



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 04:55 am BST

PDB ID : 1LGR  
Title : INTERACTIONS OF NUCLEOTIDES WITH FULLY UNADENYLYLATED  
GLUTAMINE SYNTHETASE FROM SALMONELLA TYPHIMURIUM  
Authors : Liaw, S.-H.; Eisenberg, D.  
Deposited on : 1994-08-05  
Resolution : 2.79 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

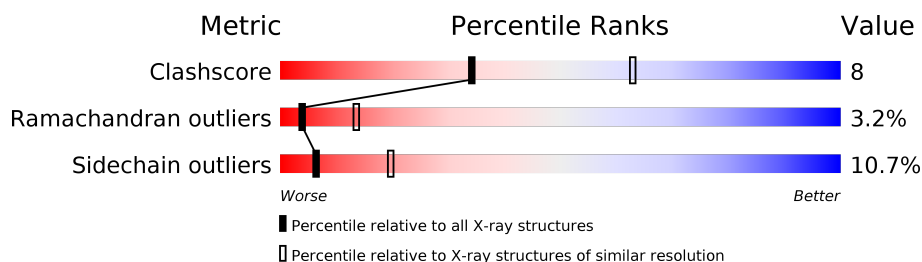
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.79 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	468	65% 24% . . 5%
1	B	468	65% 24% . . 5%
1	C	468	64% 25% . . 5%
1	D	468	66% 24% 5% . 5%
1	E	468	66% 24% . . 5%
1	F	468	66% 24% . . 5%
1	G	468	66% 24% . . 5%
1	H	468	66% 23% . . 5%

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Mol	Chain	Length	Quality of chain
1	I	468	<div><div></div><div>65%25%<div><div></div><div></div><div></div></div>5%</div></div>
1	J	468	<div><div></div><div>66%23%<div><div></div><div></div><div></div></div>5%</div></div>
1	K	468	<div><div></div><div>65%24%<div><div></div><div></div><div></div></div>5%5%</div></div>
1	L	468	<div><div></div><div>66%24%<div><div></div><div></div><div></div></div>5%</div></div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 41760 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 GLUTAMINE SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	B	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	C	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	D	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	E	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	F	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	G	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	H	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	I	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	J	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	K	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	L	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

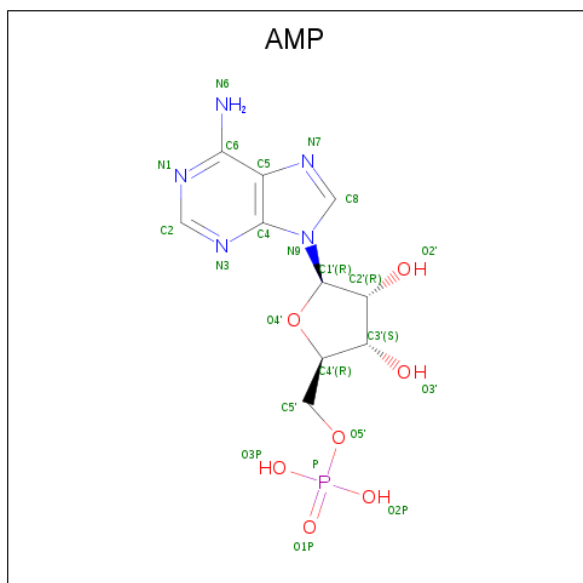
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Mn	0	0
			2	2		
2	J	2	Total	Mn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Mn	0	0
			2	2		
2	K	2	Total	Mn	0	0
			2	2		
2	E	2	Total	Mn	0	0
			2	2		
2	H	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		
2	I	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		
2	A	2	Total	Mn	0	0
			2	2		
2	L	2	Total	Mn	0	0
			2	2		
2	F	2	Total	Mn	0	0
			2	2		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

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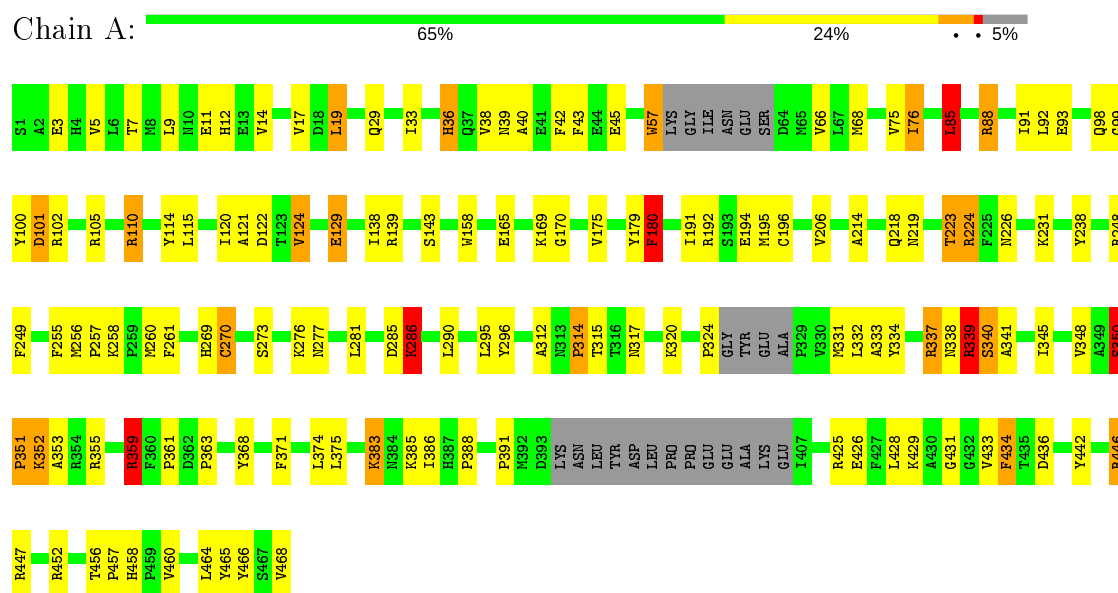
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	L	1	Total 23	C 10	N 5	O 7	P 1	0	0

### 3 Residue-property plots

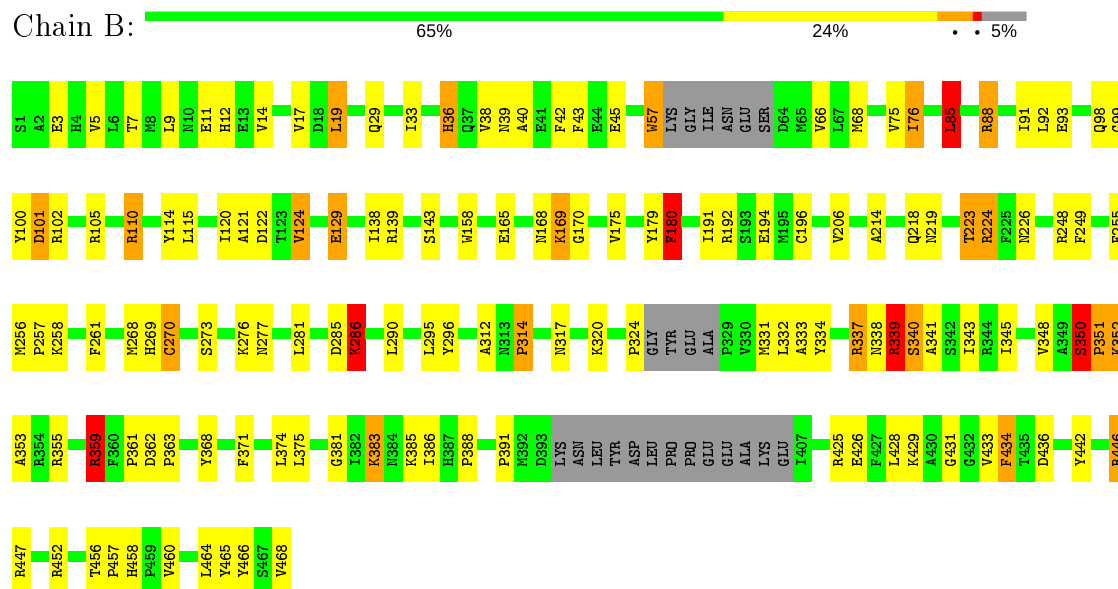
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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: GLUTAMINE SYNTHETASE

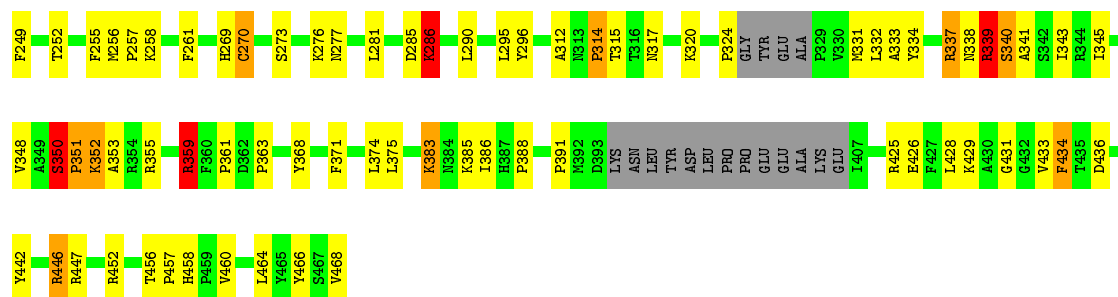


#### • Molecule 1: GLUTAMINE SYNTHETASE



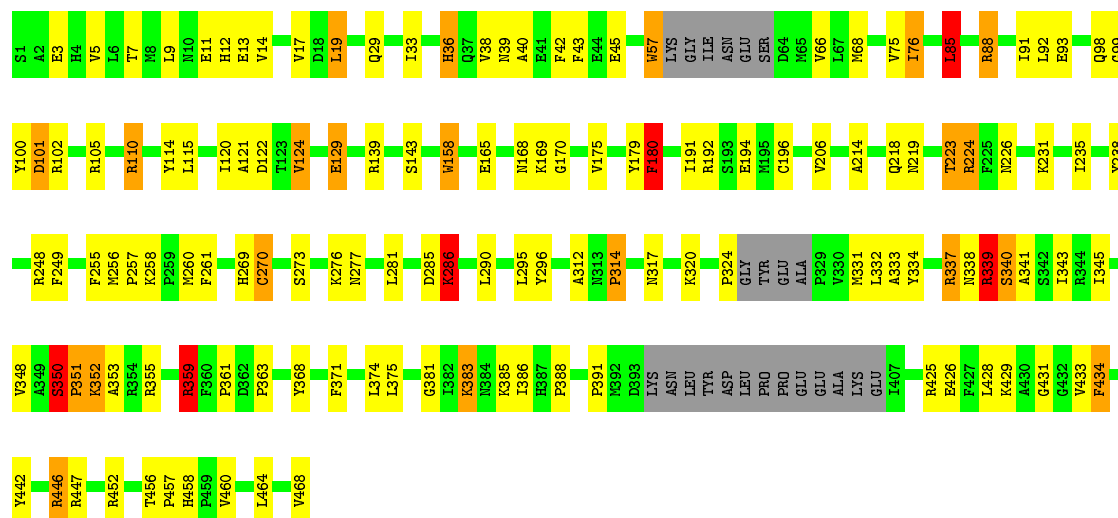






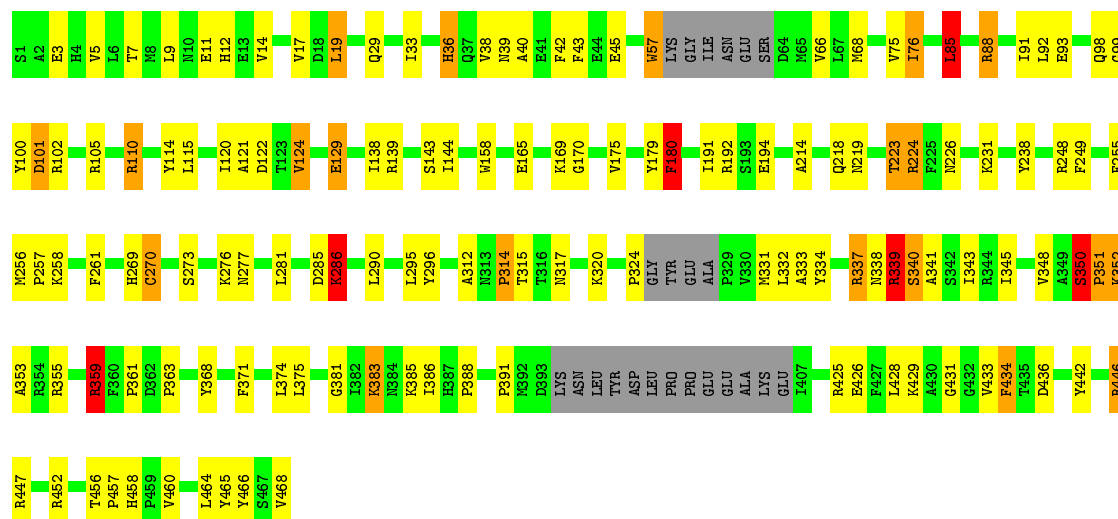
• Molecule 1: GLUTAMINE SYNTHETASE

Chain F: 66% 24% 5%



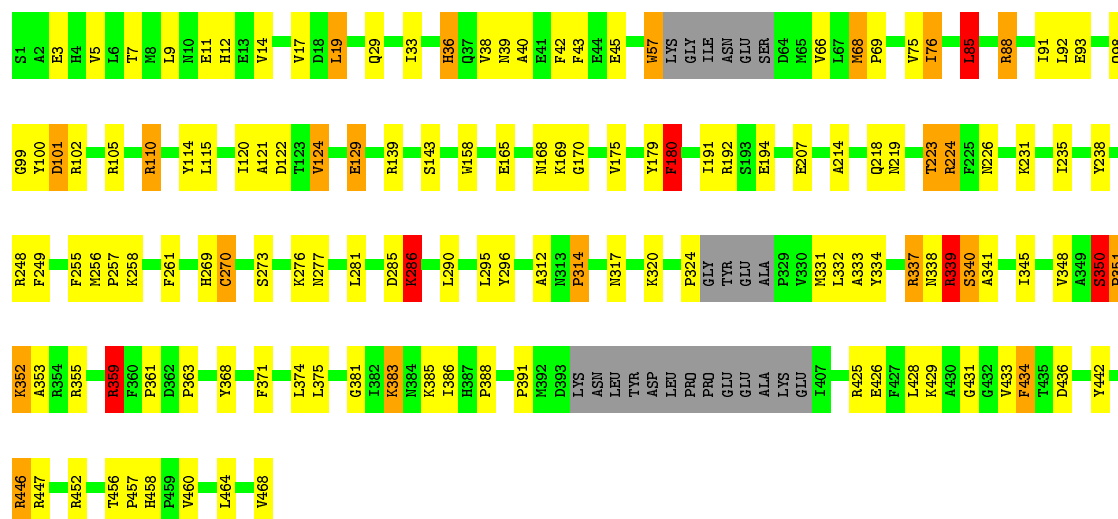
• Molecule 1: GLUTAMINE SYNTHETASE

Chain G: 66% 24% 5%



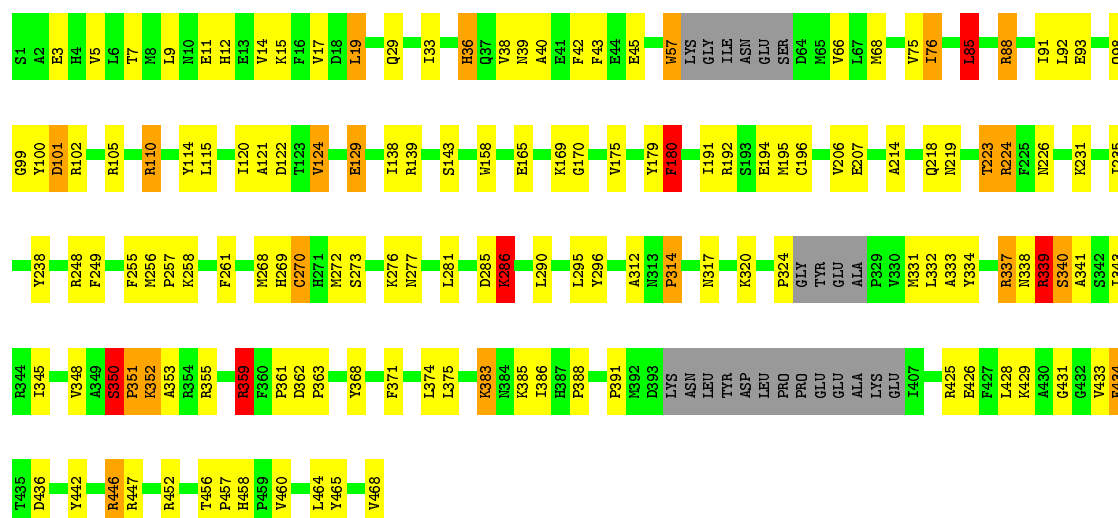
• Molecule 1: GLUTAMINE SYNTHETASE

Chain H:  66% 23% 5%



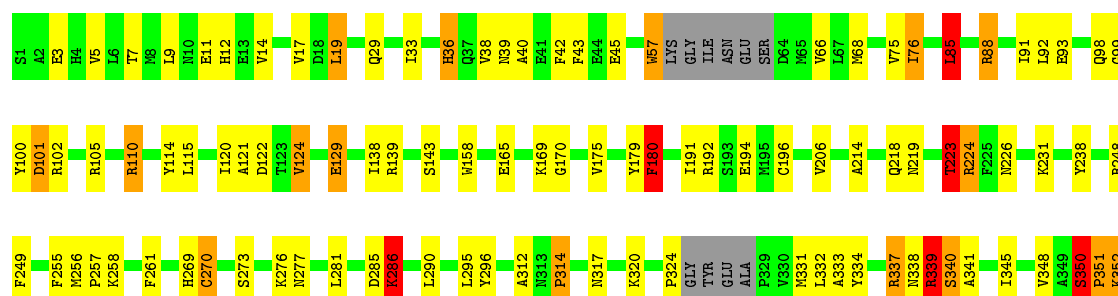
• Molecule 1: GLUTAMINE SYNTHETASE

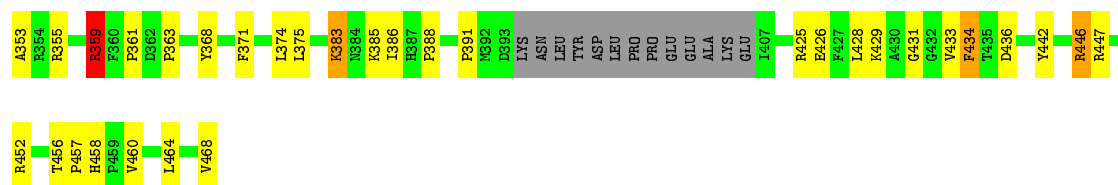
Chain I:  65% 25% 5%



• Molecule 1: GLUTAMINE SYNTHETASE

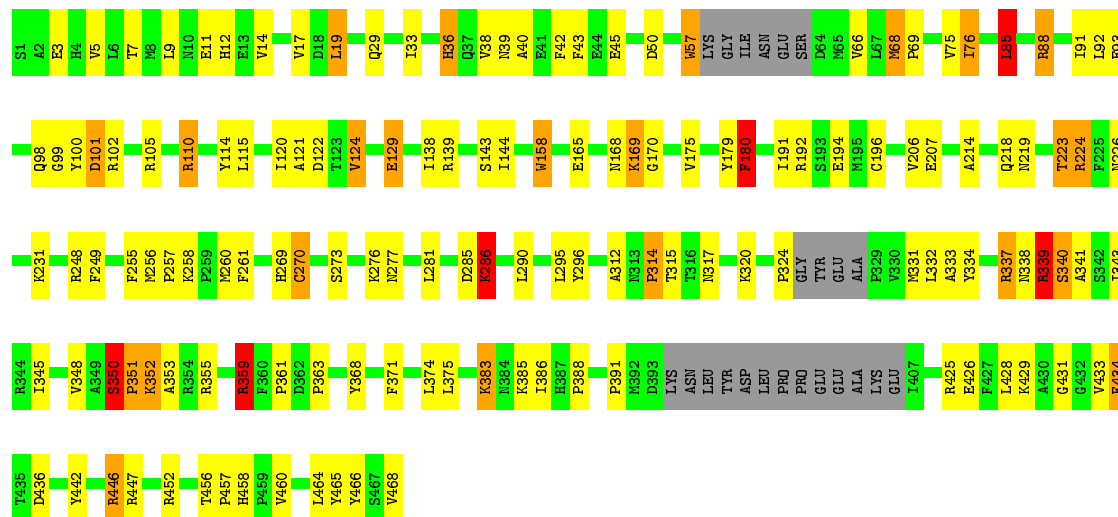
Chain J:  66% 23% 5%





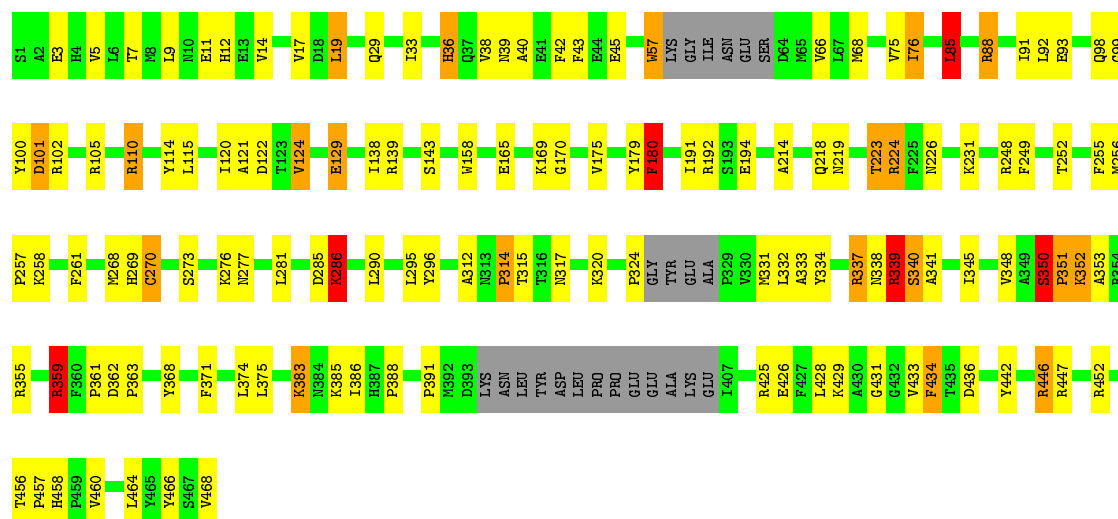
• Molecule 1: GLUTAMINE SYNTHETASE

Chain K: 65% 24% 5% • 5%



• Molecule 1: GLUTAMINE SYNTHETASE

Chain L: 66% 24% • 5%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	235.50 Å   134.50 Å   200.10 Å 90.00°   102.80°   90.00°	Depositor
Resolution (Å)	8.00 – 2.79	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.79)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.233 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	41760	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	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: AMP, MN

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	0.74	0/3535	1.51	39/4782 (0.8%)
1	B	0.74	0/3535	1.51	38/4782 (0.8%)
1	C	0.74	0/3535	1.51	39/4782 (0.8%)
1	D	0.74	0/3535	1.51	38/4782 (0.8%)
1	E	0.74	0/3535	1.51	39/4782 (0.8%)
1	F	0.74	0/3535	1.51	39/4782 (0.8%)
1	G	0.74	0/3535	1.51	39/4782 (0.8%)
1	H	0.74	0/3535	1.51	39/4782 (0.8%)
1	I	0.74	0/3535	1.51	40/4782 (0.8%)
1	J	0.74	0/3535	1.51	39/4782 (0.8%)
1	K	0.74	0/3535	1.51	38/4782 (0.8%)
1	L	0.74	0/3535	1.51	38/4782 (0.8%)
All	All	0.74	0/42420	1.51	465/57384 (0.8%)

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
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
1	I	0	2
1	J	0	2
1	K	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
All	All	0	24

There are no bond length outliers.

The worst 5 of 465 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	88	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	C	88	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	L	158	TRP	CD1-CG-CD2	9.69	114.05	106.30
1	C	158	TRP	CD1-CG-CD2	9.69	114.05	106.30
1	J	158	TRP	CD1-CG-CD2	9.68	114.05	106.30

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	ARG	Sidechain
1	A	350	SER	Peptide
1	B	224	ARG	Sidechain
1	B	350	SER	Peptide
1	C	224	ARG	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	3455	0	3371	64	0
1	B	3455	0	3371	64	0
1	C	3455	0	3371	68	2
1	D	3455	0	3371	63	0
1	E	3455	0	3371	62	0
1	F	3455	0	3371	59	2
1	G	3455	0	3371	62	0
1	H	3455	0	3371	58	0
1	I	3455	0	3371	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	3455	0	3371	59	0
1	K	3455	0	3371	69	0
1	L	3455	0	3371	61	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	23	0	12	2	0
3	B	23	0	12	2	0
3	C	23	0	12	2	0
3	D	23	0	12	3	0
3	E	23	0	12	2	0
3	F	23	0	12	2	0
3	G	23	0	12	2	0
3	H	23	0	12	3	0
3	I	23	0	12	3	0
3	J	23	0	12	2	0
3	K	23	0	12	3	0
3	L	23	0	12	2	0
All	All	41760	0	40596	689	2

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 8.

The worst 5 of 689 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:H:192:ARG:HD3	1:H:219:ASN:HD22	1.57	0.70
1:E:192:ARG:HD3	1:E:219:ASN:HD22	1.57	0.70
1:A:192:ARG:HD3	1:A:219:ASN:HD22	1.57	0.70
1:D:192:ARG:HD3	1:D:219:ASN:HD22	1.57	0.70
1:J:192:ARG:HD3	1:J:219:ASN:HD22	1.57	0.69

All (2) 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)
1:C:1:SER:OG	1:F:13:GLU:OE2[4_454]	1.08	1.12
1:C:1:SER:OG	1:F:13:GLU:CD[4_454]	2.11	0.09

## 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	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	4	13
1	B	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	4	13
1	C	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	4	13
1	D	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	4	13
1	E	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	4	13
1	F	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	4	13
1	G	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	4	13
1	H	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	4	13
1	I	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	4	13
1	J	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	4	13
1	K	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	4	13
1	L	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	4	13
All	All	5244/5616 (93%)	4704 (90%)	372 (7%)	168 (3%)	4	13

5 of 168 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	PHE
1	A	286	LYS
1	B	180	PHE

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Mol	Chain	Res	Type
1	B	286	LYS
1	C	180	PHE

### 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	365/384 (95%)	326 (89%)	39 (11%)	6	20
1	B	365/384 (95%)	326 (89%)	39 (11%)	6	20
1	C	365/384 (95%)	326 (89%)	39 (11%)	6	20
1	D	365/384 (95%)	326 (89%)	39 (11%)	6	20
1	E	365/384 (95%)	326 (89%)	39 (11%)	6	20
1	F	365/384 (95%)	326 (89%)	39 (11%)	6	20
1	G	365/384 (95%)	326 (89%)	39 (11%)	6	20
1	H	365/384 (95%)	326 (89%)	39 (11%)	6	20
1	I	365/384 (95%)	326 (89%)	39 (11%)	6	20
1	J	365/384 (95%)	326 (89%)	39 (11%)	6	20
1	K	365/384 (95%)	326 (89%)	39 (11%)	6	20
1	L	365/384 (95%)	326 (89%)	39 (11%)	6	20
All	All	4380/4608 (95%)	3912 (89%)	468 (11%)	6	20

5 of 468 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	143	SER
1	G	339	ARG
1	L	33	ILE
1	F	314	PRO
1	G	33	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	189	GLN
1	G	219	ASN
1	L	30	HIS
1	F	219	ASN
1	G	30	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 24 are monoatomic - leaving 12 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	$\# Z  > 2$
3	AMP	B	472	-	22,25,25	1.17	3 (13%)	25,38,38	1.10	2 (8%)
3	AMP	F	476	-	22,25,25	1.17	3 (13%)	25,38,38	1.10	2 (8%)
3	AMP	K	481	-	22,25,25	1.17	3 (13%)	25,38,38	1.10	2 (8%)
3	AMP	C	473	-	22,25,25	1.17	3 (13%)	25,38,38	1.10	2 (8%)
3	AMP	H	478	-	22,25,25	1.17	3 (13%)	25,38,38	1.11	2 (8%)
3	AMP	J	480	-	22,25,25	1.17	2 (9%)	25,38,38	1.10	2 (8%)
3	AMP	I	479	-	22,25,25	1.17	2 (9%)	25,38,38	1.10	2 (8%)
3	AMP	D	474	-	22,25,25	1.17	3 (13%)	25,38,38	1.10	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	AMP	G	477	-	22,25,25	1.18	3 (13%)	25,38,38	1.10	2 (8%)
3	AMP	A	471	-	22,25,25	1.17	3 (13%)	25,38,38	1.10	2 (8%)
3	AMP	L	482	-	22,25,25	1.17	2 (9%)	25,38,38	1.11	2 (8%)
3	AMP	E	475	-	22,25,25	1.18	3 (13%)	25,38,38	1.11	2 (8%)

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
3	AMP	B	472	-	-	5/6/26/26	0/3/3/3
3	AMP	F	476	-	-	5/6/26/26	0/3/3/3
3	AMP	K	481	-	-	5/6/26/26	0/3/3/3
3	AMP	C	473	-	-	5/6/26/26	0/3/3/3
3	AMP	H	478	-	-	5/6/26/26	0/3/3/3
3	AMP	J	480	-	-	5/6/26/26	0/3/3/3
3	AMP	I	479	-	-	5/6/26/26	0/3/3/3
3	AMP	D	474	-	-	5/6/26/26	0/3/3/3
3	AMP	G	477	-	-	5/6/26/26	0/3/3/3
3	AMP	A	471	-	-	5/6/26/26	0/3/3/3
3	AMP	L	482	-	-	5/6/26/26	0/3/3/3
3	AMP	E	475	-	-	5/6/26/26	0/3/3/3

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	478	AMP	P-O1P	2.89	1.59	1.50
3	L	482	AMP	P-O1P	2.88	1.59	1.50
3	F	476	AMP	P-O1P	2.88	1.59	1.50
3	E	475	AMP	P-O1P	2.88	1.59	1.50
3	I	479	AMP	P-O1P	2.88	1.59	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	482	AMP	O3'-C3'-C4'	-2.11	104.94	111.05
3	J	480	AMP	O3'-C3'-C4'	-2.10	104.96	111.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	478	AMP	O3'-C3'-C4'	-2.10	104.97	111.05
3	B	472	AMP	O3'-C3'-C4'	-2.10	104.97	111.05
3	C	473	AMP	O3'-C3'-C4'	-2.10	104.99	111.05

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	473	AMP	C5'-O5'-P-O1P
3	C	473	AMP	C5'-O5'-P-O2P
3	C	473	AMP	C5'-O5'-P-O3P
3	C	473	AMP	O4'-C4'-C5'-O5'
3	C	473	AMP	C3'-C4'-C5'-O5'

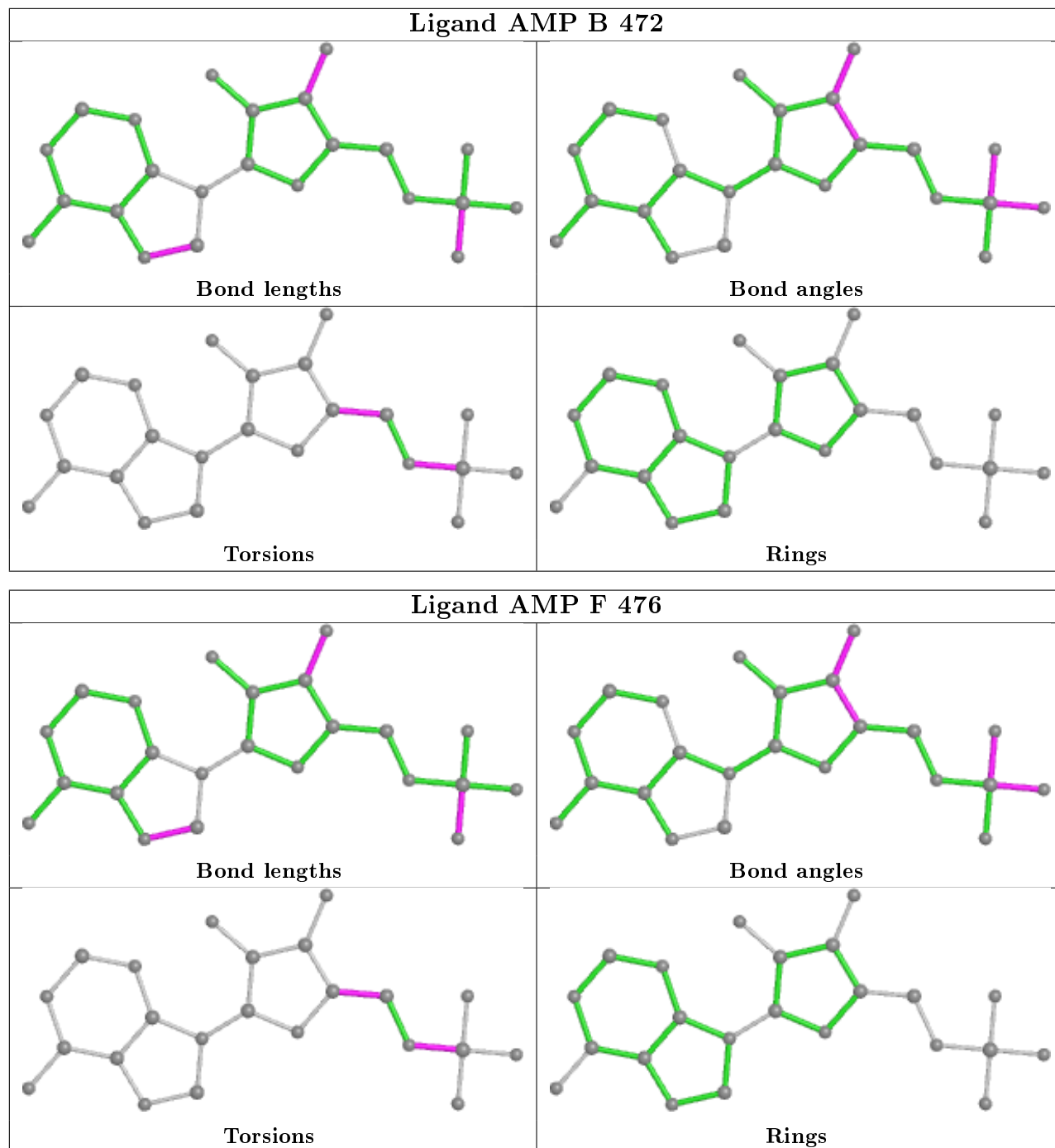
There are no ring outliers.

12 monomers are involved in 28 short contacts:

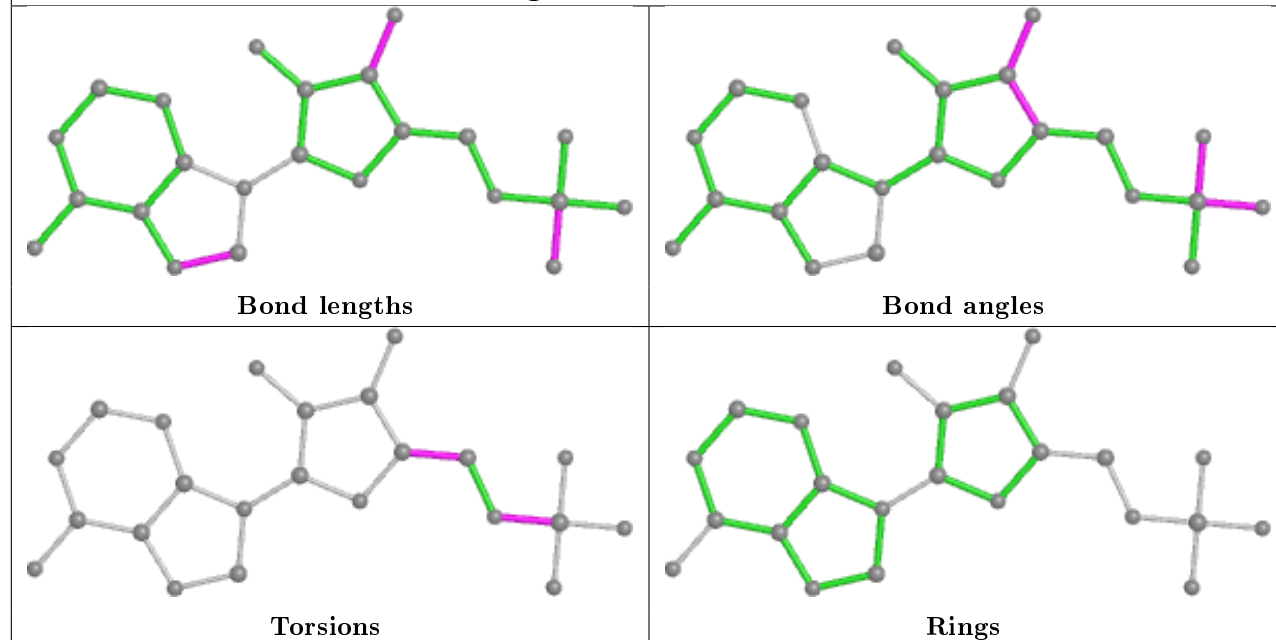
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	472	AMP	2	0
3	F	476	AMP	2	0
3	K	481	AMP	3	0
3	C	473	AMP	2	0
3	H	478	AMP	3	0
3	J	480	AMP	2	0
3	I	479	AMP	3	0
3	D	474	AMP	3	0
3	G	477	AMP	2	0
3	A	471	AMP	2	0
3	L	482	AMP	2	0
3	E	475	AMP	2	0

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

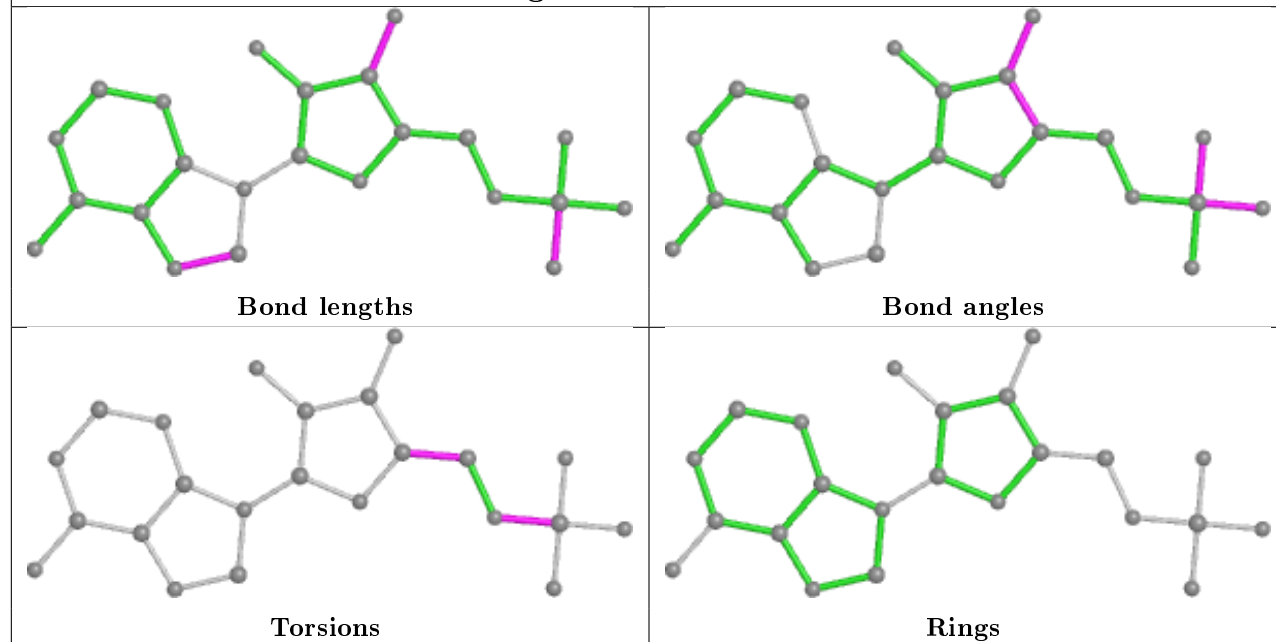
equivalents in the CSD to analyse the geometry.



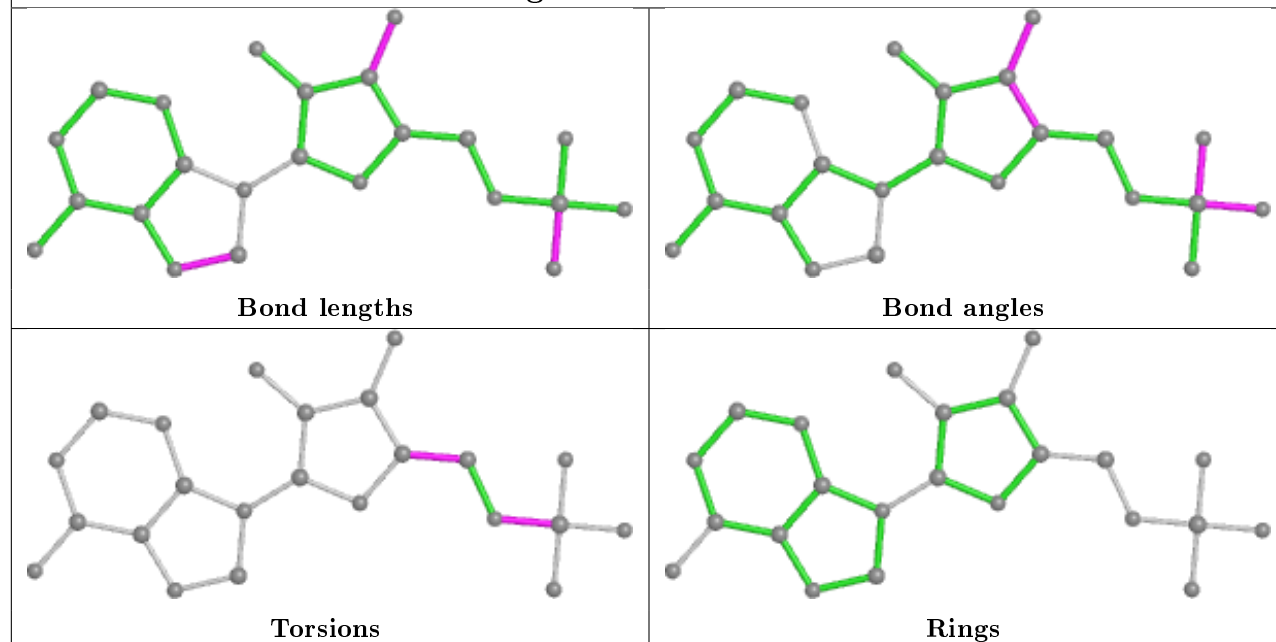
## Ligand AMP K 481



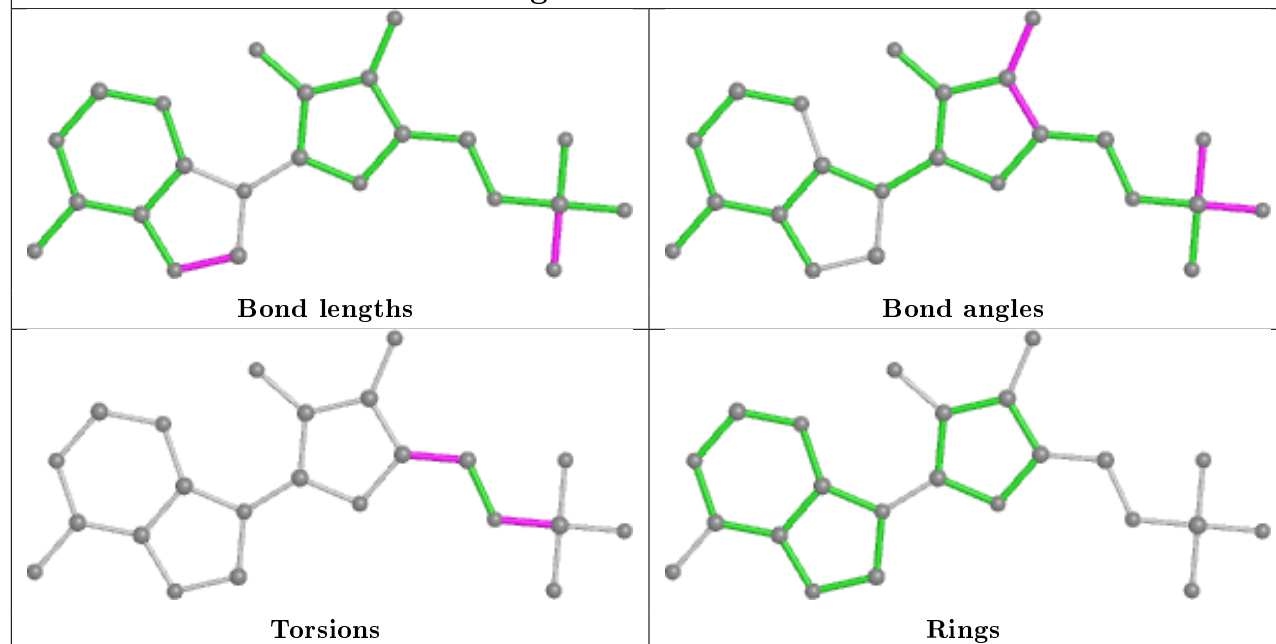
## Ligand AMP C 473



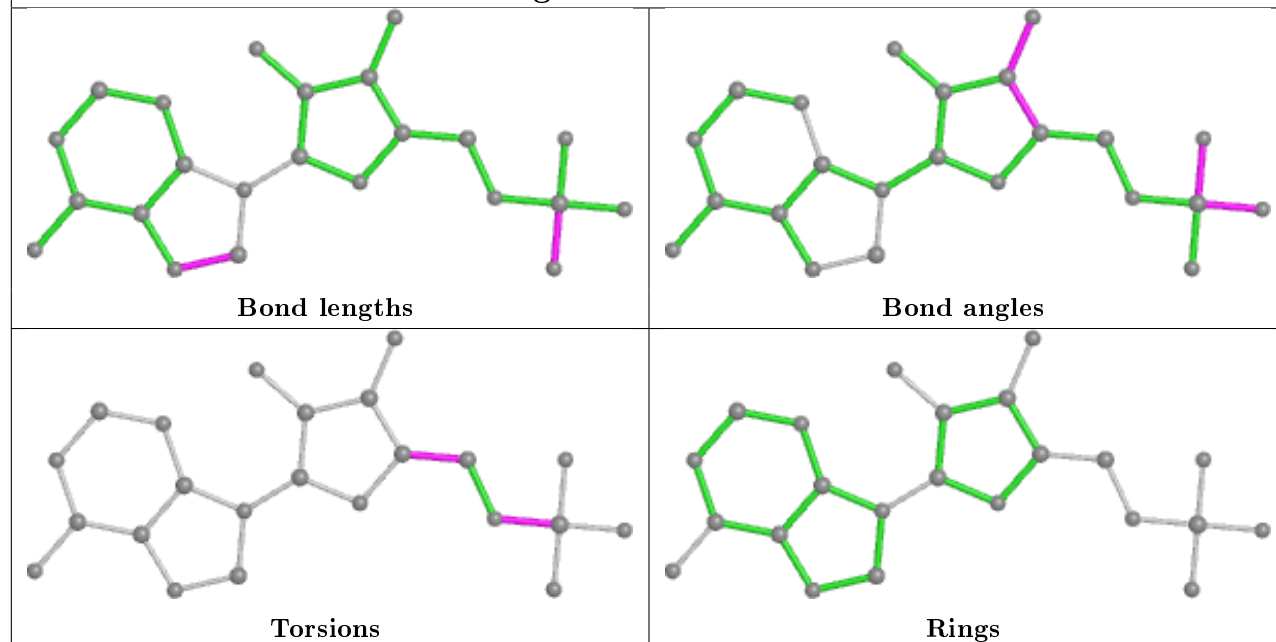
## Ligand AMP H 478



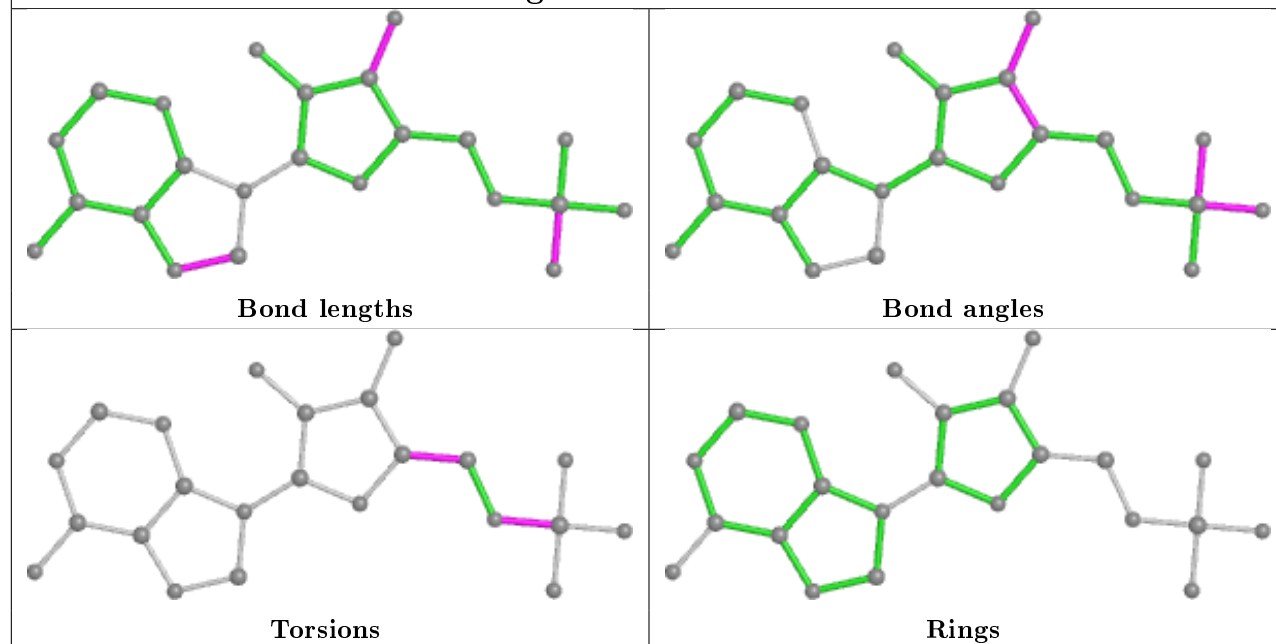
## Ligand AMP J 480



## Ligand AMP I 479

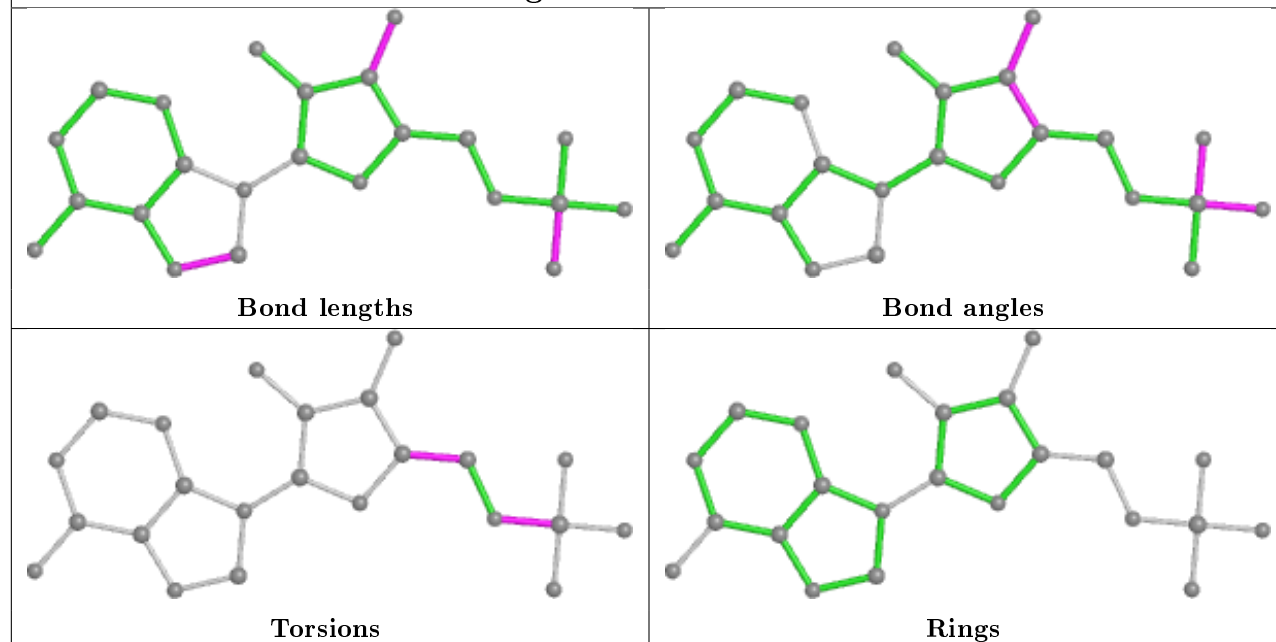


## Ligand AMP D 474

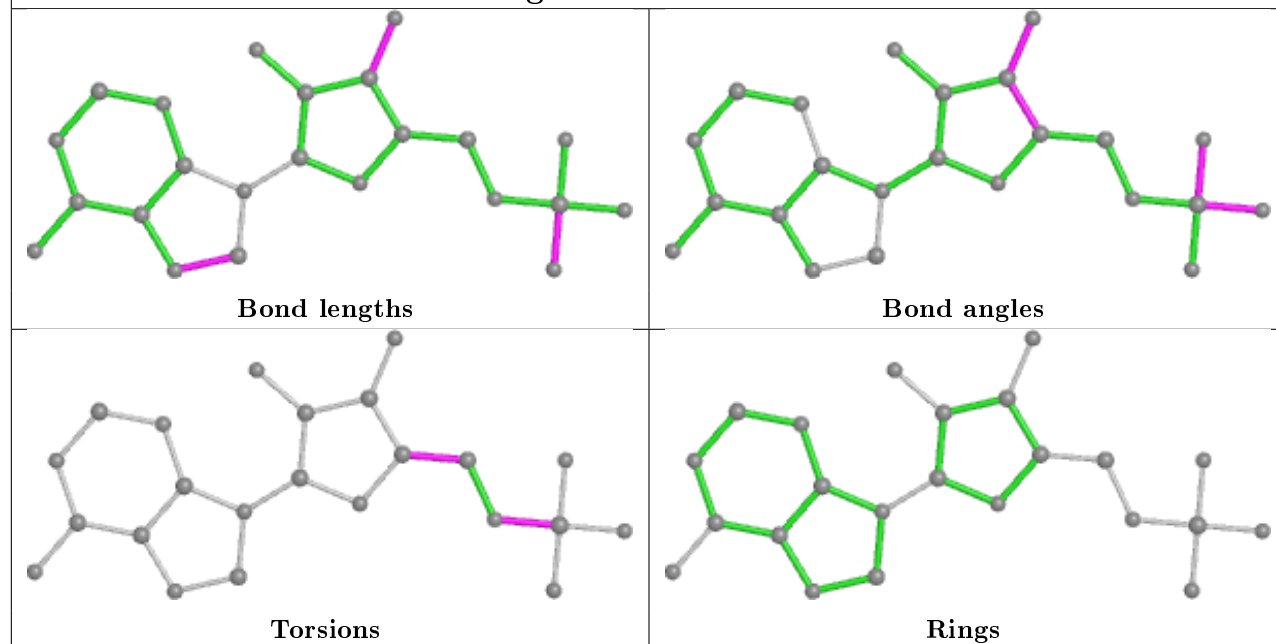


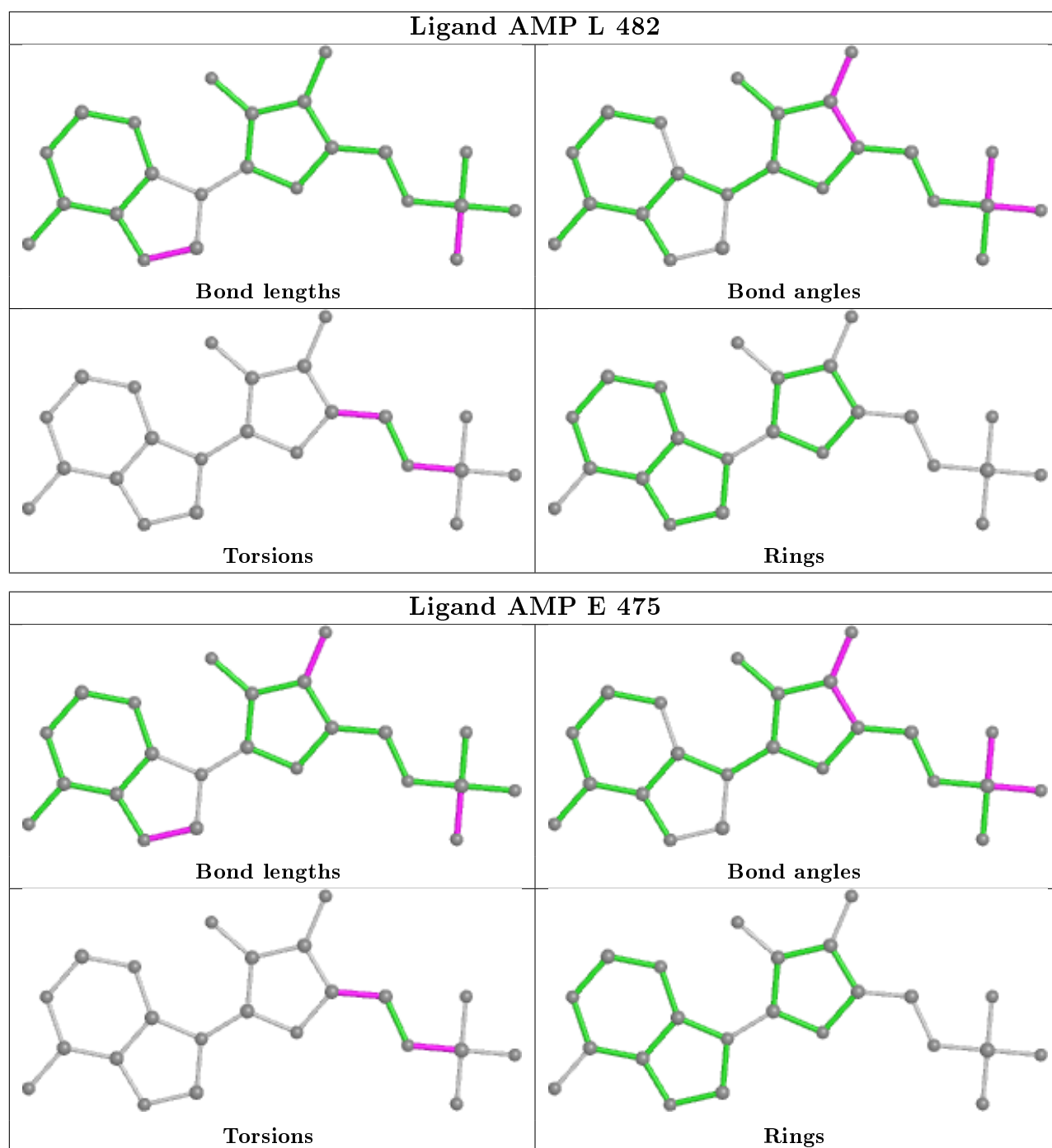


## Ligand AMP G 477



## Ligand AMP A 471





## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.