



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:22 AM UTC

PDB ID : 1GPH / pdb\_00001gph  
Title : STRUCTURE OF THE ALLOSTERIC REGULATORY ENZYME OF PURINE BIOSYNTHESIS  
Authors : Smith, J.L.  
Deposited on : 1994-04-20  
Resolution : 3.00 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

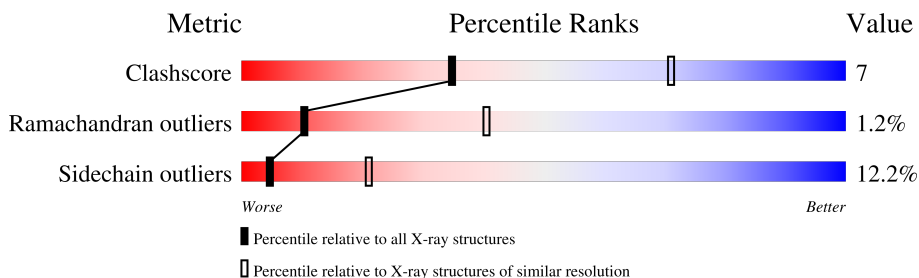
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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  $\geq 3$ , 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	1	465	
1	2	465	
1	3	465	
1	4	465	

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	SF4	1	466	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14676 atoms, of which 304 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 PHOSPHORIBOSYL-PYROPHOSPHATE AMIDOTRANSFERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	1	465	3615	2212	76	620	687	20	0	0	0
1	2	465	3615	2212	76	620	687	20	0	0	0
1	3	465	3615	2212	76	620	687	20	0	0	0
1	4	465	3615	2212	76	620	687	20	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

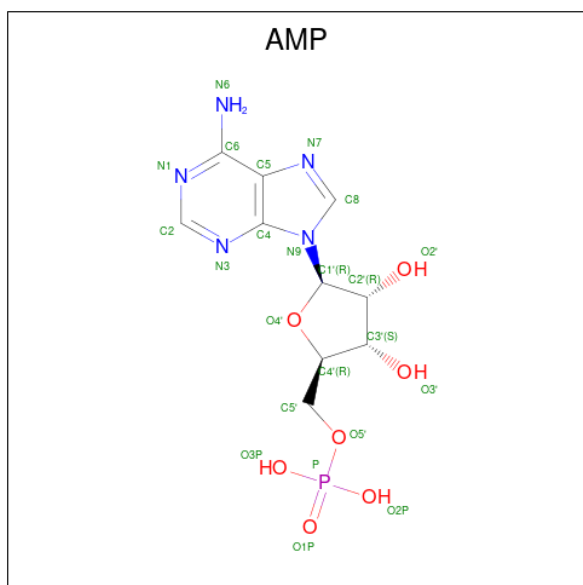
Chain	Residue	Modelled	Actual	Comment	Reference
1	402	ASP	GLY	conflict	UNP P00497
2	402	ASP	GLY	conflict	UNP P00497
3	402	ASP	GLY	conflict	UNP P00497
4	402	ASP	GLY	conflict	UNP P00497

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1	1	Total Fe S 8 4 4	0	0
2	2	1	Total Fe S 8 4 4	0	0
2	3	1	Total Fe S 8 4 4	0	0
2	4	1	Total Fe S 8 4 4	0	0

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula:  $C_{10}H_{14}N_5O_7P$ ).



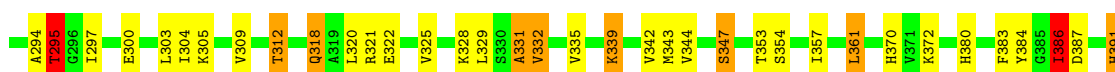
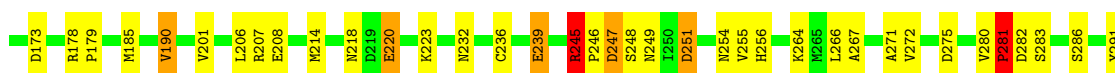
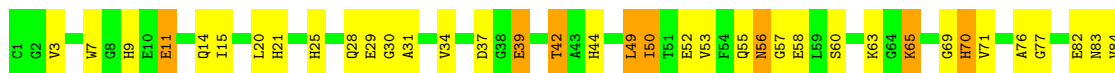
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	1	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4	1	Total 23	C 10	N 5	O 7	P 1	0	0





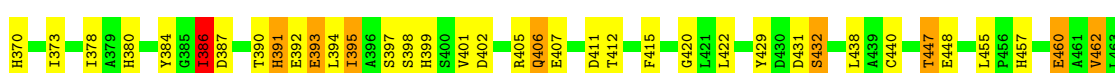
• Molecule 1: GLUTAMINE PHOSPHORIBOSYL-PYROPHOSPHATE AMIDOTRANSFERASE

Chain 3: 63% 31% 5%



• Molecule 1: GLUTAMINE PHOSPHORIBOSYL-PYROPHOSPHATE AMIDOTRANSFERASE

Chain 4: 59% 30% 9%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.80Å 75.70Å 94.10Å 90.00° 91.40° 90.00°	Depositor
Resolution (Å)	7.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	14676	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

## 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: SF4, AMP

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	1	1.13	32/3597 (0.9%)	1.97	118/4857 (2.4%)
1	2	1.09	28/3597 (0.8%)	1.92	105/4857 (2.2%)
1	3	1.08	26/3597 (0.7%)	1.95	112/4857 (2.3%)
1	4	1.08	28/3597 (0.8%)	1.93	115/4857 (2.4%)
All	All	1.10	114/14388 (0.8%)	1.95	450/19428 (2.3%)

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	1	0	1

The worst 5 of 114 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	370	HIS	CD2-NE2	-7.73	1.29	1.37
1	1	25	HIS	CD2-NE2	-7.68	1.29	1.37
1	4	332	VAL	CA-CB	7.57	1.62	1.53
1	3	70	HIS	CD2-NE2	-7.51	1.29	1.37
1	2	25	HIS	CD2-NE2	-7.29	1.29	1.37

The worst 5 of 450 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	118	GLN	OE1-CD-NE2	-13.84	108.76	122.60
1	3	57	GLY	N-CA-C	-13.57	99.06	113.58
1	2	430	ASP	CA-CB-CG	10.91	123.51	112.60
1	1	281	PRO	O-C-N	10.34	136.60	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	295	THR	N-CA-CB	-10.19	94.61	110.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	18	TYR	Sidechain

## 5.2 Too-close contacts [i](#)

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	1	3539	76	3524	52	0
1	2	3539	76	3524	50	0
1	3	3539	76	3524	57	0
1	4	3539	76	3524	66	0
2	1	8	0	0	2	0
2	2	8	0	0	0	0
2	3	8	0	0	0	0
2	4	8	0	0	0	0
3	1	46	0	24	2	0
3	2	46	0	24	0	0
3	3	46	0	24	1	0
3	4	46	0	24	1	0
All	All	14372	304	14192	214	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 7.

The worst 5 of 214 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)
1:4:275:ASP:HB2	1:4:339:LYS:HG3	1.61	0.82
1:4:41:LEU:HD12	1:4:88:LEU:HD21	1.63	0.81
1:4:316:PRO:HG2	1:4:321:ARG:HD3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:264:LYS:HG2	1:3:294:ALA:HB2	1.69	0.74
1:1:291:TYR:O	1:1:295:THR:HB	1.92	0.68

There are no symmetry-related clashes.

## 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	1	463/465 (100%)	436 (94%)	19 (4%)	8 (2%)	7	32
1	2	463/465 (100%)	433 (94%)	23 (5%)	7 (2%)	8	35
1	3	463/465 (100%)	437 (94%)	23 (5%)	3 (1%)	21	56
1	4	463/465 (100%)	434 (94%)	24 (5%)	5 (1%)	11	43
All	All	1852/1860 (100%)	1740 (94%)	89 (5%)	23 (1%)	10	40

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	56	ASN
1	2	282	ASP
1	2	431	ASP
1	3	94	ASN
1	4	56	ASN

### 5.3.2 Protein sidechains [i](#)

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	1	382/382 (100%)	332 (87%)	50 (13%)	4	19
1	2	382/382 (100%)	338 (88%)	44 (12%)	5	24
1	3	382/382 (100%)	337 (88%)	45 (12%)	5	22
1	4	382/382 (100%)	335 (88%)	47 (12%)	4	21
All	All	1528/1528 (100%)	1342 (88%)	186 (12%)	5	21

5 of 186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3	223	LYS
1	4	60	SER
1	3	272	VAL
1	3	386	ILE
1	4	121	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	2	391	HIS
1	3	55	GLN
1	4	380	HIS
1	2	436	GLN
1	3	123	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

12 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	SF4	4	466	1	0,12,12	-	-	-		
3	AMP	4	467	-	25,25,25	0.79	0	37,38,38	0.93	1 (2%)
3	AMP	1	467	-	25,25,25	1.00	2 (8%)	37,38,38	1.48	7 (18%)
2	SF4	1	466	1	0,12,12	-	-	-		
3	AMP	4	468	-	25,25,25	0.89	1 (4%)	37,38,38	1.08	3 (8%)
2	SF4	2	466	1	0,12,12	-	-	-		
2	SF4	3	466	1	0,12,12	-	-	-		
3	AMP	1	468	-	25,25,25	1.04	1 (4%)	37,38,38	0.96	1 (2%)
3	AMP	3	467	-	25,25,25	1.02	3 (12%)	37,38,38	1.12	4 (10%)
3	AMP	3	468	-	25,25,25	0.90	0	37,38,38	1.12	3 (8%)
3	AMP	2	468	-	25,25,25	1.24	2 (8%)	37,38,38	1.25	4 (10%)
3	AMP	2	467	-	25,25,25	0.97	2 (8%)	37,38,38	1.26	4 (10%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	4	466	1	-	-	0/6/5/5
3	AMP	4	467	-	-	3/10/26/26	0/3/3/3
3	AMP	1	467	-	-	3/10/26/26	0/3/3/3
2	SF4	1	466	1	-	-	0/6/5/5
3	AMP	4	468	-	-	3/10/26/26	0/3/3/3
3	AMP	3	467	-	-	1/10/26/26	0/3/3/3
3	AMP	1	468	-	-	4/10/26/26	0/3/3/3
2	SF4	2	466	1	-	-	0/6/5/5
2	SF4	3	466	1	-	-	0/6/5/5
3	AMP	3	468	-	-	4/10/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	2	468	-	-	2/10/26/26	0/3/3/3
3	AMP	2	467	-	-	1/10/26/26	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1	468	AMP	P-O3P	-2.37	1.46	1.54
3	1	467	AMP	O3'-C3'	2.29	1.48	1.43
3	3	467	AMP	O4'-C4'	-2.25	1.40	1.45
3	2	468	AMP	C3'-C4'	-2.21	1.47	1.53
3	2	468	AMP	C2'-C1'	-2.21	1.46	1.53

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1	467	AMP	C3'-C2'-C1'	4.41	109.80	101.46
3	2	468	AMP	O3'-C3'-C4'	-3.66	100.56	111.08
3	1	467	AMP	C5'-C4'-C3'	3.39	127.42	115.21
3	2	468	AMP	O4'-C1'-N9	3.15	114.13	108.09
3	3	468	AMP	C3'-C2'-C1'	3.00	107.13	101.46

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	1	467	AMP	C5'-O5'-P-O2P
3	1	467	AMP	C5'-O5'-P-O3P
3	3	468	AMP	C5'-O5'-P-O2P
3	3	468	AMP	C5'-O5'-P-O3P
3	4	467	AMP	C5'-O5'-P-O2P

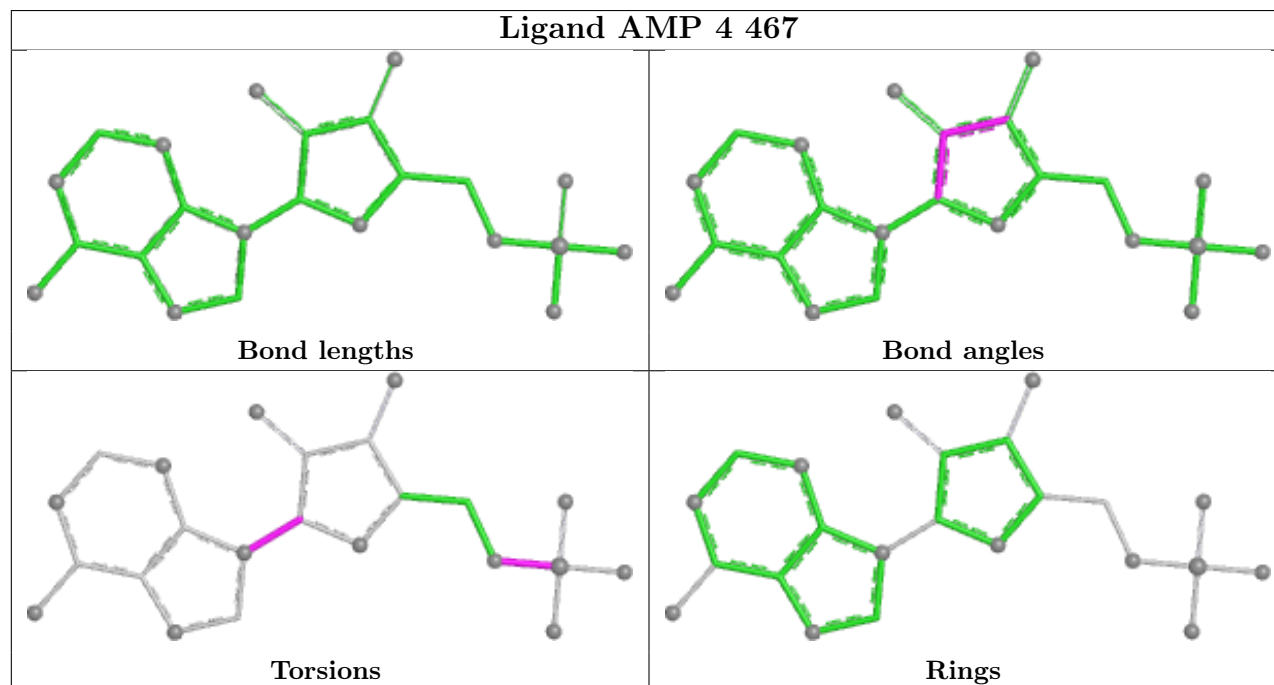
There are no ring outliers.

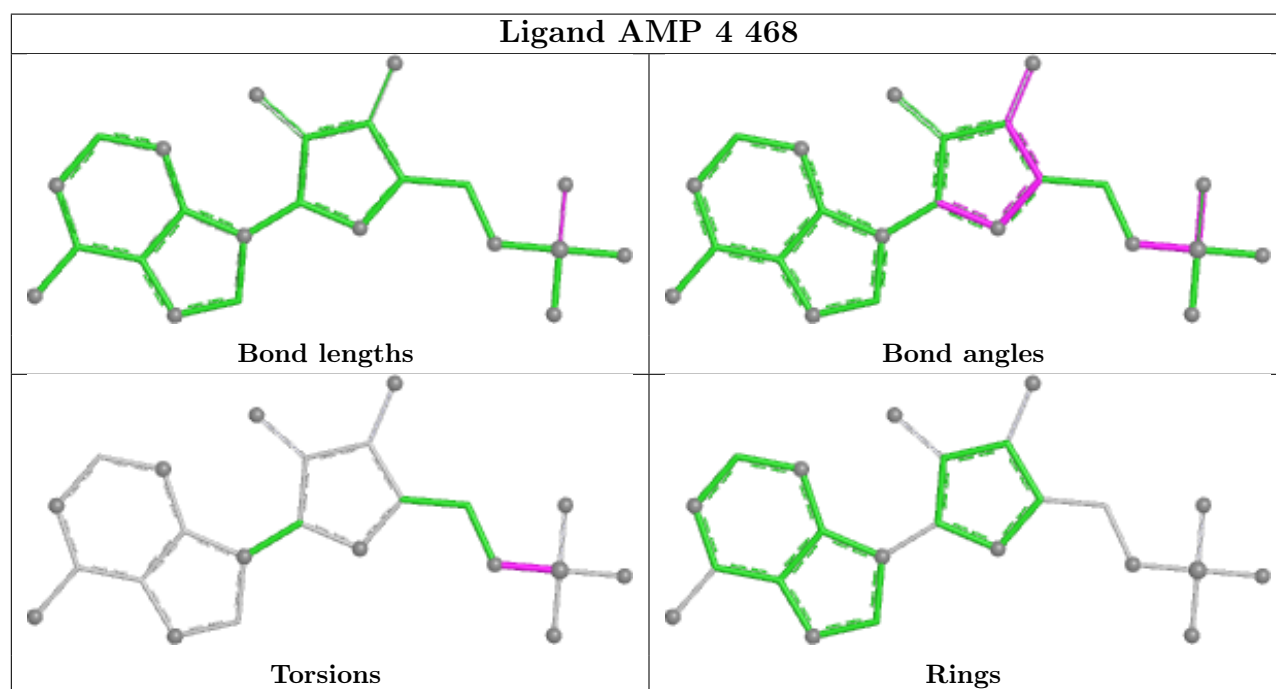
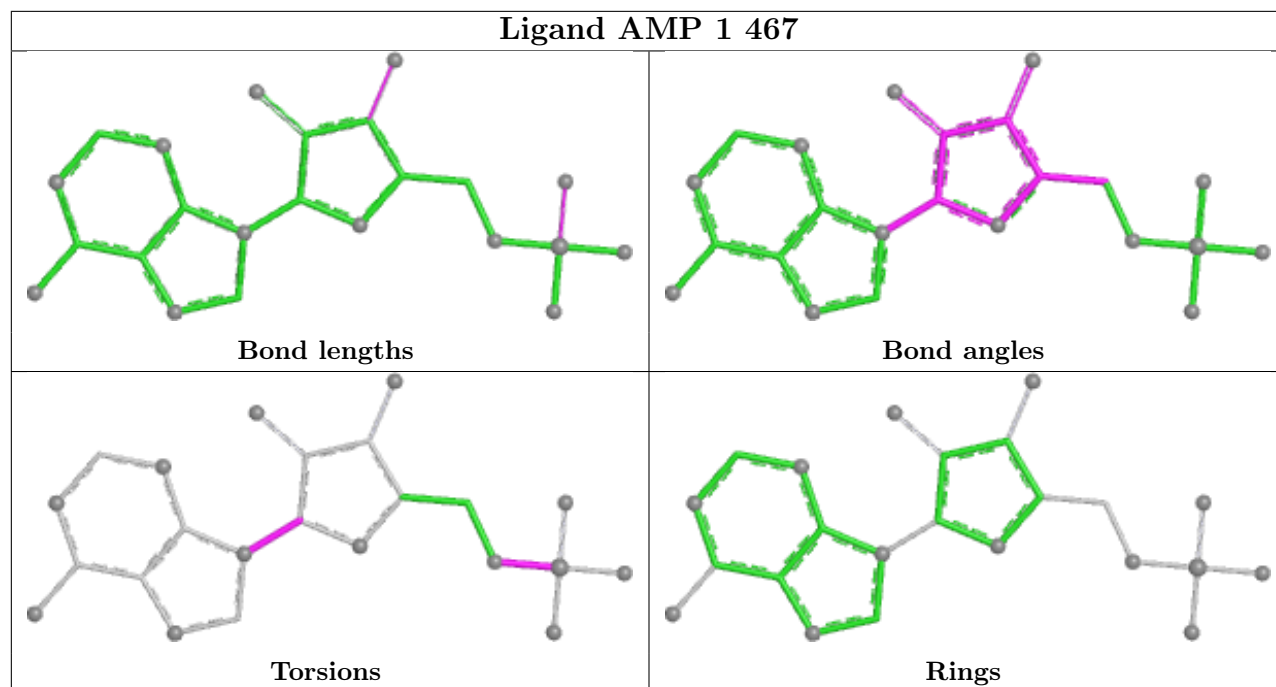
4 monomers are involved in 6 short contacts:

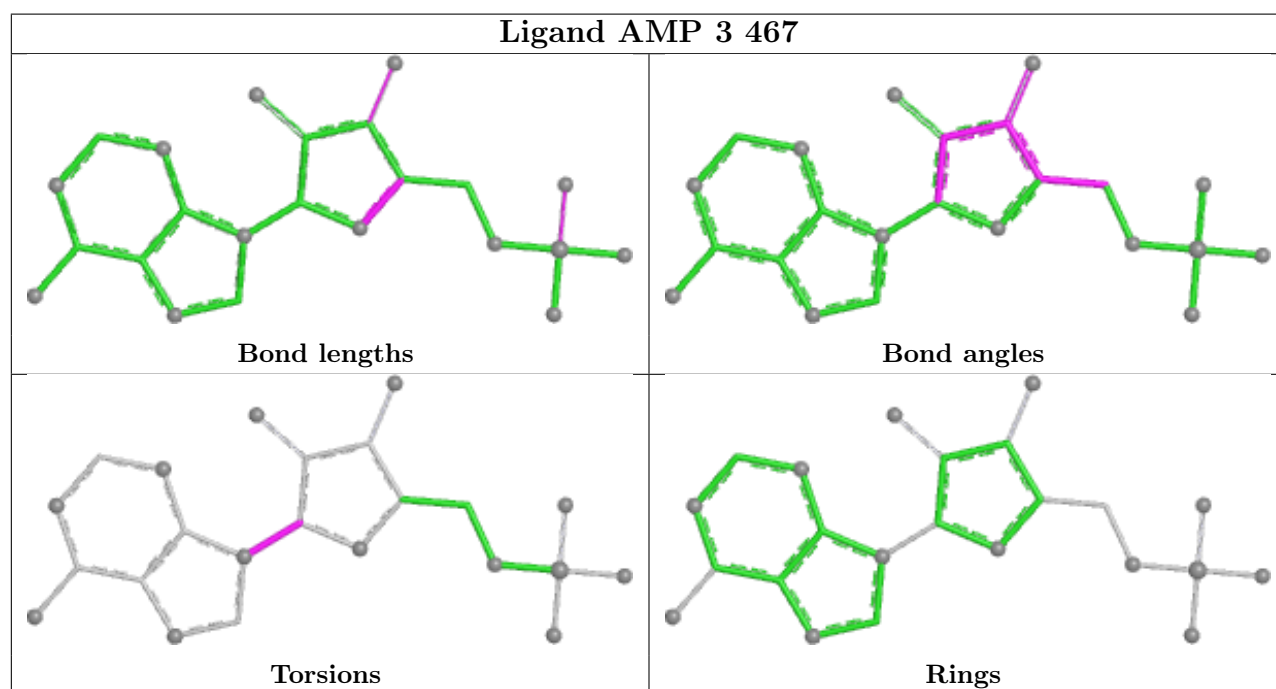
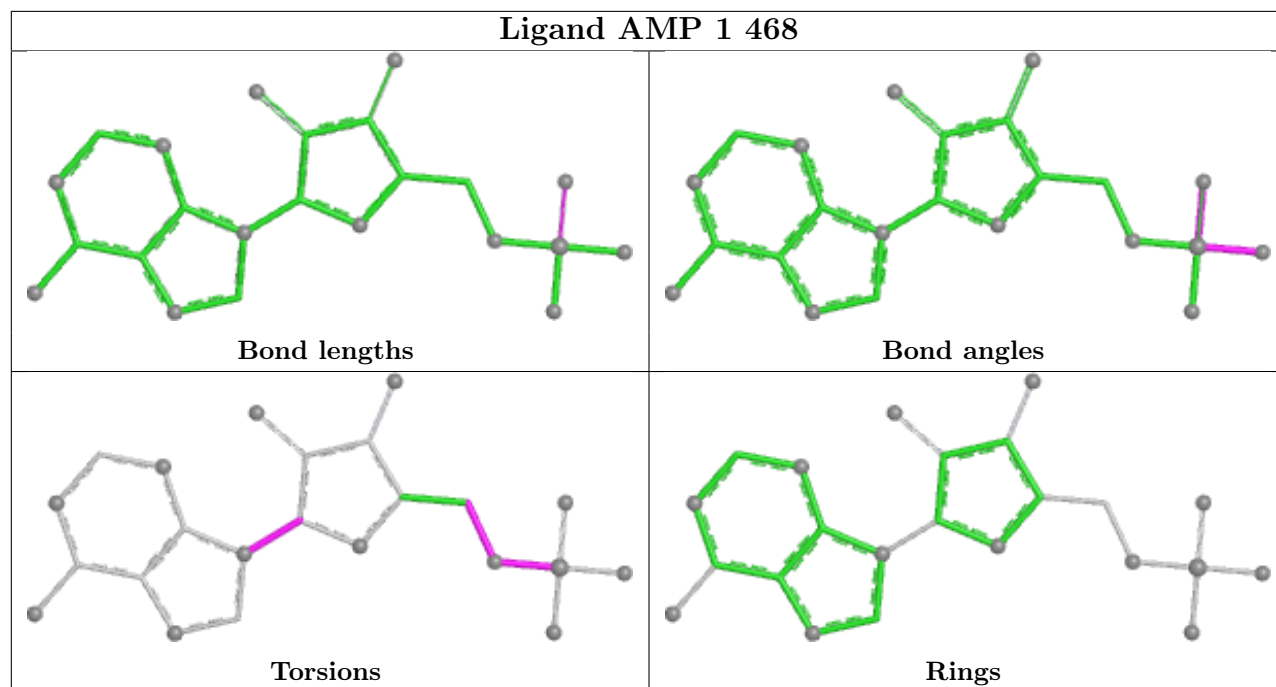
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1	466	SF4	2	0
3	4	468	AMP	1	0
3	1	468	AMP	2	0
3	3	467	AMP	1	0

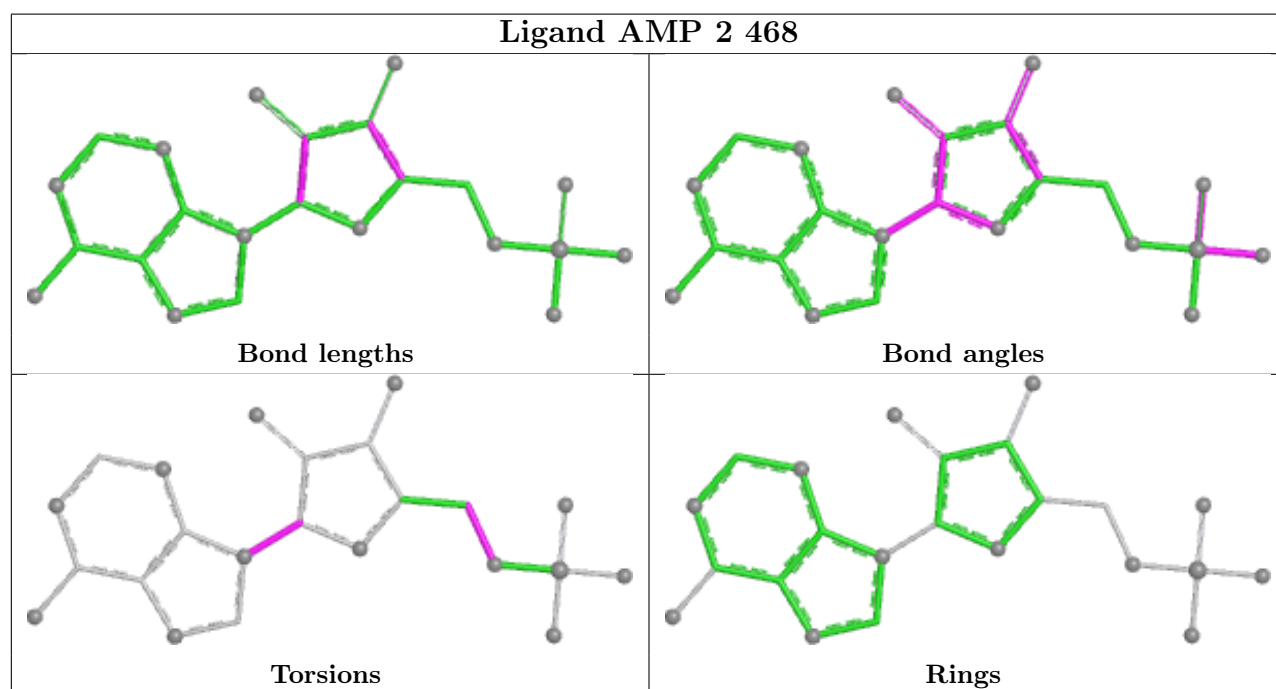
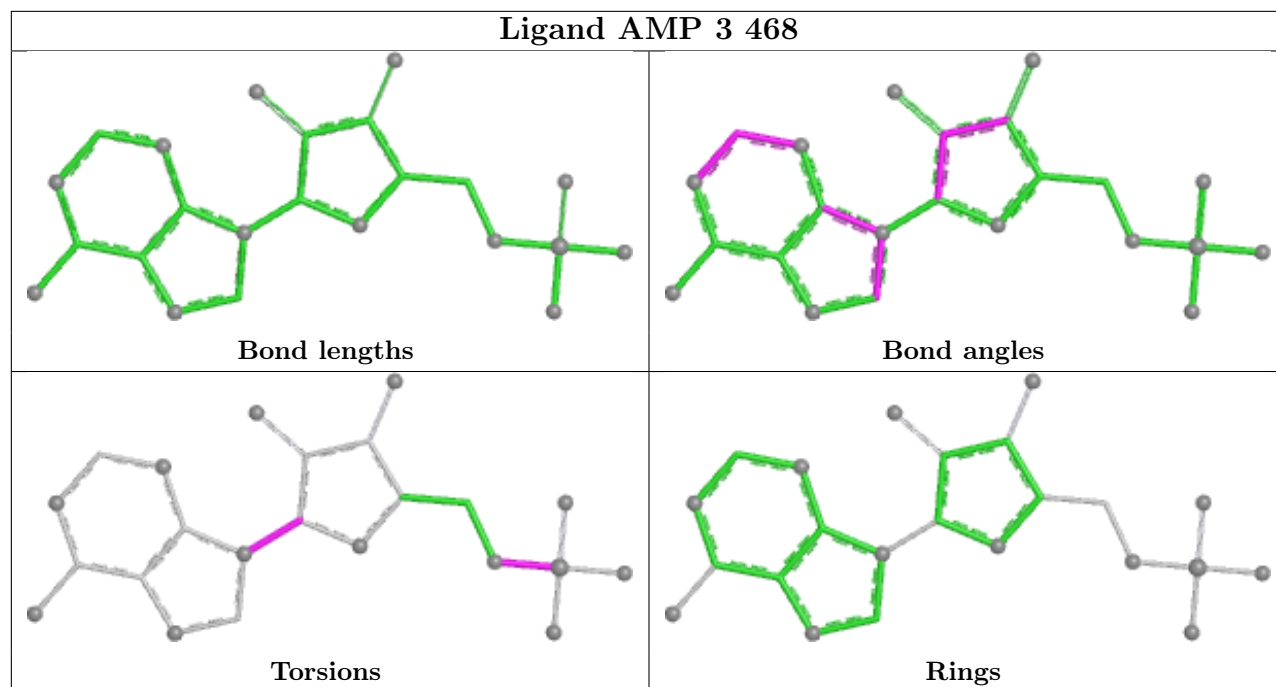
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

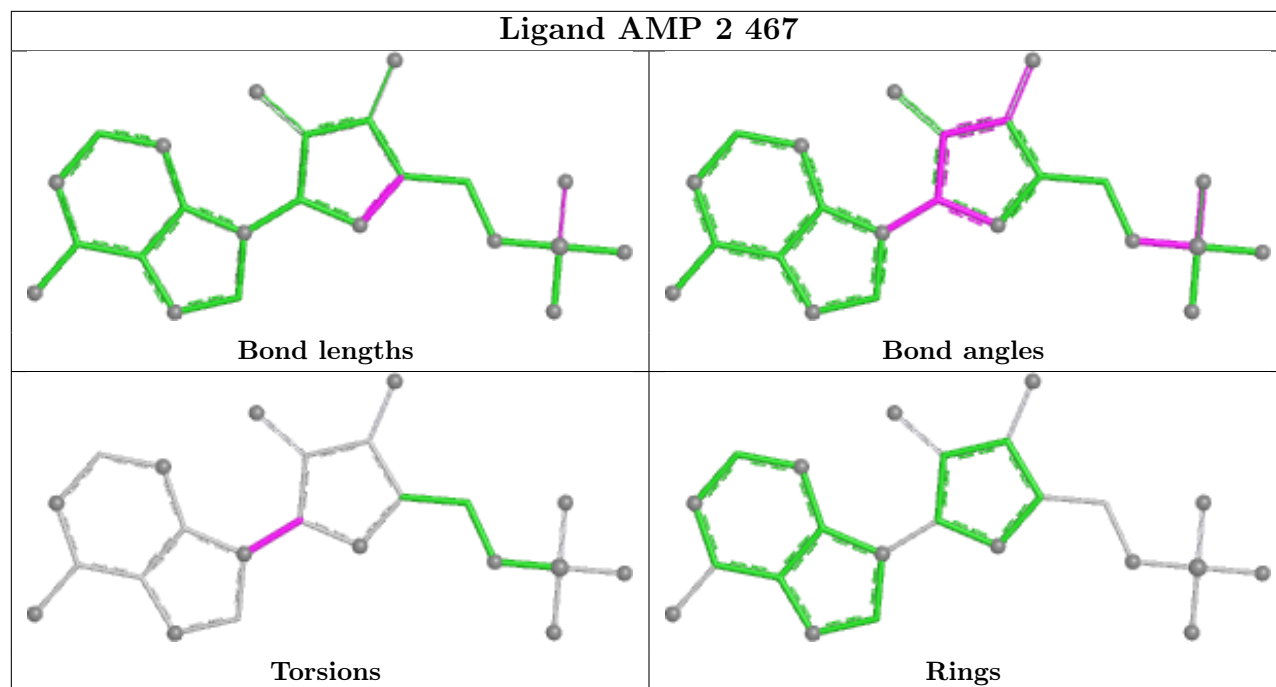
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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

### 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.