



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 27, 2020 – 12:20 am BST

PDB ID : 4FBP  
Title : CONFORMATIONAL TRANSITION OF FRUCTOSE-1,6-BISPHOSPHATASE: STRUCTURE COMPARISON BETWEEN THE AMP COMPLEX (T FORM) AND THE FRUCTOSE 6-PHOSPHATE COMPLEX (R FORM)  
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Deposited on : 1991-02-11  
Resolution : 2.50 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

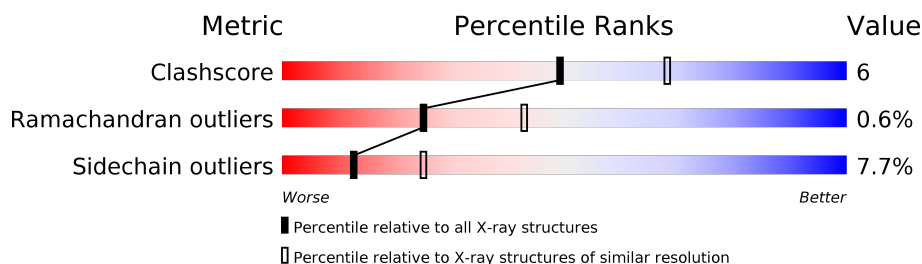
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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	335	
1	B	335	
1	C	335	
1	D	335	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12988 atoms, of which 2840 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 FRUCTOSE 1,6-BISPHOSPHATASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	318	Total	C	H	N	O	S	0	0	1
			2963	1546	536	410	456	15			
1	B	318	Total	C	H	N	O	S	0	0	1
			2963	1546	536	410	456	15			
1	C	318	Total	C	H	N	O	S	0	0	1
			2963	1546	536	410	456	15			
1	D	318	Total	C	H	N	O	S	0	0	1
			2963	1546	536	410	456	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLN	GLU	CONFLICT	UNP P00636
A	96	THR	SER	CONFLICT	UNP P00636
A	199	ASN	ASP	CONFLICT	UNP P00636
B	20	GLN	GLU	CONFLICT	UNP P00636
B	96	THR	SER	CONFLICT	UNP P00636
B	199	ASN	ASP	CONFLICT	UNP P00636
C	20	GLN	GLU	CONFLICT	UNP P00636
C	96	THR	SER	CONFLICT	UNP P00636
C	199	ASN	ASP	CONFLICT	UNP P00636
D	20	GLN	GLU	CONFLICT	UNP P00636
D	96	THR	SER	CONFLICT	UNP P00636
D	199	ASN	ASP	CONFLICT	UNP P00636

- Molecule 2 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
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is water.


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	98	Total	H	O	0	0
			294	196	98		
3	B	81	Total	H	O	0	0
			243	162	81		
3	C	81	Total	H	O	0	0
			243	162	81		
3	D	88	Total	H	O	0	0
			264	176	88		

**i**

Note EDS was not executed.

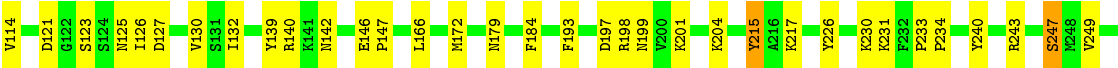
- Chain A:
- 
- 75% 18% 5%
- E300 I305 R313 I317 V324 L327 Y331 A335 S124 N125 V130 Y139 M142 S143 T144 D145 E146 E149 M182 D187 R198 K201 Y215 D220 P221 Y226 R229 K230 Y240 V249 R254 K268 A269 S270 K274 L275 R276 L277 E280 C281 K290 A291 L294 T297 G298 V299

- Chain B:
- 
- 73% 18% 5%
- Legend: 73% 18% 5%
- Residues (from top to bottom):
- TTR, ASP, GLN, ALA, PHE, ASP, THR, I9, I10, R15, F16, V17, K30, T31, L37, R49, K50, E53, A54, H55, L56, V57, G58, I59, S62, THR, ASN, VAL, THR, GLY, ASP, GLN, VAL, LYS, K72, M78, D79, L80, K86, L94, V95, T96, E97, E98, D99, I103, E106, F109
  - E108, Y113, D121, G122, S123, S124, N125, Y130, M142, D145, Q154, R157, M158, L166, T171, M179, N182, C183, F184, F193, I194, L195, R198, E218, Y226, I227, Q228, R229, K230, K231, F232, P233, P234, Y240, R243, Y244, S247, M248, V249, Y264, D265
  - K266, K267, K274, L275, E280, P283, V287, L294, K299, R313, I317, P321, V324, L327, K333, R334, A335

- Chain C: 



● Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.50Å 88.50Å 211.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12988	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	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: 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	A	0.74	0/2468	1.41	15/3337 (0.4%)
1	B	0.74	0/2468	1.43	18/3337 (0.5%)
1	C	0.73	0/2468	1.40	16/3337 (0.5%)
1	D	0.70	0/2468	1.35	18/3337 (0.5%)
All	All	0.73	0/9872	1.40	67/13348 (0.5%)

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	3
1	B	0	5
1	C	0	4
1	D	0	4
All	All	0	16

There are no bond length outliers.

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	ARG	NE-CZ-NH2	-15.13	112.73	120.30
1	C	49	ARG	NE-CZ-NH2	-13.95	113.33	120.30
1	B	49	ARG	NE-CZ-NH2	-13.62	113.49	120.30
1	B	313	ARG	NE-CZ-NH1	10.85	125.72	120.30
1	C	15	ARG	NE-CZ-NH2	-9.94	115.33	120.30

There are no chirality outliers.

5 of 16 planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	139	TYR	Sidechain
1	A	226	TYR	Sidechain
1	A	240	TYR	Sidechain
1	B	226	TYR	Sidechain
1	B	57	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	2427	536	2486	27	0
1	B	2427	536	2486	34	0
1	C	2427	536	2486	33	0
1	D	2427	536	2486	33	0
2	A	23	0	12	0	0
2	B	23	0	12	0	0
2	C	23	0	12	0	0
2	D	23	0	12	0	0
3	A	98	196	0	0	0
3	B	81	162	0	0	0
3	C	81	162	0	2	0
3	D	88	176	0	2	0
All	All	10148	2840	9992	117	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 117 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:B:125:ASN:HB3	1:B:130:VAL:HG12	1.57	0.85
1:D:126:ILE:HG12	1:D:132:ILE:HD13	1.70	0.73
1:A:125:ASN:HB3	1:A:130:VAL:HB	1.70	0.72
1:B:274:LYS:HD3	1:B:275:LEU:HD23	1.74	0.69
1:B:78:ASN:OD1	1:B:96:THR:HG21	1.94	0.68

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 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	314/335 (94%)	297 (95%)	15 (5%)	2 (1%)	25	43
1	B	314/335 (94%)	302 (96%)	12 (4%)	0	100	100
1	C	314/335 (94%)	294 (94%)	16 (5%)	4 (1%)	12	21
1	D	314/335 (94%)	295 (94%)	17 (5%)	2 (1%)	25	43
All	All	1256/1340 (94%)	1188 (95%)	60 (5%)	8 (1%)	25	43

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	270	SER
1	C	237	SER
1	A	268	LYS
1	C	207	SER
1	C	178	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	263/278 (95%)	246 (94%)	17 (6%)	17	33
1	B	263/278 (95%)	244 (93%)	19 (7%)	14	28
1	C	263/278 (95%)	235 (89%)	28 (11%)	6	13
1	D	263/278 (95%)	246 (94%)	17 (6%)	17	33
All	All	1052/1112 (95%)	971 (92%)	81 (8%)	13	25

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	30	MET
1	C	121	ASP
1	D	247	SER
1	C	37	LEU
1	C	56	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	154	GLN
1	B	182	ASN
1	D	182	ASN
1	B	179	ASN
1	B	282	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 ⓘ

4 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	AMP	D	338	-	22,25,25	1.14	3 (13%)	25,38,38	1.64	4 (16%)
2	AMP	A	338	-	22,25,25	1.10	1 (4%)	25,38,38	1.37	3 (12%)
2	AMP	C	338	-	22,25,25	1.19	3 (13%)	25,38,38	1.32	3 (12%)
2	AMP	B	338	-	22,25,25	1.08	1 (4%)	25,38,38	1.22	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
2	AMP	D	338	-	-	1/6/26/26	0/3/3/3
2	AMP	A	338	-	-	0/6/26/26	0/3/3/3
2	AMP	C	338	-	-	0/6/26/26	0/3/3/3
2	AMP	B	338	-	-	0/6/26/26	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	338	AMP	C2-N3	3.45	1.37	1.32
2	C	338	AMP	C2-N3	3.33	1.37	1.32
2	A	338	AMP	C2-N3	3.26	1.37	1.32
2	B	338	AMP	C2-N3	3.21	1.37	1.32
2	C	338	AMP	C5'-C4'	-2.31	1.44	1.51

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	338	AMP	N3-C2-N1	-5.12	120.68	128.68
2	A	338	AMP	N3-C2-N1	-3.73	122.86	128.68
2	C	338	AMP	N3-C2-N1	-3.52	123.18	128.68
2	D	338	AMP	C5-C6-N1	-3.47	112.49	120.35
2	B	338	AMP	O2P-P-O5'	3.31	115.53	106.73

There are no chirality outliers.

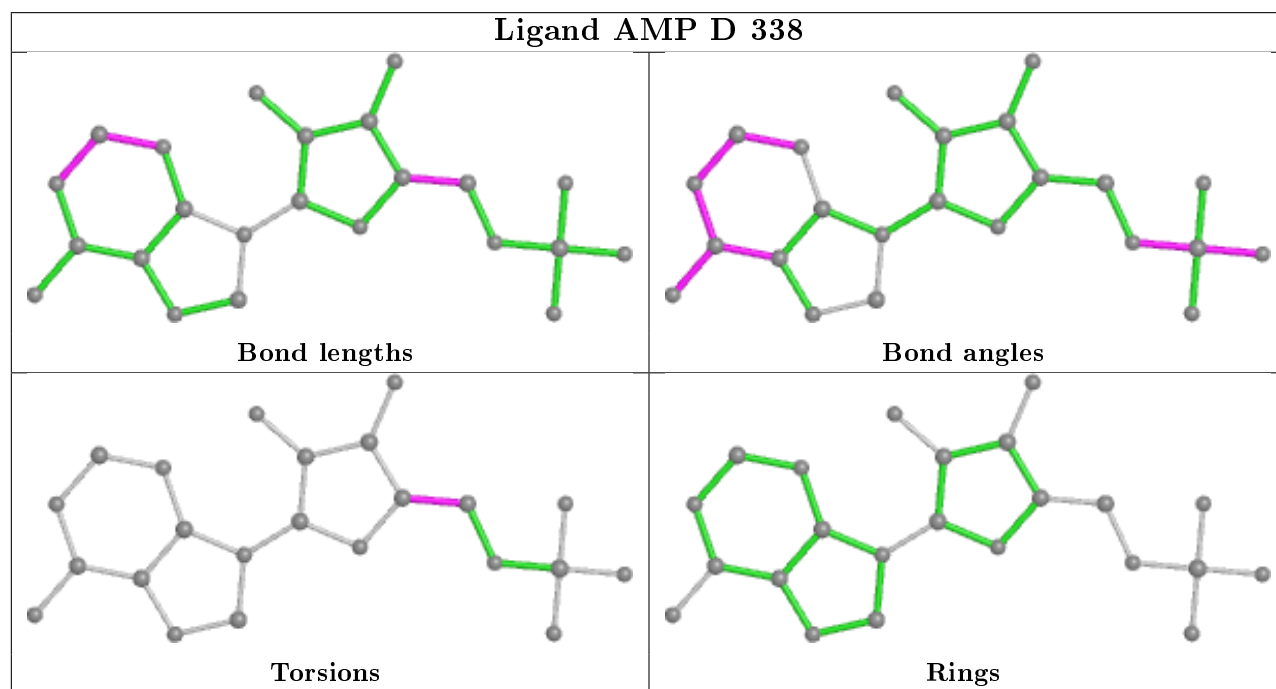
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	338	AMP	O4'-C4'-C5'-O5'

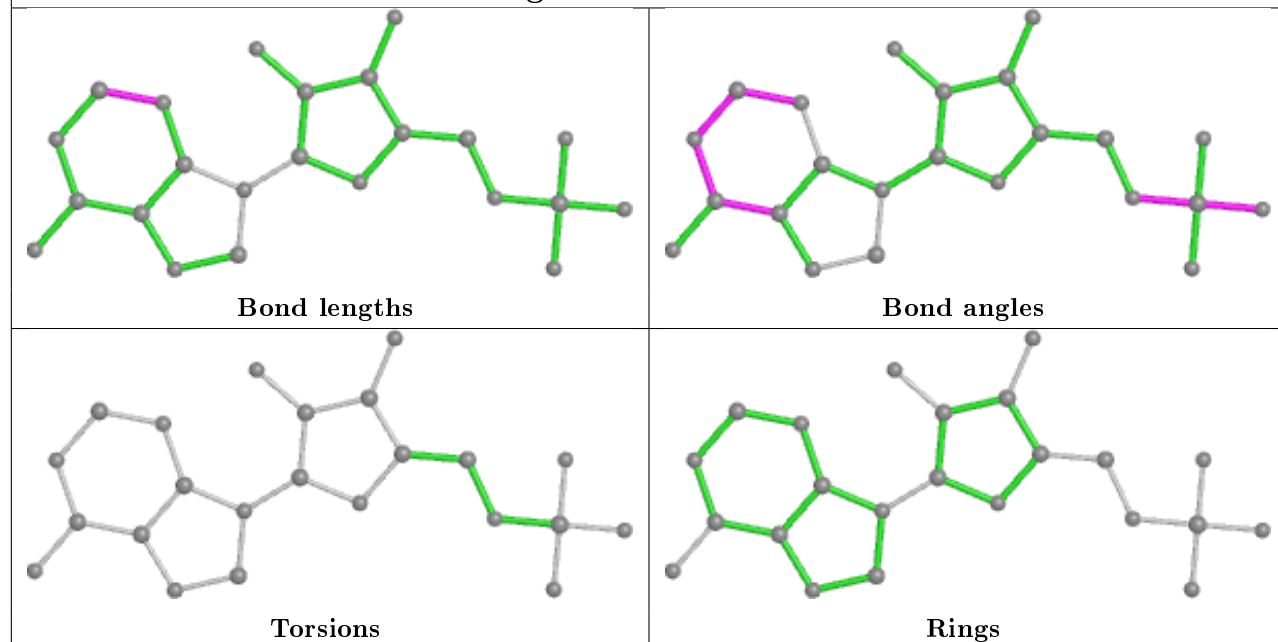
There are no ring outliers.

No monomer is involved in short contacts.

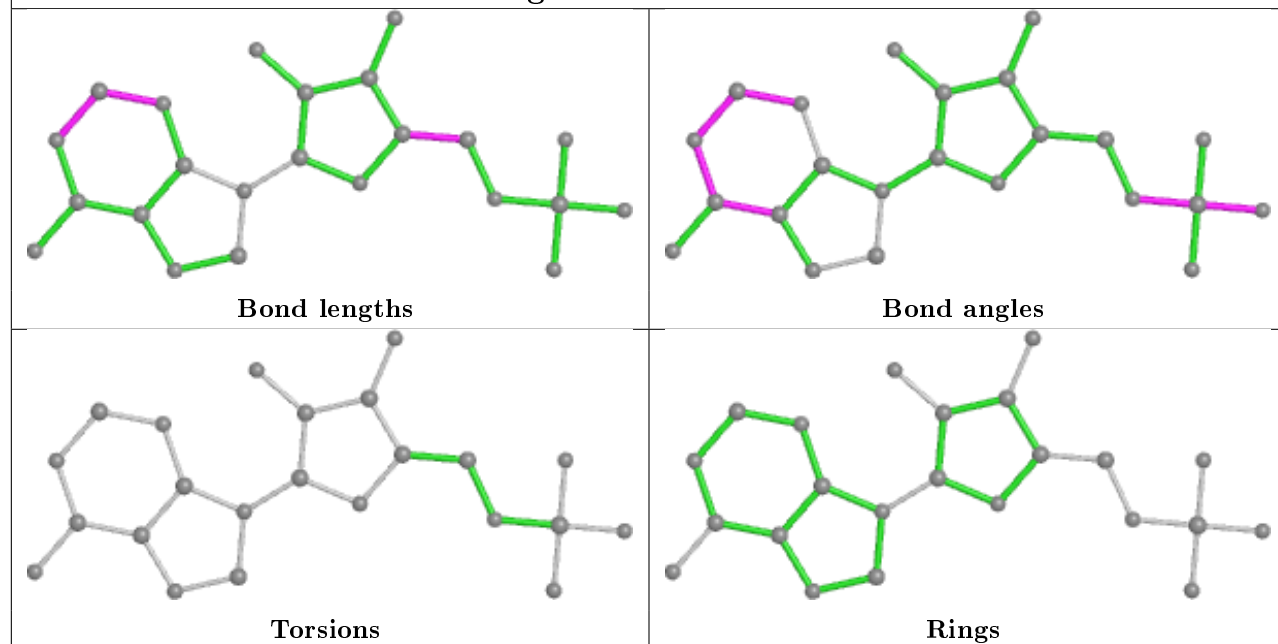
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

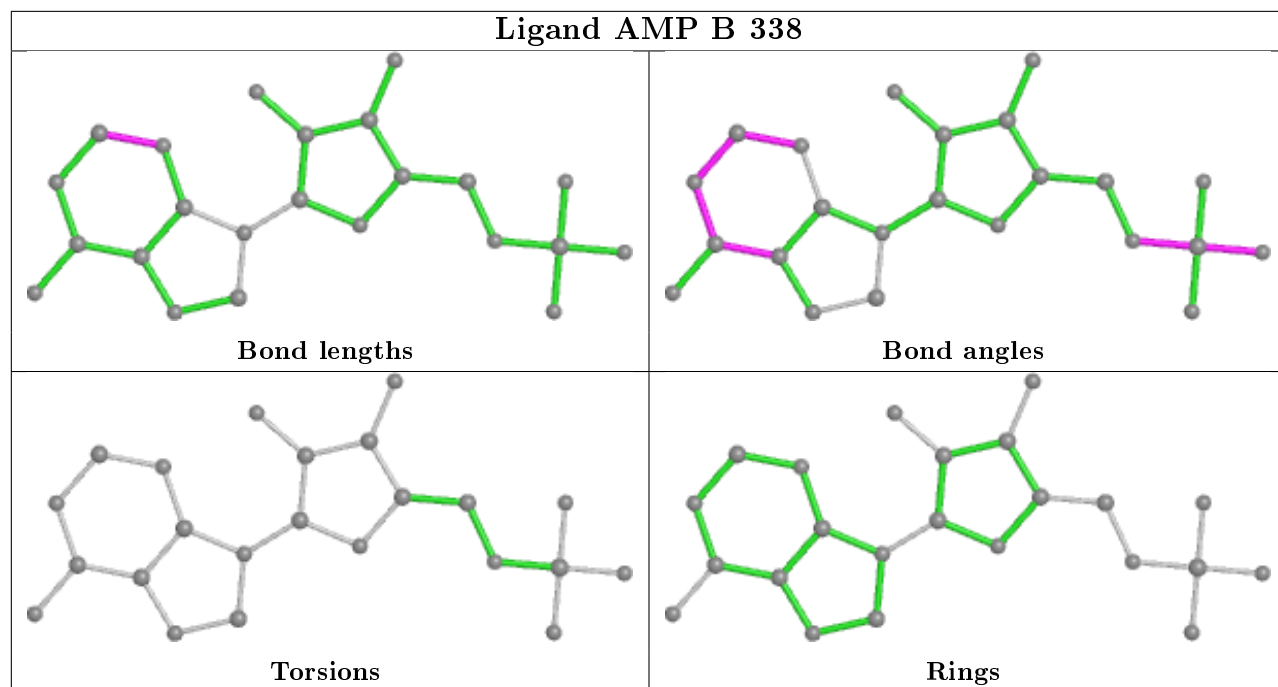


## Ligand AMP A 338



## Ligand AMP C 338





## 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.