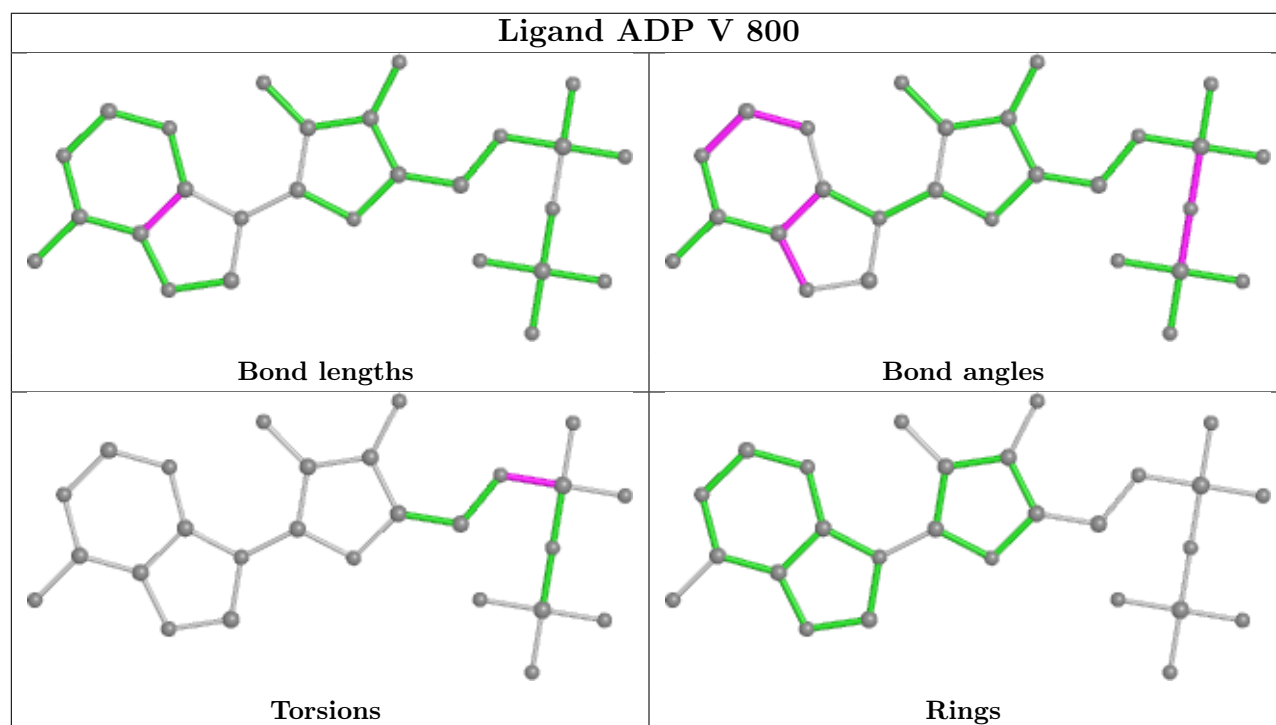
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	PLP	1	0
4	B	801	PLP	2	0
4	C	801	PLP	1	0
4	D	801	PLP	2	0
4	E	801	PLP	2	0
4	F	801	PLP	1	0
4	G	801	PLP	3	0
4	H	801	PLP	2	0
4	J	801	PLP	2	0
4	K	801	PLP	1	0
4	L	801	PLP	3	0
4	M	801	PLP	2	0
4	N	801	PLP	2	0
4	O	801	PLP	1	0
4	P	801	PLP	2	0
4	Q	801	PLP	1	0
4	R	801	PLP	1	0
4	S	801	PLP	2	0
4	T	801	PLP	1	0
5	V	800	ADP	2	0
5	W	800	ADP	2	0
5	X	800	ADP	2	0

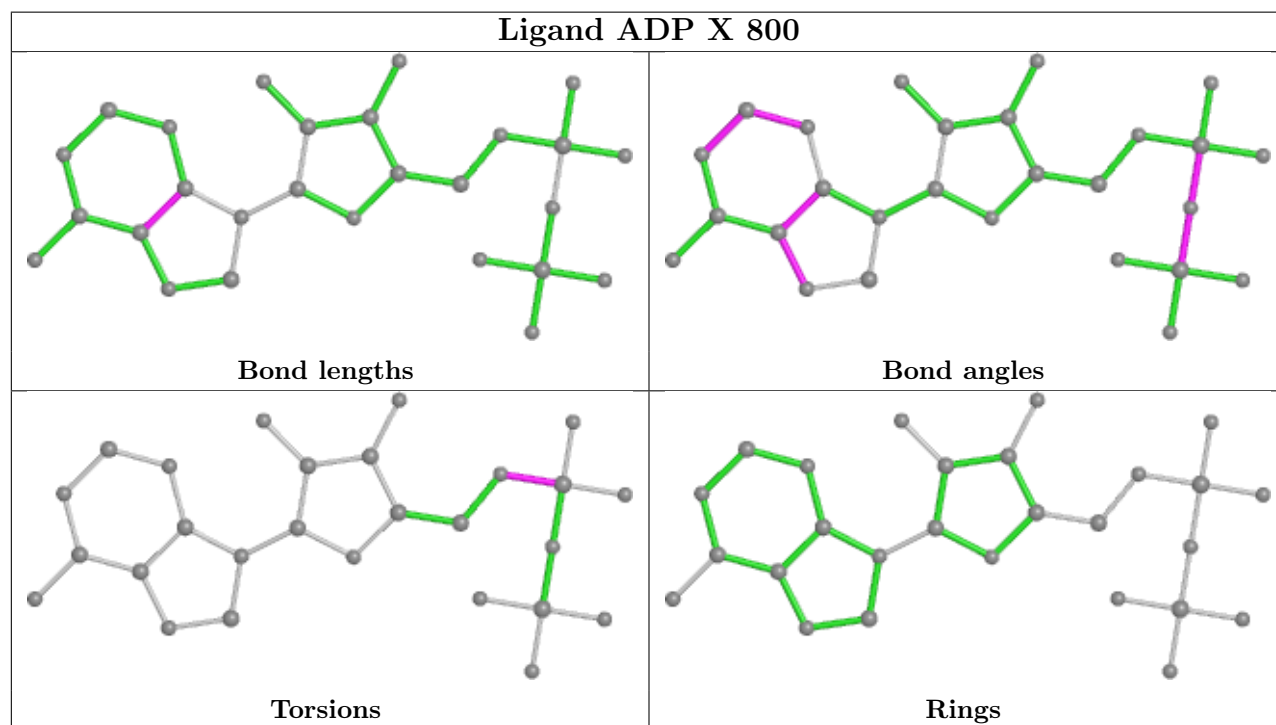
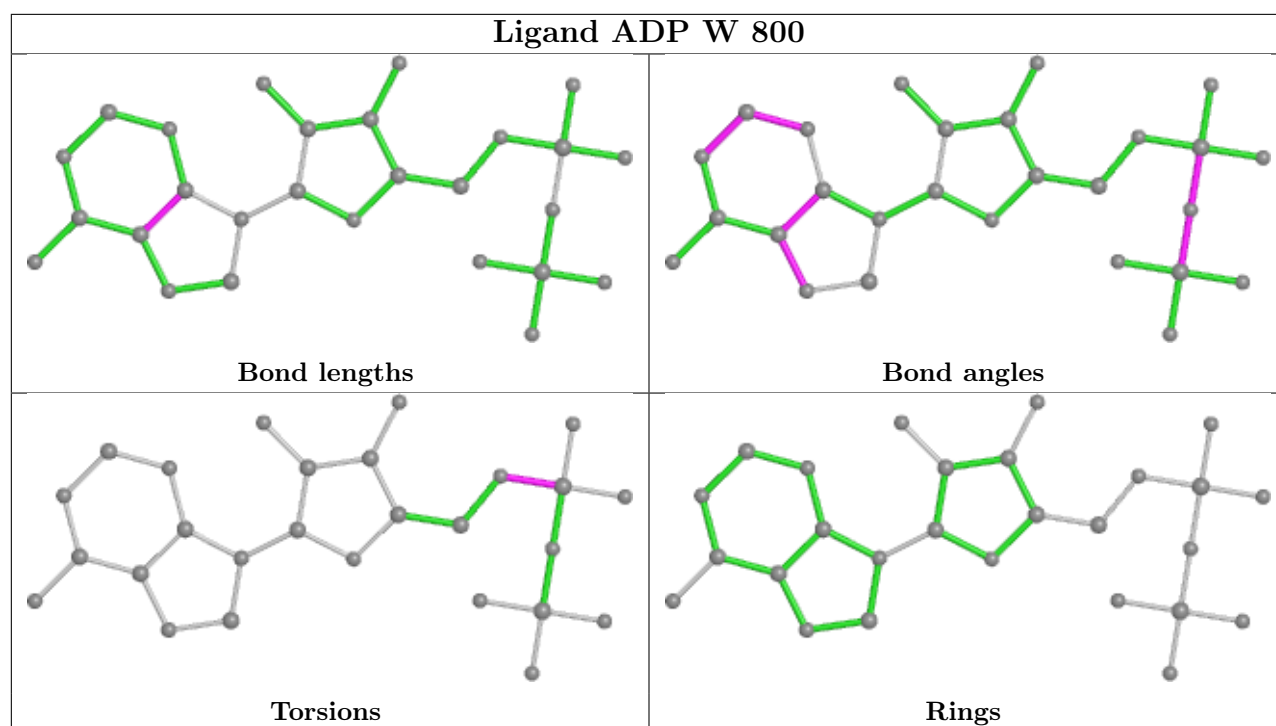
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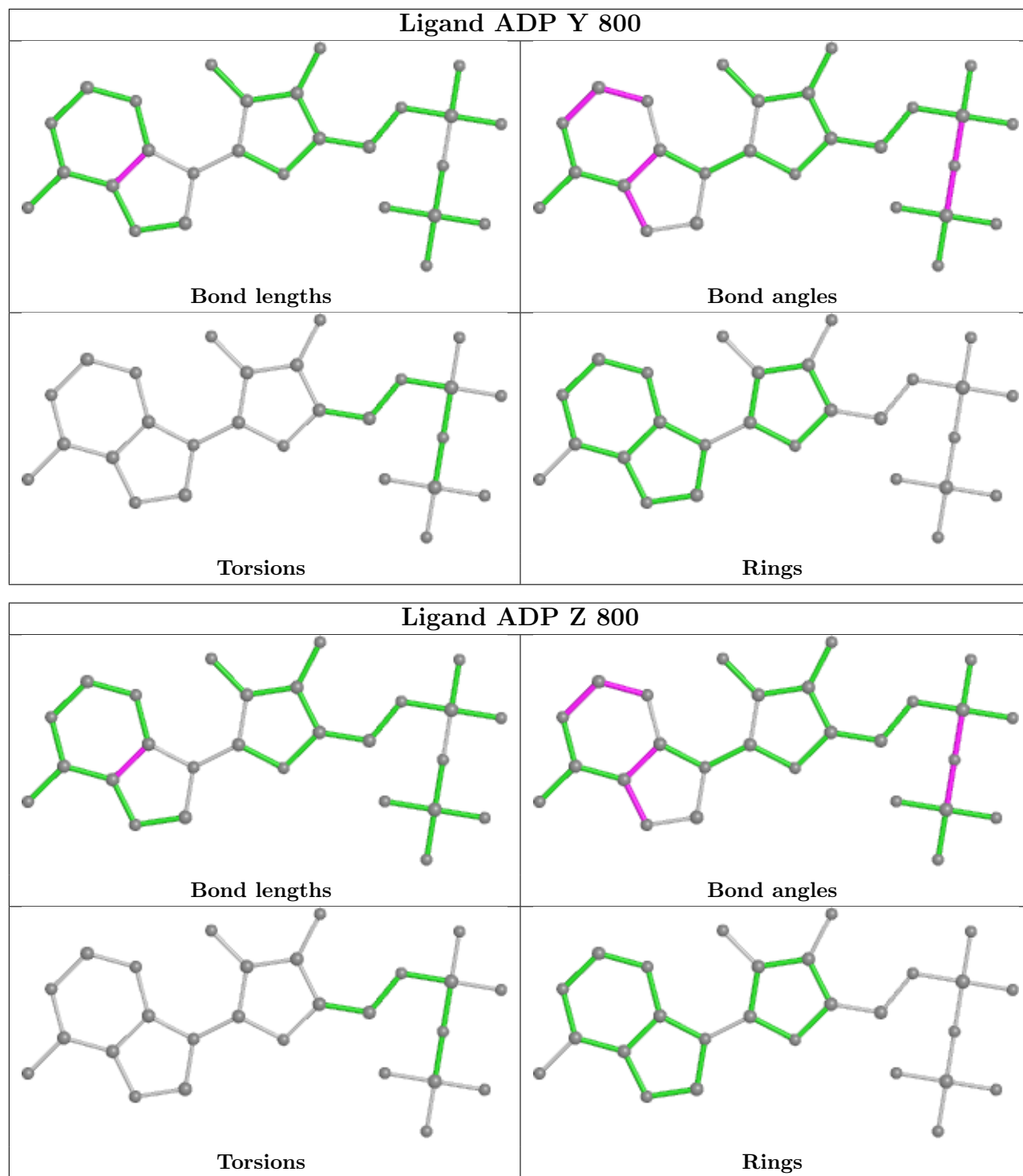
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Y	800	ADP	3	0
5	Z	800	ADP	2	0

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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.