



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

Dec 9, 2019 – 02:07 AM EST

PDB ID : 6RN2  
EMDB ID: : EMD-4940  
Title : ClpB (DWB mutant) bound to casein in presence of ATPgammaS - state WT-1  
Authors : Deville, C.; Saibil, H.R.  
Deposited on : 2019-05-07  
Resolution : 6.20 Å(reported)  
Based on PDB ID : 1CIU

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

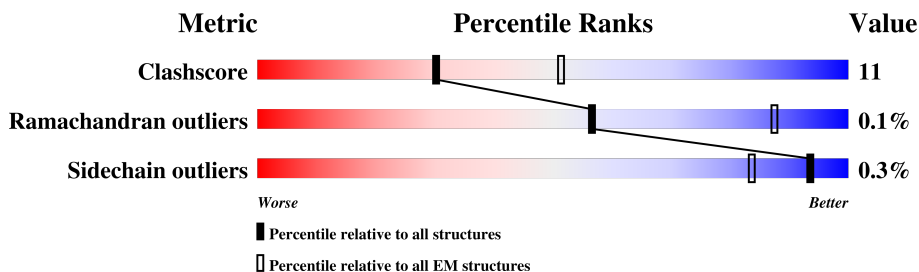
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.20 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	858	56% 23% • 20%
1	B	858	60% 20% • 20%
1	C	858	60% 20% 20%
1	D	858	57% 22% 20%
1	E	858	53% 26% • 20%
1	F	858	58% 22% 20%
2	S	24	79% 21%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32937 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 Chaperone protein ClpB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	684	Total	C	N	O	S	0	0
			5406	3386	976	1024	20		
1	B	689	Total	C	N	O	S	0	0
			5430	3400	981	1029	20		
1	C	689	Total	C	N	O	S	0	0
			5430	3400	981	1029	20		
1	D	684	Total	C	N	O	S	0	0
			5406	3386	976	1024	20		
1	E	684	Total	C	N	O	S	0	0
			5406	3386	976	1024	20		
1	F	684	Total	C	N	O	S	0	0
			5406	3386	976	1024	20		

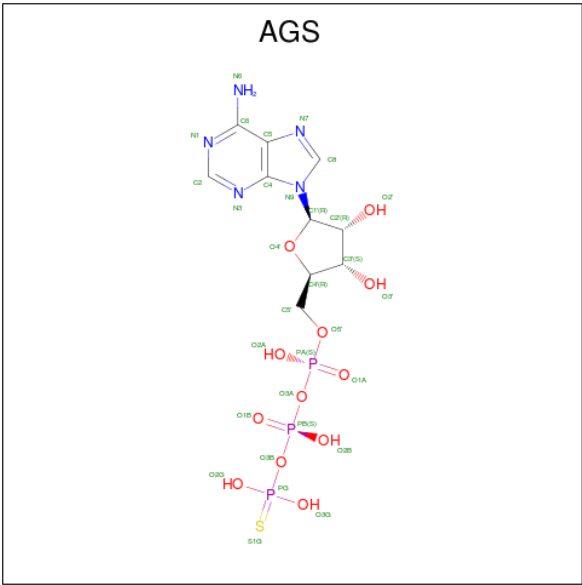
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	ALA	GLU	engineered mutation	UNP V2RJ62
A	678	ALA	GLU	engineered mutation	UNP V2RJ62
A	858	HIS	-	expression tag	UNP V2RJ62
B	279	ALA	GLU	engineered mutation	UNP V2RJ62
B	678	ALA	GLU	engineered mutation	UNP V2RJ62
B	858	HIS	-	expression tag	UNP V2RJ62
C	279	ALA	GLU	engineered mutation	UNP V2RJ62
C	678	ALA	GLU	engineered mutation	UNP V2RJ62
C	858	HIS	-	expression tag	UNP V2RJ62
D	279	ALA	GLU	engineered mutation	UNP V2RJ62
D	678	ALA	GLU	engineered mutation	UNP V2RJ62
D	858	HIS	-	expression tag	UNP V2RJ62
E	279	ALA	GLU	engineered mutation	UNP V2RJ62
E	678	ALA	GLU	engineered mutation	UNP V2RJ62
E	858	HIS	-	expression tag	UNP V2RJ62
F	279	ALA	GLU	engineered mutation	UNP V2RJ62
F	678	ALA	GLU	engineered mutation	UNP V2RJ62
F	858	HIS	-	expression tag	UNP V2RJ62

- Molecule 2 is a protein called casein.

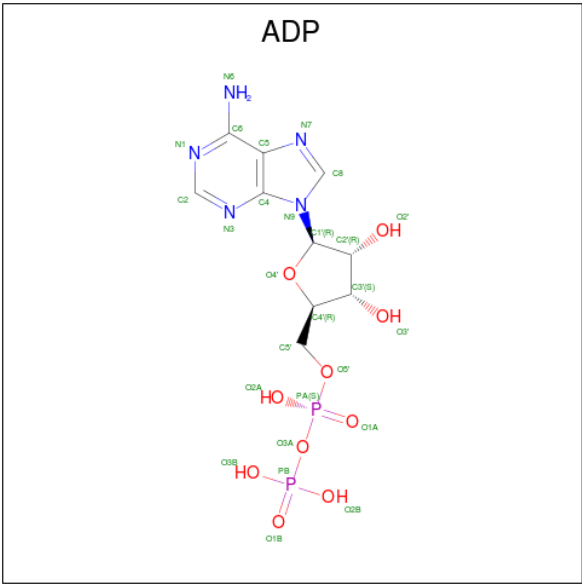
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	S	24	120	72	24	24	0	0

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S) (labeled as "Ligand of Interest" by author).

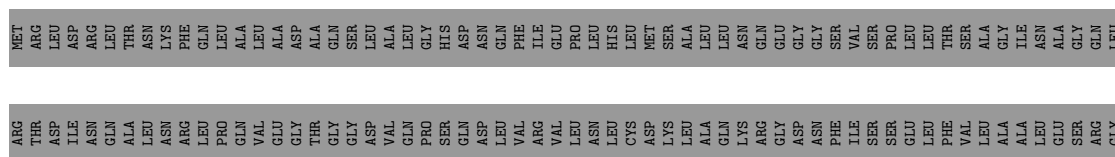


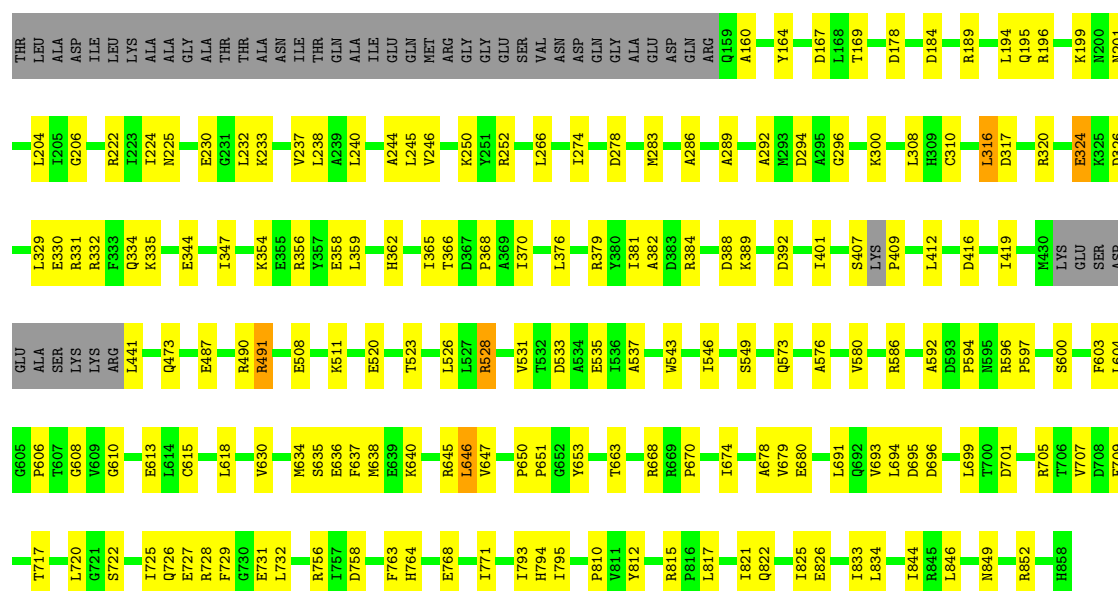
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
3	A	1	31	10	5	12	3	1	0
3	B	1	62	20	10	24	6	2	0
3	B	1	62	20	10	24	6	2	0
3	C	1	62	20	10	24	6	2	0
3	C	1	62	20	10	24	6	2	0
3	D	1	62	20	10	24	6	2	0
3	D	1	62	20	10	24	6	2	0
3	E	1	62	20	10	24	6	2	0
3	E	1	62	20	10	24	6	2	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by author).



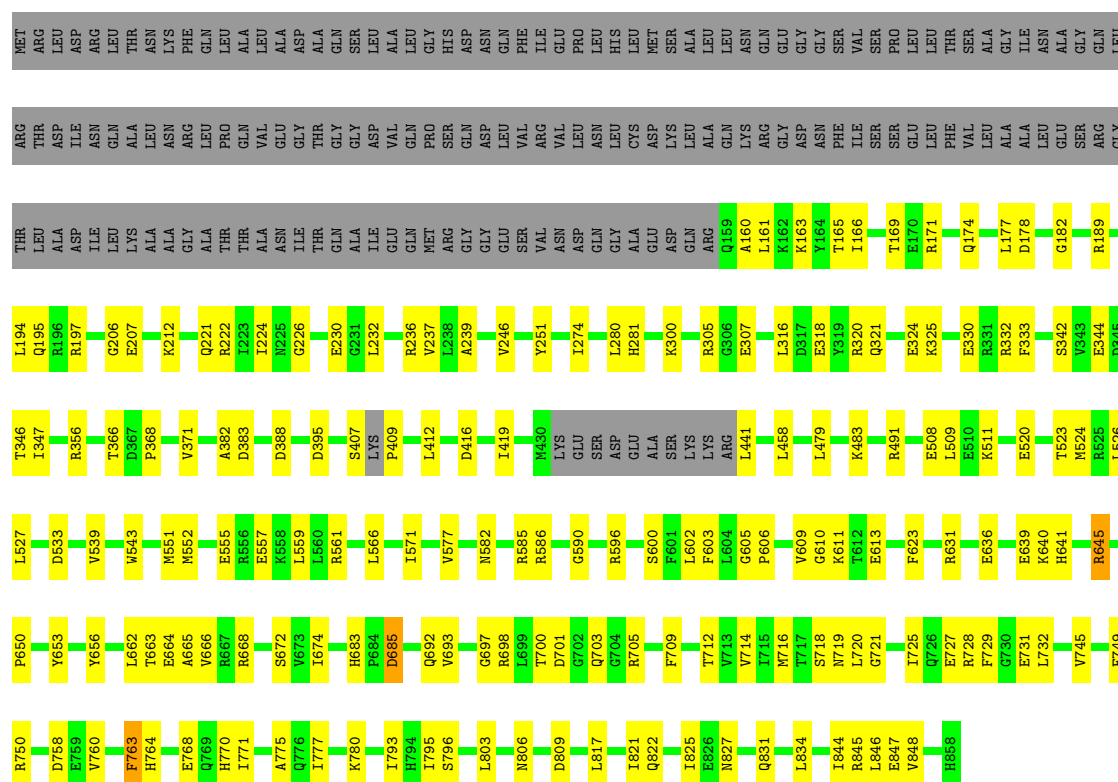
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	





### • Molecule 1: Chaperone protein ClpB

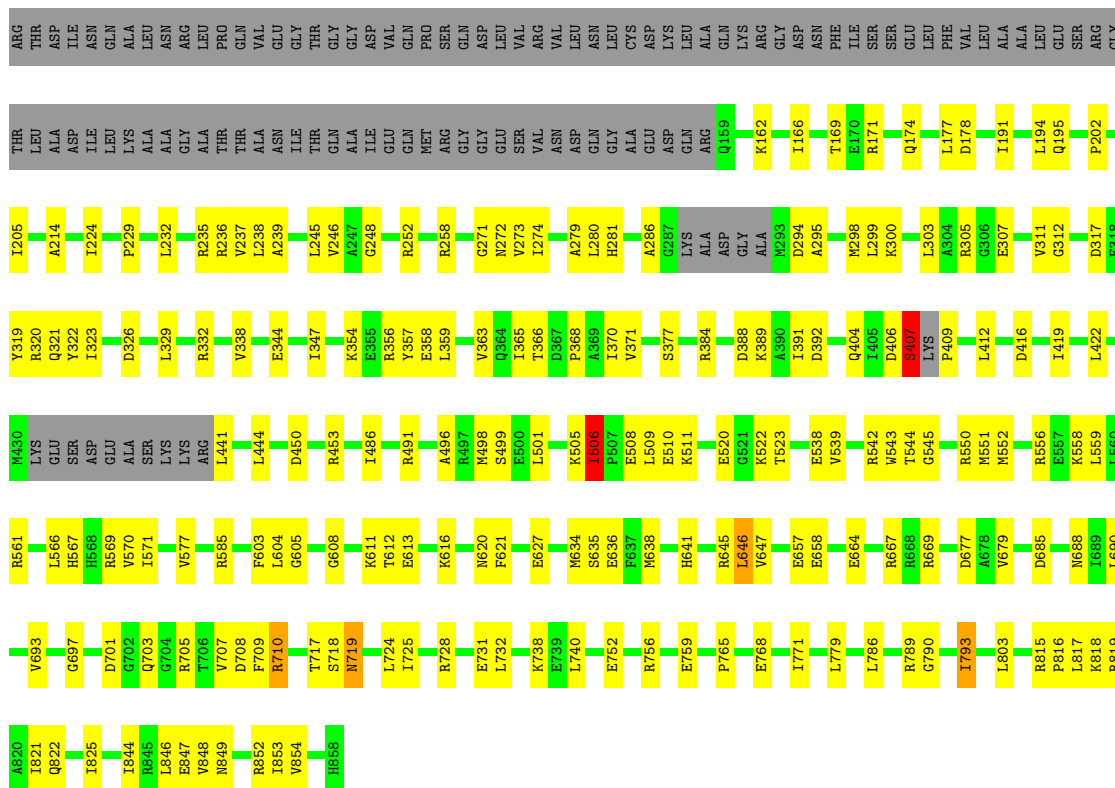
Chain C: 60% 20% 20%



### • Molecule 1: Chaperone protein ClpB

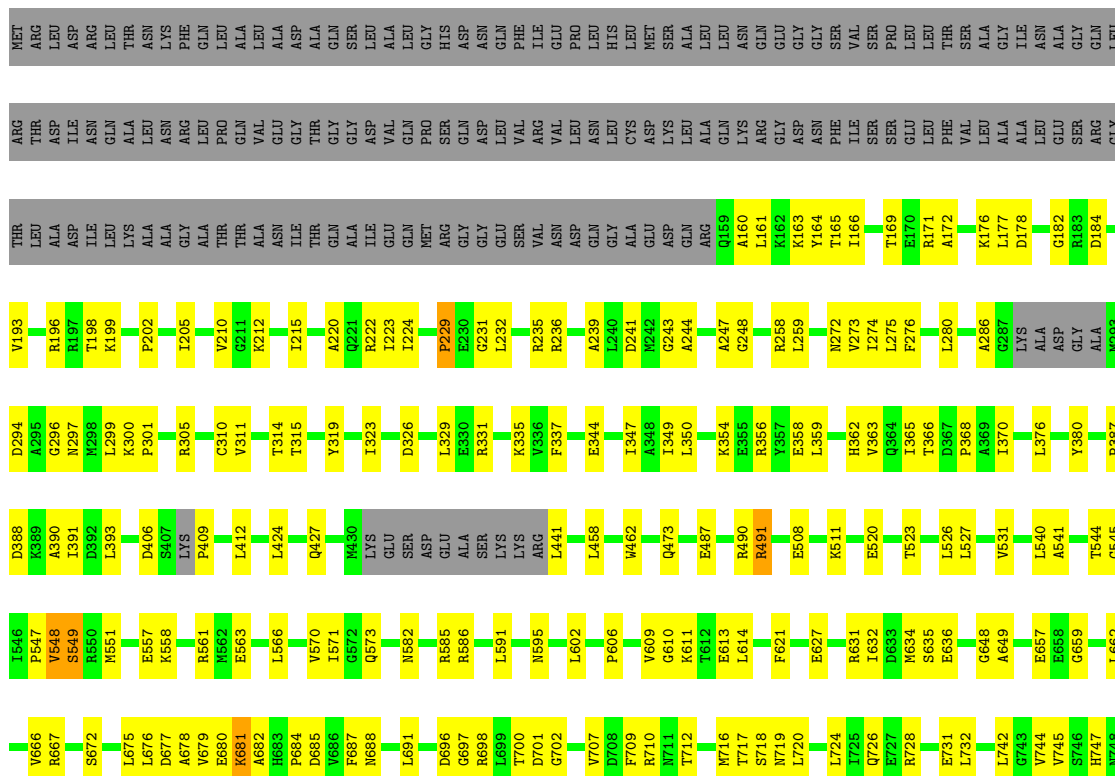
Chain D: 57% 22% 20%



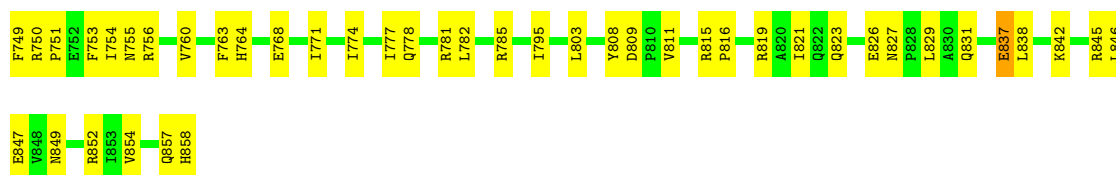


- Molecule 1: Chaperone protein ClpB

Chain E:  53% 26% . 20%

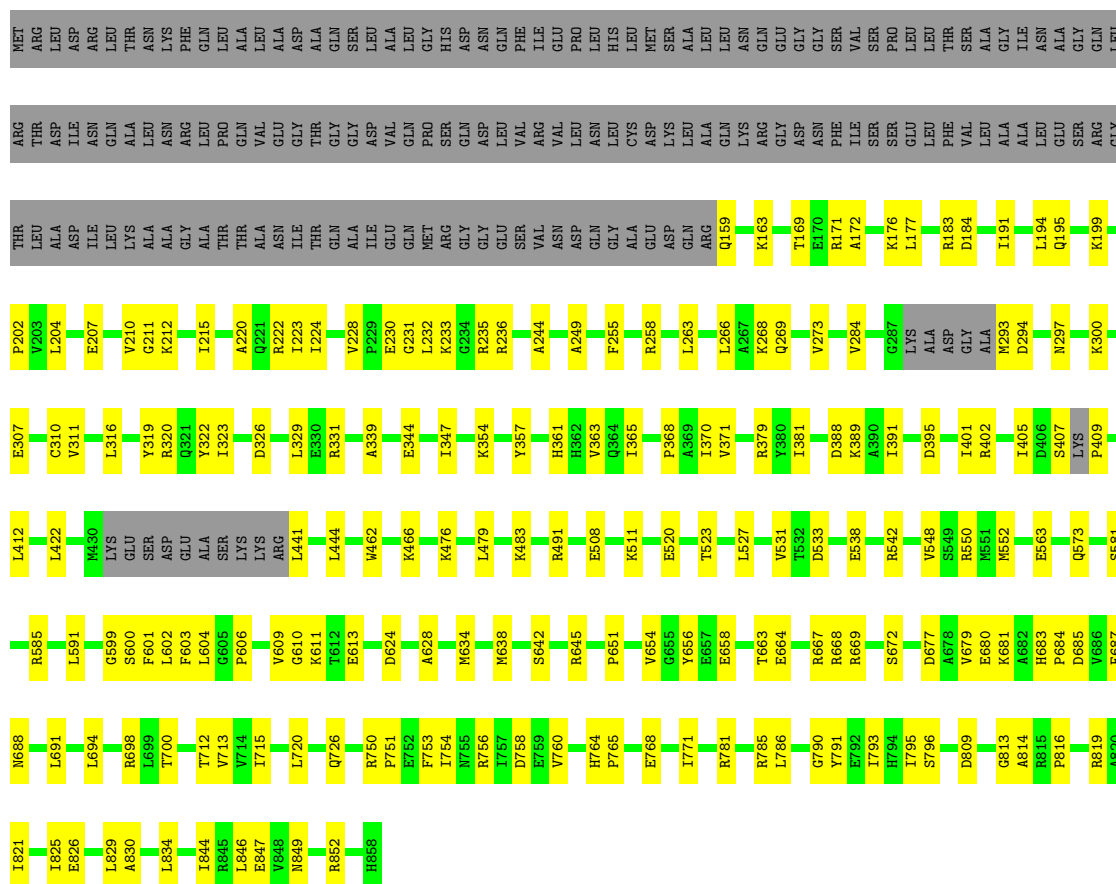






• Molecule 1: Chaperone protein ClpB

Chain F: 58% 22% 20%



• Molecule 2: casein

Chain S: 79% 21%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	21927	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.0	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AGS, ADP

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	0.50	1/5479 (0.0%)	0.62	0/7383
1	B	0.60	0/5504	0.71	7/7419 (0.1%)
1	C	0.63	1/5504 (0.0%)	0.69	1/7419 (0.0%)
1	D	0.55	0/5478	0.69	5/7380 (0.1%)
1	E	0.43	0/5477	0.61	0/7376
1	F	0.41	0/5478	0.57	0/7380
2	S	0.41	0/119	0.70	0/165
All	All	0.53	2/33039 (0.0%)	0.65	13/44522 (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	A	0	10
1	B	0	11
1	C	0	15
1	D	0	13
1	E	0	12
1	F	0	6
All	All	0	67

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	613	GLU	CD-OE1	5.74	1.31	1.25
1	C	763	PHE	C-N	-5.40	1.21	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	407	SER	C-N-CD	-8.72	101.41	120.60
1	B	316	LEU	CB-CG-CD2	-8.21	97.04	111.00
1	B	407	SER	C-N-CD	-6.60	106.08	120.60
1	D	646	LEU	CA-CB-CG	6.46	130.16	115.30
1	D	407	SER	C-N-CA	6.30	148.46	122.00

There are no chirality outliers.

5 of 67 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	407	SER	Peptide
1	A	441	LEU	Peptide
1	A	526	LEU	Peptide
1	A	528	ARG	Peptide
1	A	549	SER	Peptide

## 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	5406	0	5486	136	0
1	B	5430	0	5507	119	0
1	C	5430	0	5505	113	0
1	D	5406	0	5486	128	0
1	E	5406	0	5484	151	0
1	F	5406	0	5487	111	0
2	S	120	0	122	5	0
3	A	31	0	10	4	0
3	B	62	0	23	9	0
3	C	62	0	24	5	0
3	D	62	0	24	10	0
3	E	62	0	21	10	0
4	A	27	0	10	4	0
4	E	27	0	8	1	0
All	All	32937	0	33197	714	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 11.

The worst 5 of 714 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:D:539:VAL:O	1:D:543:TRP:HB2	1.65	0.97
1:A:618:LEU:O	1:A:622:MET:HB3	1.86	0.75
1:F:672:SER:H	1:F:712:THR:HG22	1.52	0.73
1:D:538:GLU:HB3	1:D:542:ARG:HH21	1.53	0.72
1:C:692:GLN:HE22	1:D:636:GLU:HG3	1.54	0.71

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 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	678/858 (79%)	614 (91%)	63 (9%)	1 (0%)	53	88
1	B	685/858 (80%)	627 (92%)	58 (8%)	0	100	100
1	C	685/858 (80%)	621 (91%)	64 (9%)	0	100	100
1	D	676/858 (79%)	624 (92%)	50 (7%)	2 (0%)	43	81
1	E	674/858 (79%)	615 (91%)	59 (9%)	0	100	100
1	F	676/858 (79%)	617 (91%)	59 (9%)	0	100	100
2	S	22/24 (92%)	17 (77%)	5 (23%)	0	100	100
All	All	4096/5172 (79%)	3735 (91%)	358 (9%)	3 (0%)	56	88

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	527	LEU
1	D	407	SER
1	D	506	ILE

### 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	574/714 (80%)	573 (100%)	1 (0%)	94	96
1	B	574/714 (80%)	572 (100%)	2 (0%)	93	96
1	C	574/714 (80%)	572 (100%)	2 (0%)	93	96
1	D	574/714 (80%)	572 (100%)	2 (0%)	93	96
1	E	574/714 (80%)	573 (100%)	1 (0%)	94	96
1	F	574/714 (80%)	573 (100%)	1 (0%)	94	96
All	All	3444/4284 (80%)	3435 (100%)	9 (0%)	93	96

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	491	ARG
1	F	491	ARG
1	D	710	ARG
1	B	705	ARG
1	D	491	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	688	ASN
1	D	297	ASN
1	F	281	HIS
1	C	692	GLN
1	C	858	HIS

### 5.3.3 RNA ⓘ

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](#)

11 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	$\# Z  > 2$
3	AGS	A	1001	-	25,33,33	0.76	0	24,52,52	1.49	3 (12%)
4	ADP	A	1002	-	24,29,29	1.27	3 (12%)	25,45,45	2.17	6 (24%)
3	AGS	B	1001	-	25,33,33	0.83	0	24,52,52	1.46	2 (8%)
3	AGS	B	1002	-	25,33,33	0.73	0	24,52,52	1.72	3 (12%)
3	AGS	C	1001	-	25,33,33	0.80	0	24,52,52	1.82	3 (12%)
3	AGS	C	1002	-	25,33,33	0.85	0	24,52,52	1.89	2 (8%)
3	AGS	D	1001	-	25,33,33	0.80	0	24,52,52	1.61	2 (8%)
3	AGS	D	1002	-	25,33,33	0.89	0	24,52,52	1.79	2 (8%)
3	AGS	E	1001	-	25,33,33	0.79	1 (4%)	24,52,52	1.09	2 (8%)
3	AGS	E	1002	-	25,33,33	0.76	0	24,52,52	1.50	2 (8%)
4	ADP	E	1003	-	24,29,29	1.02	1 (4%)	25,45,45	1.96	5 (20%)

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	AGS	A	1001	-	-	5/17/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	1002	-	-	6/12/32/32	0/3/3/3
3	AGS	B	1001	-	-	3/17/38/38	0/3/3/3
3	AGS	B	1002	-	-	4/17/38/38	0/3/3/3
3	AGS	C	1001	-	-	1/17/38/38	0/3/3/3
3	AGS	C	1002	-	-	4/17/38/38	0/3/3/3
3	AGS	D	1001	-	-	6/17/38/38	0/3/3/3
3	AGS	D	1002	-	-	2/17/38/38	0/3/3/3
3	AGS	E	1001	-	-	5/17/38/38	0/3/3/3
3	AGS	E	1002	-	-	7/17/38/38	0/3/3/3
4	ADP	E	1003	-	-	4/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	ADP	C5-C4	3.54	1.48	1.40
4	A	1002	ADP	C2-N3	2.99	1.37	1.32
4	E	1003	ADP	C5-C4	2.83	1.46	1.40
4	A	1002	ADP	O4'-C1'	2.43	1.44	1.41
3	E	1001	AGS	PG-S1G	2.25	1.94	1.90

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1002	AGS	PA-O3A-PB	-7.76	107.89	132.57
4	A	1002	ADP	C1'-N9-C4	7.55	139.68	126.64
3	C	1001	AGS	PA-O3A-PB	-7.41	109.01	132.57
3	D	1002	AGS	PA-O3A-PB	-7.18	109.74	132.57
3	B	1002	AGS	PA-O3A-PB	-6.92	110.59	132.57

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1001	AGS	PB-O3B-PG-O2G
3	D	1001	AGS	PB-O3B-PG-O3G
3	D	1001	AGS	C5'-O5'-PA-O3A
4	E	1003	ADP	C5'-O5'-PA-O1A
3	B	1002	AGS	PB-O3B-PG-O2G

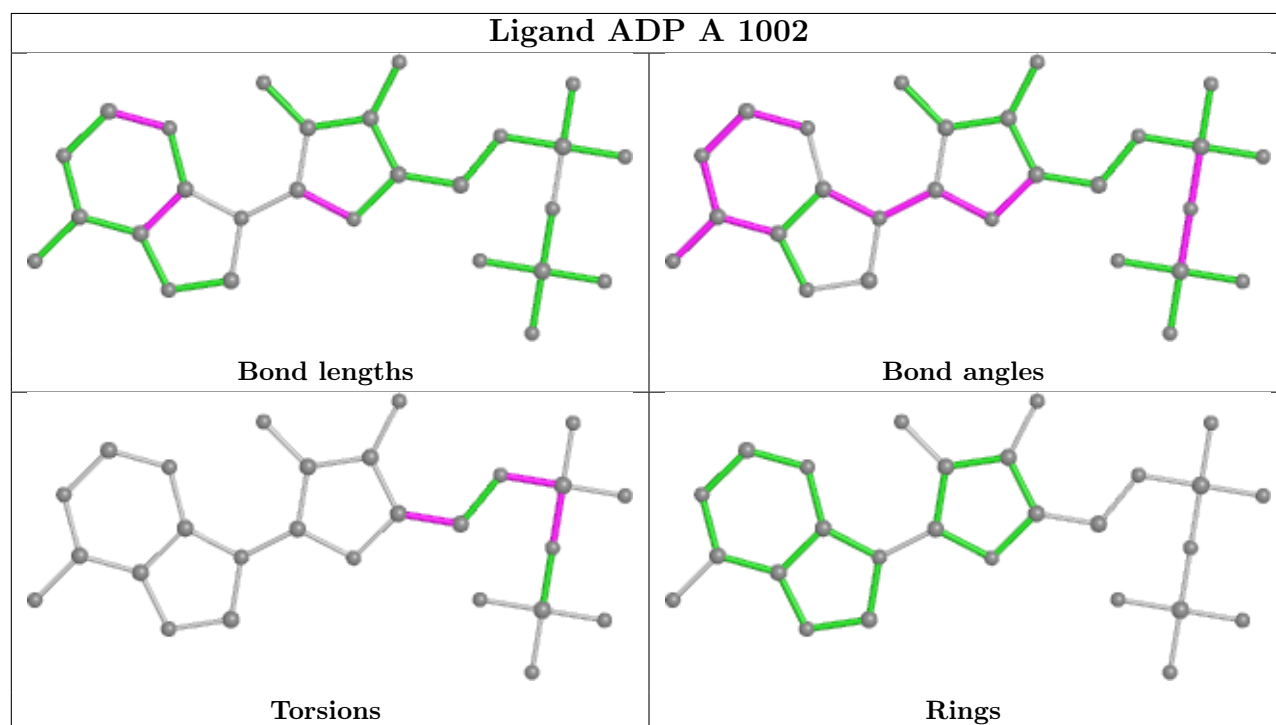
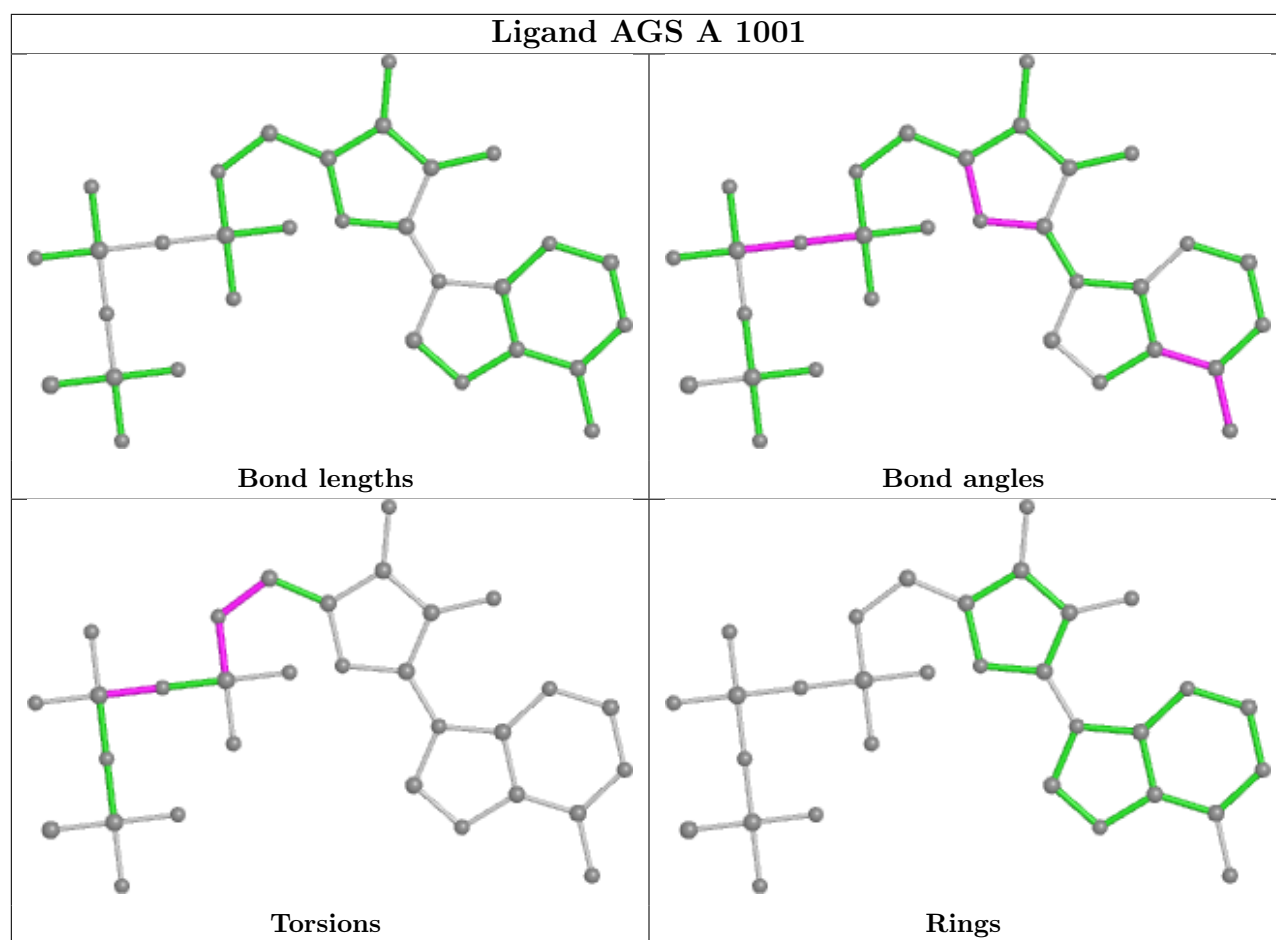


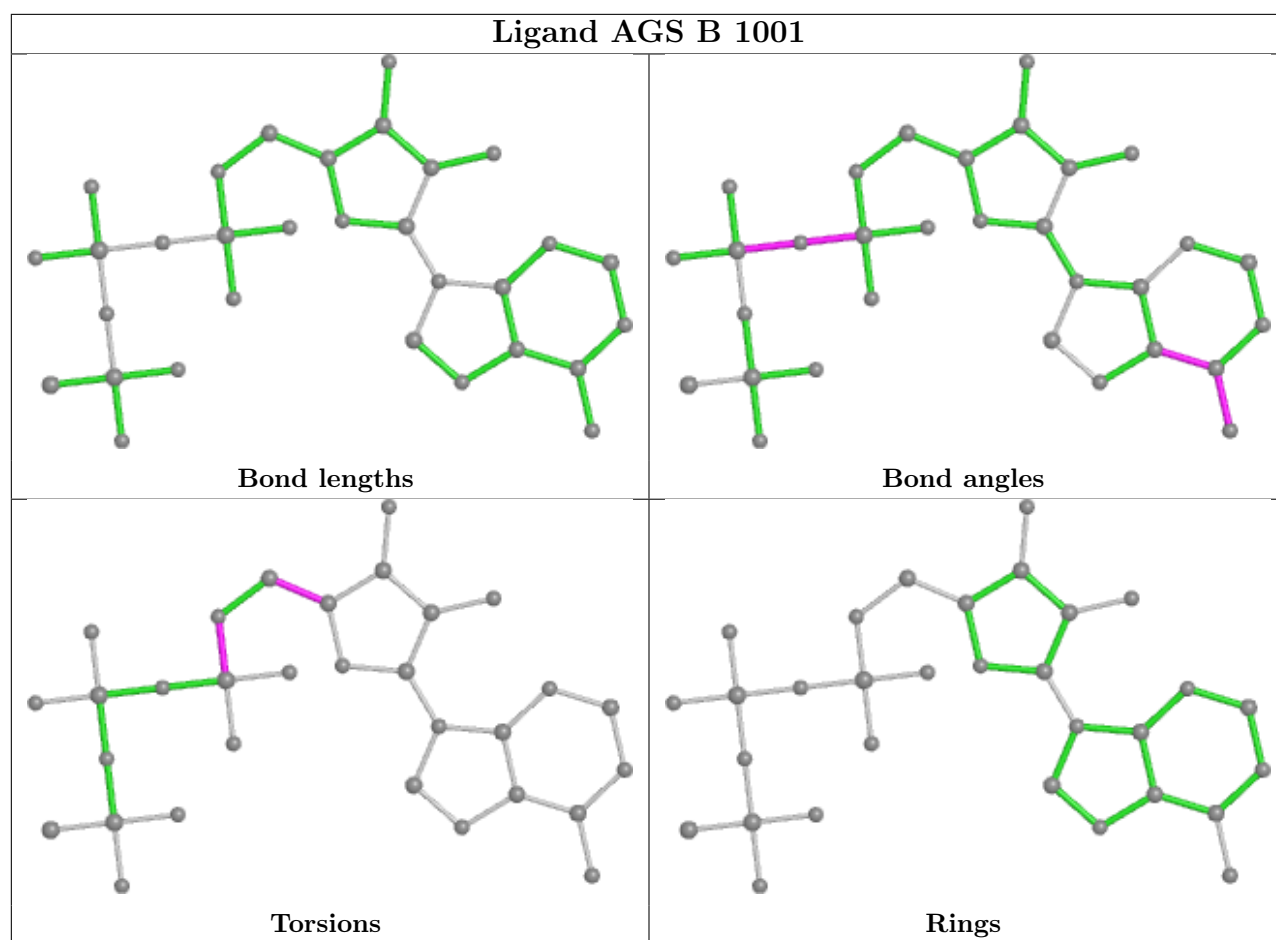
There are no ring outliers.

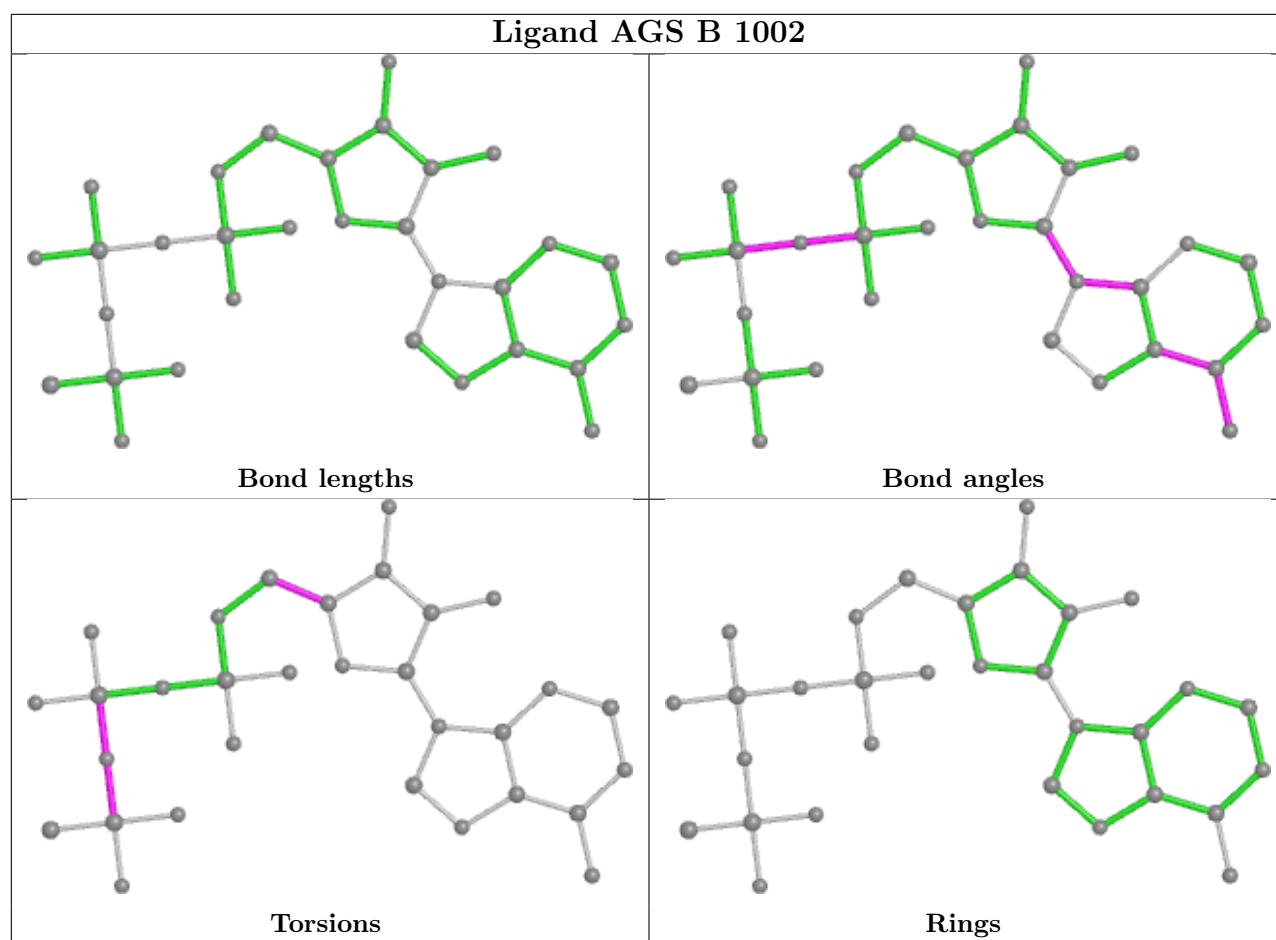
11 monomers are involved in 43 short contacts:

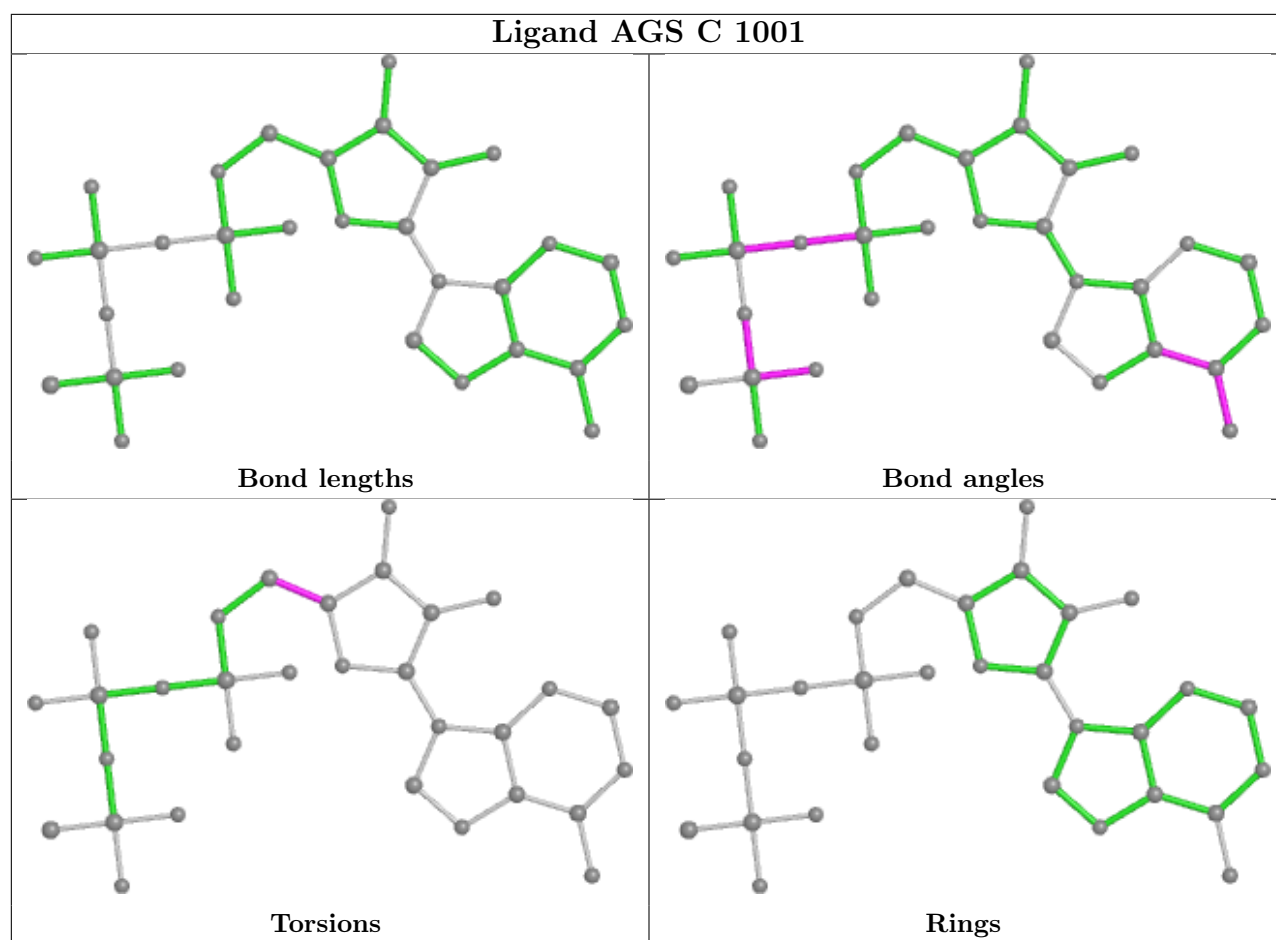
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	AGS	4	0
4	A	1002	ADP	4	0
3	B	1001	AGS	2	0
3	B	1002	AGS	7	0
3	C	1001	AGS	3	0
3	C	1002	AGS	2	0
3	D	1001	AGS	3	0
3	D	1002	AGS	7	0
3	E	1001	AGS	4	0
3	E	1002	AGS	6	0
4	E	1003	ADP	1	0

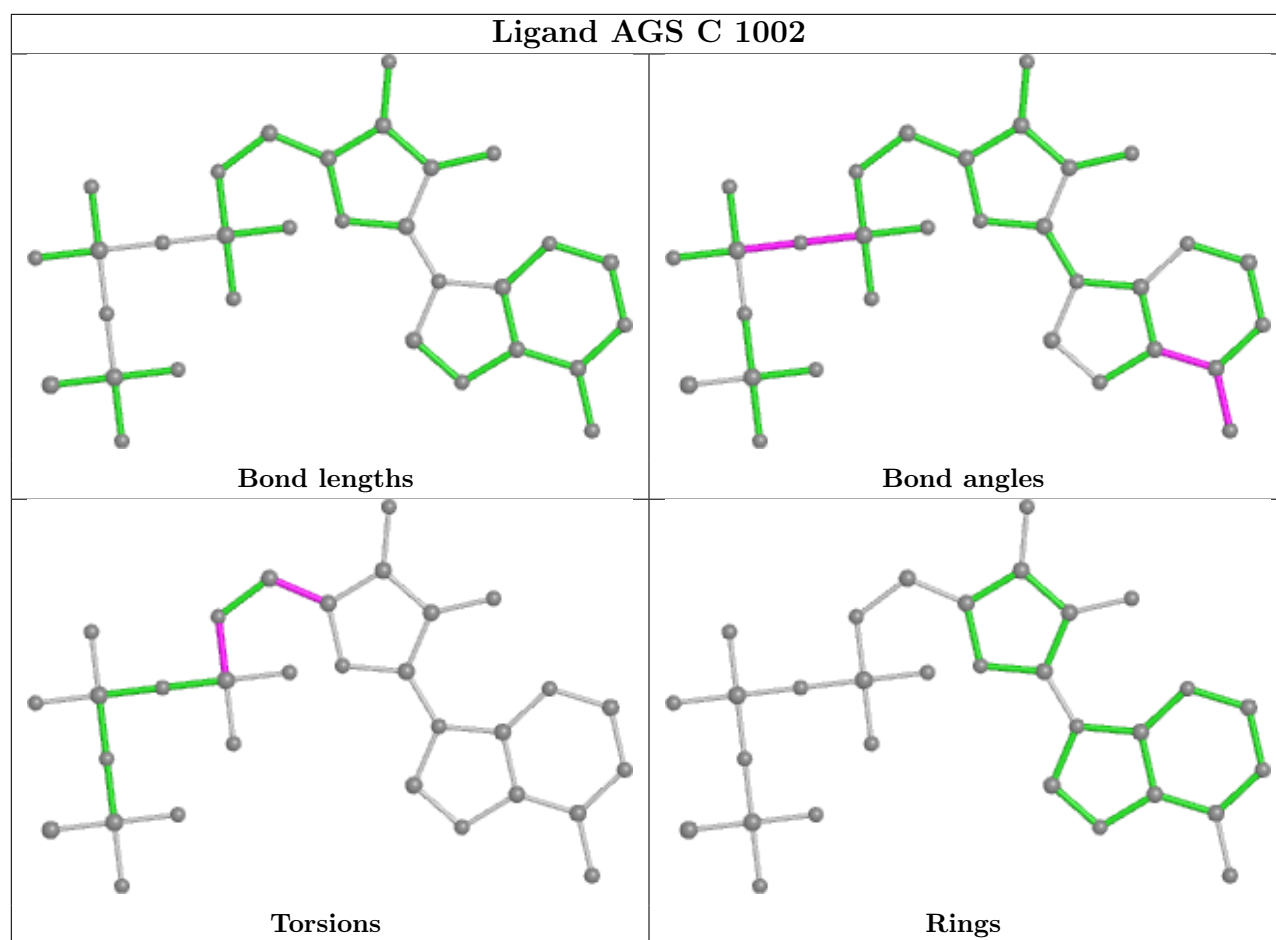
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

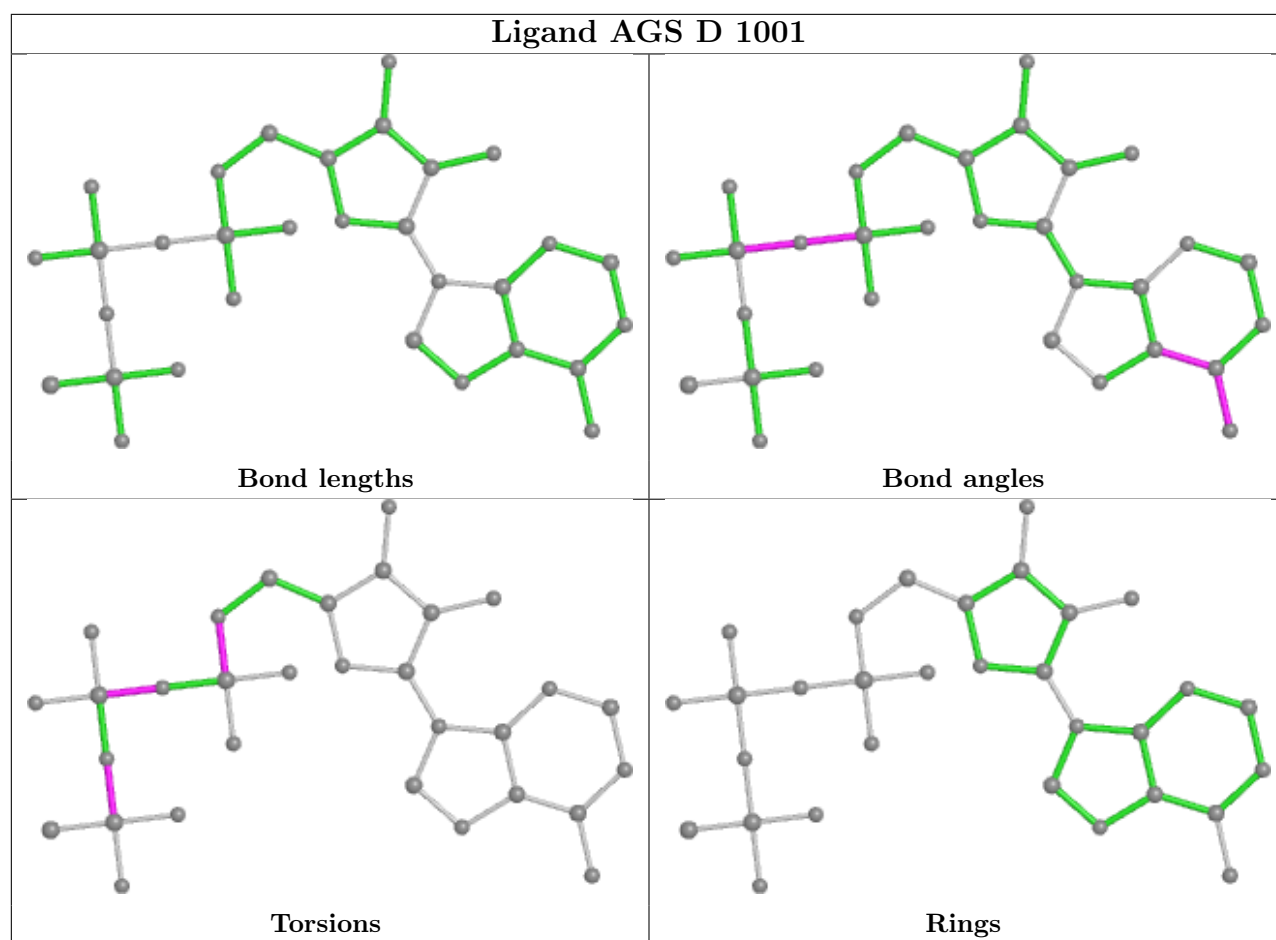


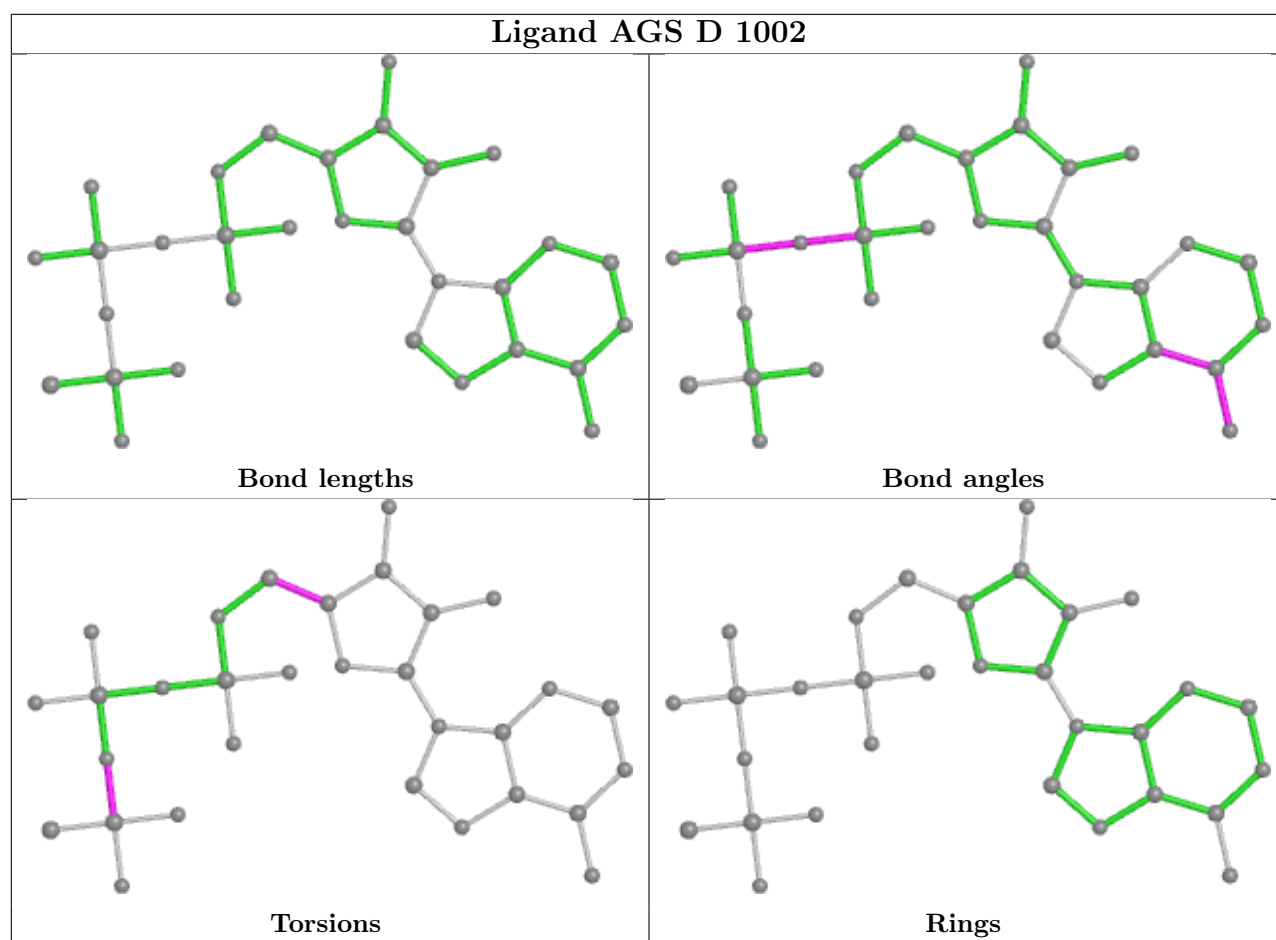




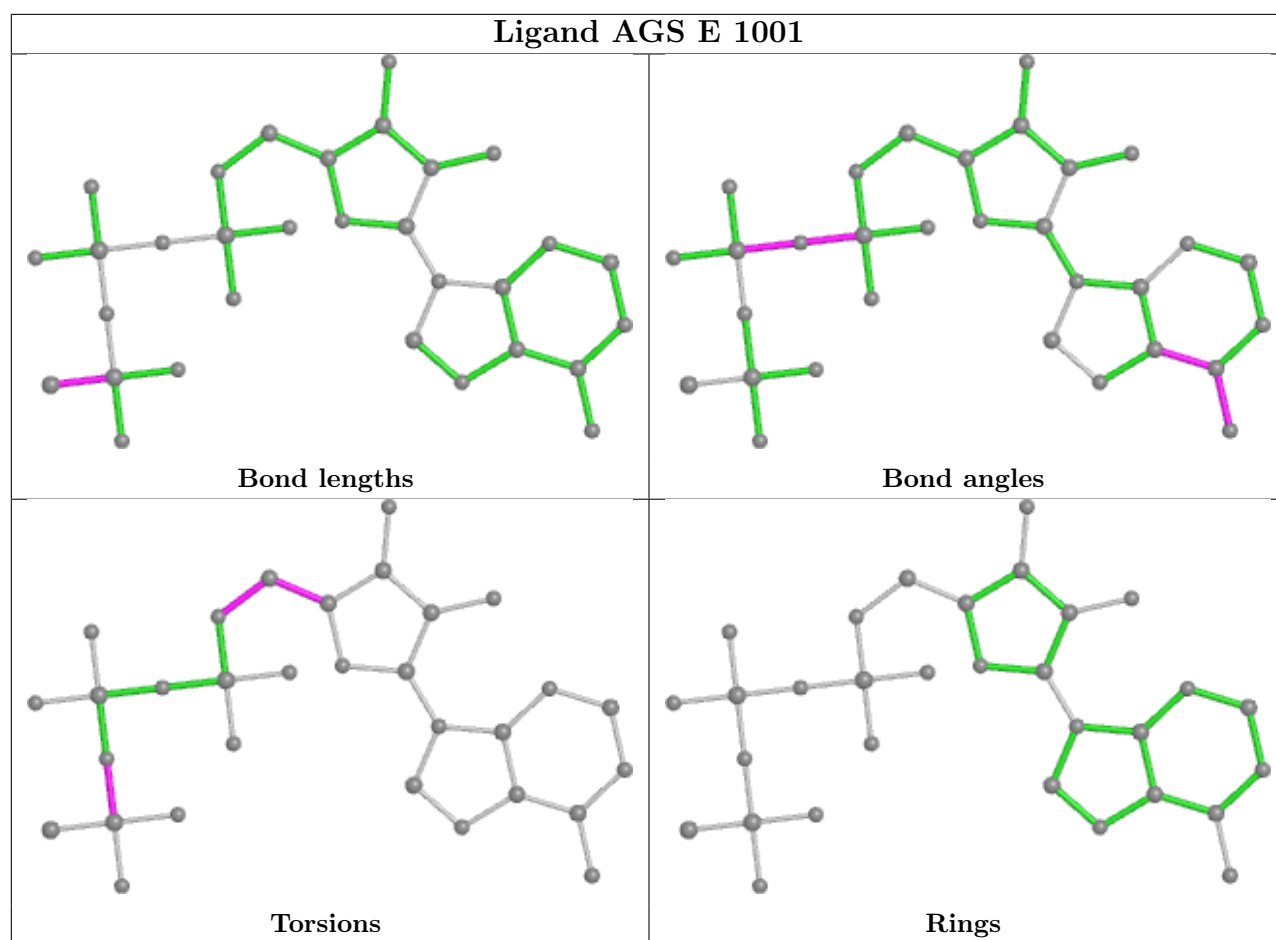


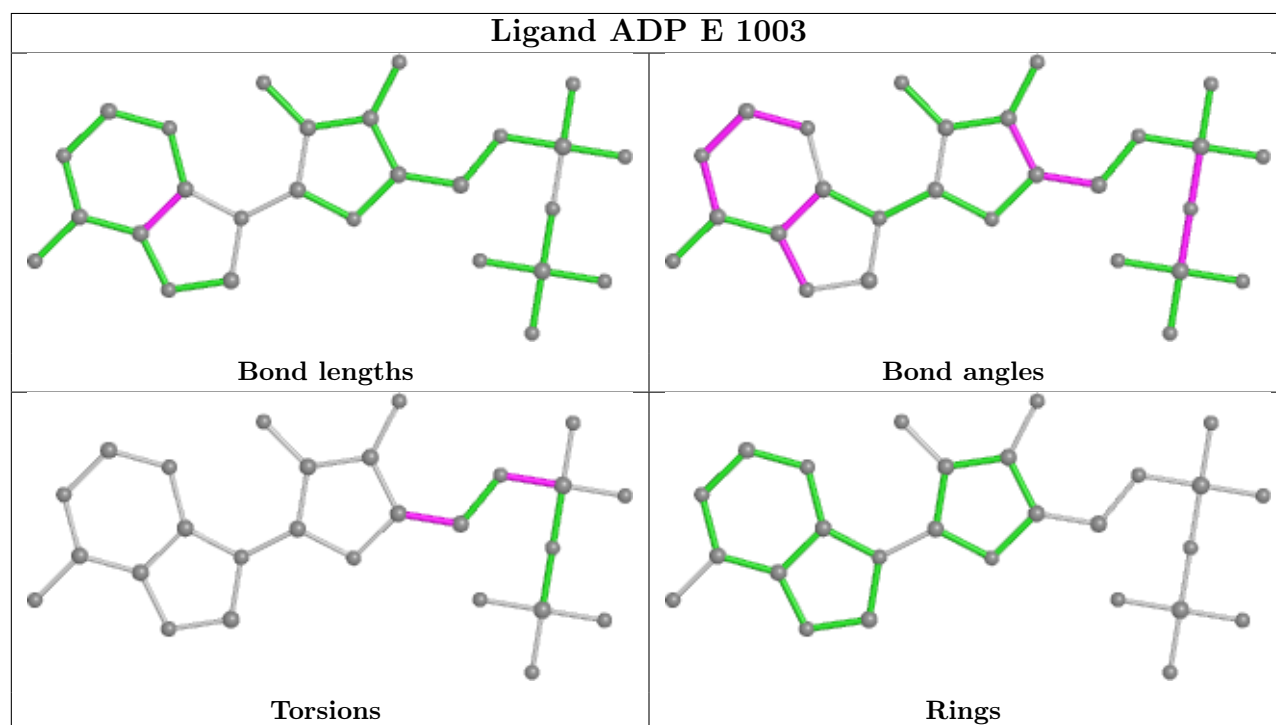
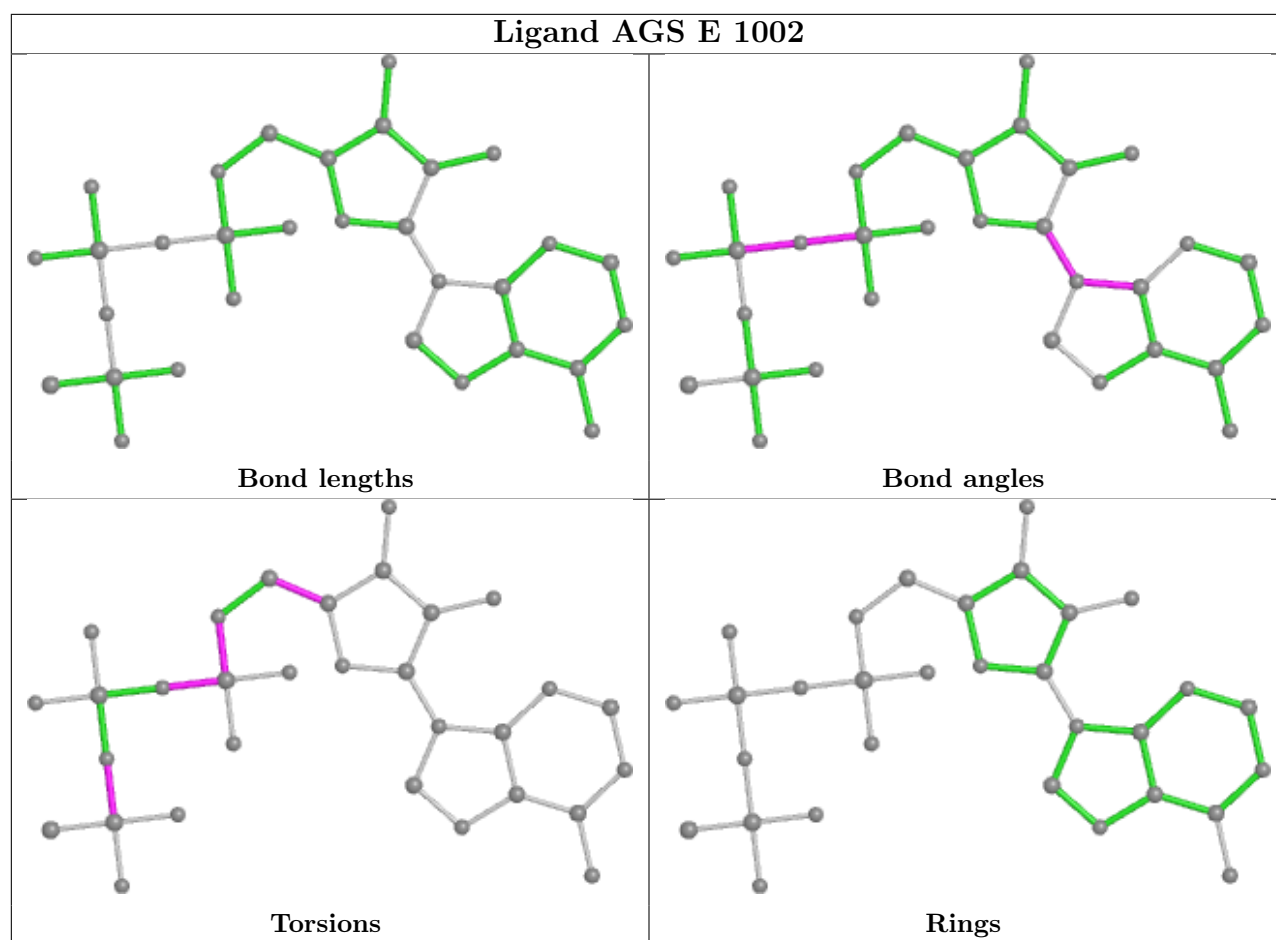












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	2
1	D	1
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	546:ILE	C	547:PRO	N	7.97
1	E	526:LEU	C	527:LEU	N	5.85
1	F	526:LEU	C	527:LEU	N	5.69
1	D	526:LEU	C	527:LEU	N	4.02