wwPDB EM Validation Summary Report

Dec 12, 2022 – 09:02 AM EST

PDB ID	:	6UQE
EMDB ID	:	EMD-20845
Title	:	ClpA/ClpP Disengaged State bound to RepA-GFP
Authors	:	Lopez, K.L.; Rizo, A.R.; Southworth, D.R.
Deposited on	:	2019-10-18
Resolution	:	3.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

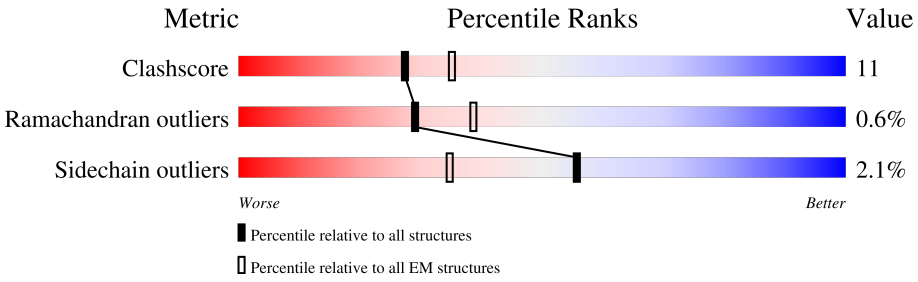
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	578	84% 10% • • •
1	B	578	81% 15% • •
1	C	578	88% 10% •
1	D	578	86% 12% •
1	E	578	87% 11% •
1	F	578	90% 10%
2	G	192	85% 12% •
2	H	192	68% 22% 8% •
2	I	192	84% 14% • •

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Mol	Chain	Length	Quality of chain
2	J	192	91% 8%
2	K	192	88% 11%
2	L	192	86% 11%
2	M	192	92% 6%
2	N	192	90% 9%
2	O	192	90% 10%
2	P	192	91% 8%
2	Q	192	91% 9%
2	R	192	92% 8%
2	S	192	93% 7%
2	T	192	92% 8%
3	X	10	50% 50%
4	Y	11	64% 36%

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
5	ADP	A	801	X	-	-	-
5	ADP	A	802	X	-	-	-
5	ADP	E	801	X	-	-	-
5	ADP	E	802	X	-	X	-
5	ADP	F	801	X	-	-	-
6	AGS	B	801	X	-	-	-
6	AGS	B	802	X	-	-	-
6	AGS	C	801	X	-	-	-
6	AGS	C	802	X	-	-	-
6	AGS	D	801	X	-	-	-
6	AGS	D	802	X	-	-	-
6	AGS	E	803	X	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 48402 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 ATP-dependent Clp protease ATP-binding subunit ClpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	562	Total	C	N	O	S	0	0
			4377	2760	778	825	14		
1	B	578	Total	C	N	O	S	0	0
			4511	2841	805	851	14		
1	C	578	Total	C	N	O	S	0	0
			4511	2841	805	851	14		
1	D	578	Total	C	N	O	S	0	0
			4510	2841	805	850	14		
1	E	578	Total	C	N	O	S	0	0
			4511	2841	805	851	14		
1	F	578	Total	C	N	O	S	0	0
			4511	2841	805	851	14		

- Molecule 2 is a protein called ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	192	Total	C	N	O	S	0	0
			1501	946	260	283	12		
2	H	192	Total	C	N	O	S	0	0
			1501	946	260	283	12		
2	I	192	Total	C	N	O	S	0	0
			1501	946	260	283	12		
2	J	192	Total	C	N	O	S	0	0
			1501	946	260	283	12		
2	K	192	Total	C	N	O	S	0	0
			1501	946	260	283	12		
2	L	192	Total	C	N	O	S	0	0
			1501	946	260	283	12		
2	M	192	Total	C	N	O	S	0	0
			1501	946	260	283	12		
2	N	192	Total	C	N	O	S	0	0
			1501	946	260	283	12		
2	O	192	Total	C	N	O	S	0	0
			1501	946	260	283	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	192	Total	C	N	O	S	0	0
			1501	946	260	283	12		
2	Q	192	Total	C	N	O	S	0	0
			1501	946	260	283	12		
2	R	192	Total	C	N	O	S	0	0
			1501	946	260	283	12		
2	S	192	Total	C	N	O	S	0	0
			1501	946	260	283	12		
2	T	192	Total	C	N	O	S	0	0
			1501	946	260	283	12		

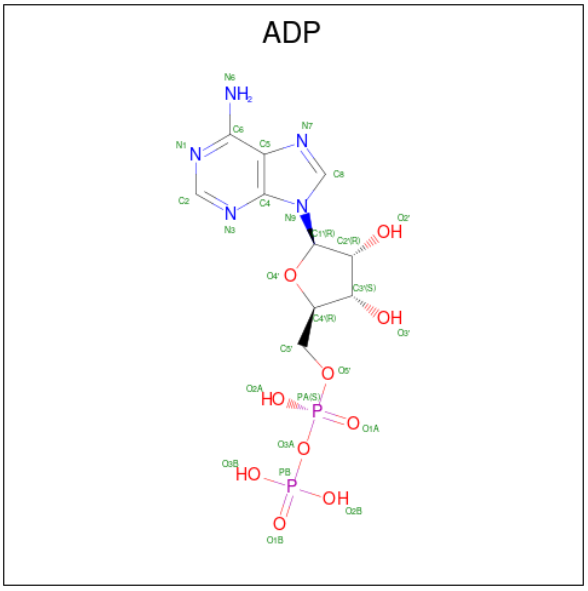
- Molecule 3 is a protein called RepA-GFP.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	X	10	Total	C	N	O	0	0
			50	30	10	10		

- Molecule 4 is a protein called RepA-GFP.

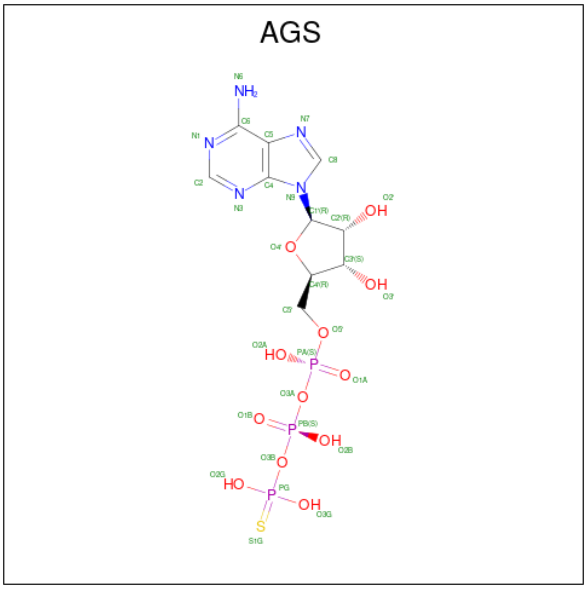
Mol	Chain	Residues	Atoms				AltConf	Trace
4	Y	11	Total	C	N	O	0	0
			55	33	11	11		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			54	20	10	20	4	
5	A	1	Total	C	N	O	P	0
			54	20	10	20	4	
5	E	1	Total	C	N	O	P	0
			54	20	10	20	4	
5	E	1	Total	C	N	O	P	0
			54	20	10	20	4	
5	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 6 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						AltConf
6	B	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
6	B	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
6	C	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
6	C	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
6	D	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
6	D	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	

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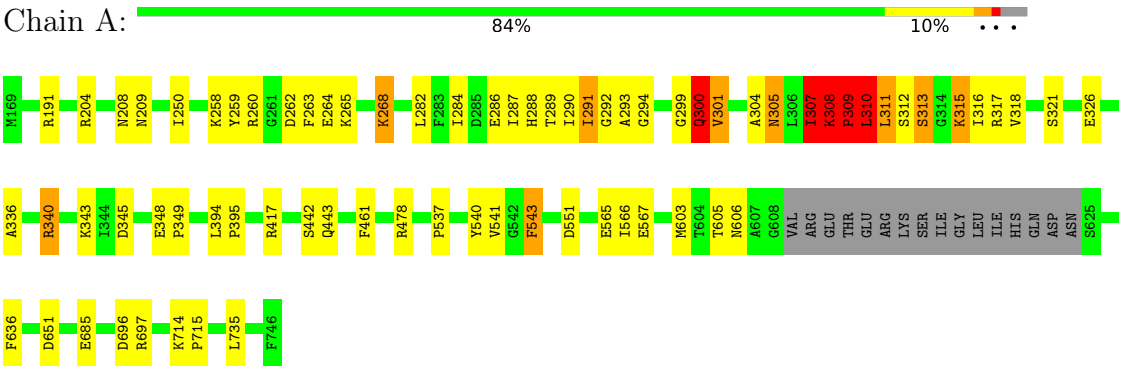
Mol	Chain	Residues	Atoms						AltConf
6	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

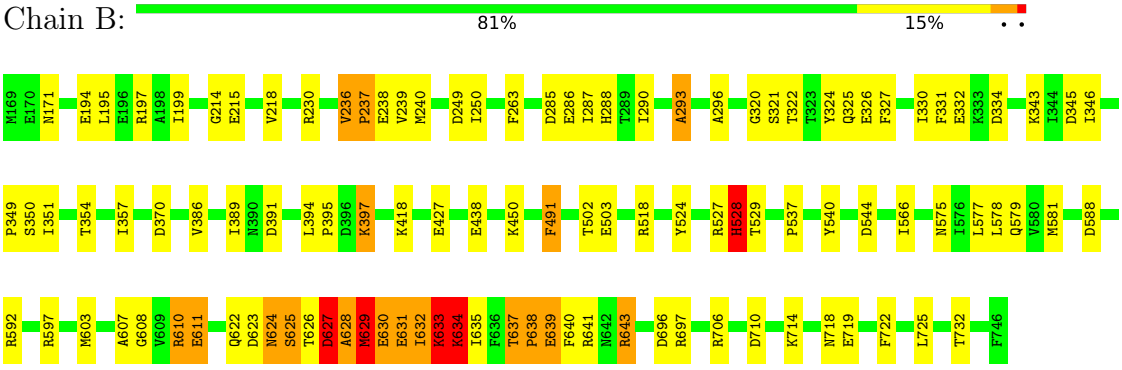
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA

Chain A:



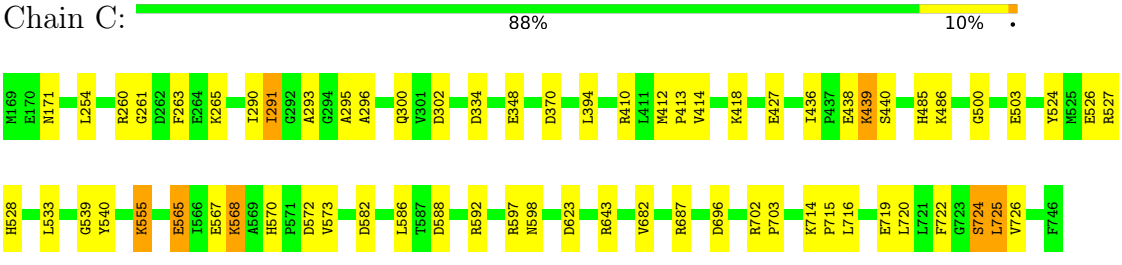
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA

Chain B:



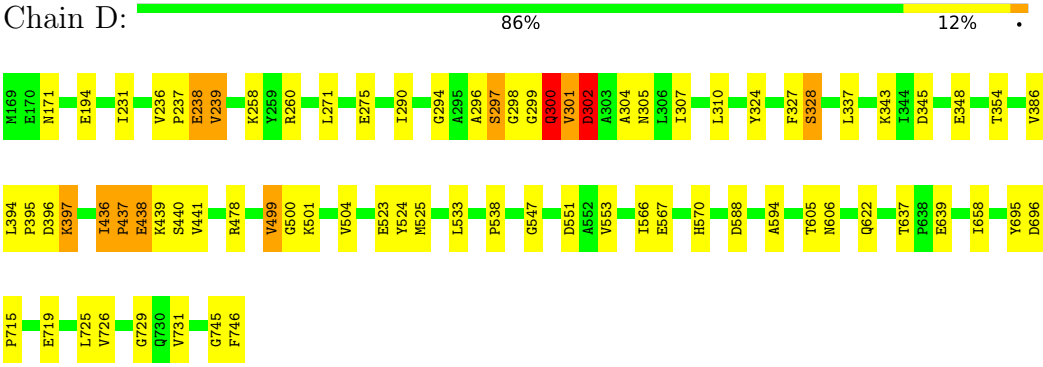
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA

Chain C:



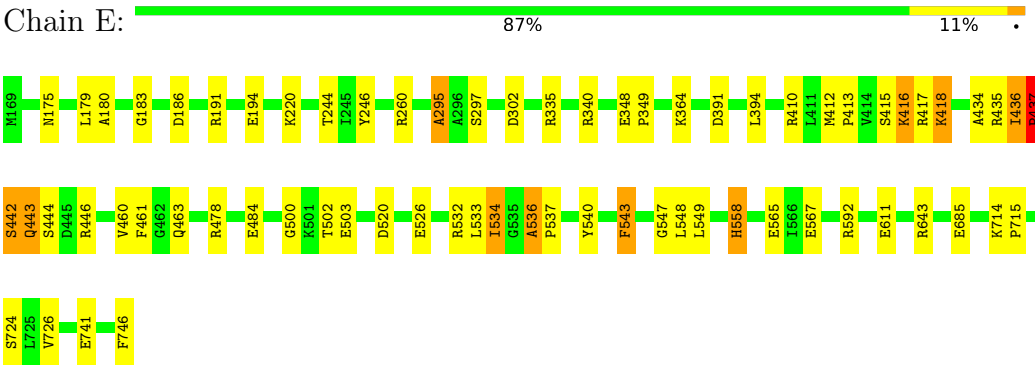
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA

Chain D:



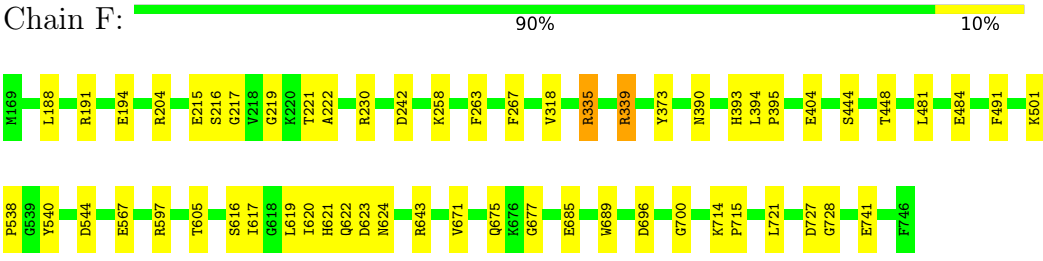
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA

Chain E:



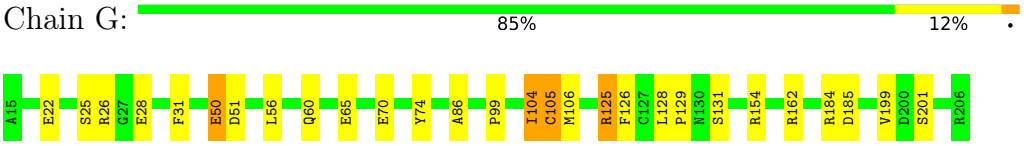
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA

Chain F:



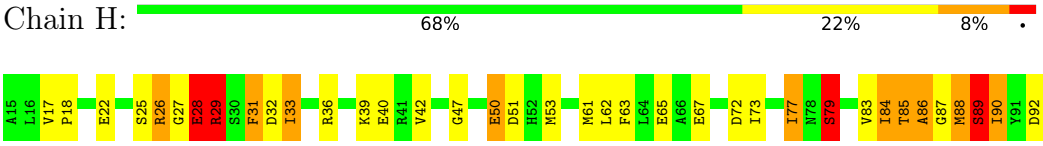
• Molecule 2: ATP-dependent Clp protease proteolytic subunit

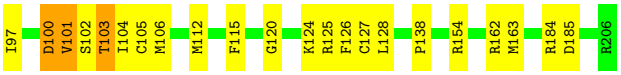
Chain G:



• Molecule 2: ATP-dependent Clp protease proteolytic subunit

Chain H:





• Molecule 2: ATP-dependent Clp protease proteolytic subunit

Chain I:

• Molecule 2: ATP-dependent Clp protease proteolytic subunit

Chain J:

• Molecule 2: ATP-dependent Clp protease proteolytic subunit

Chain K:

• Molecule 2: ATP-dependent Clp protease proteolytic subunit

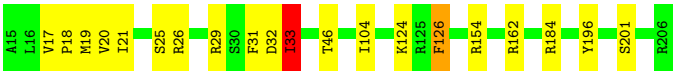
Chain L:

• Molecule 2: ATP-dependent Clp protease proteolytic subunit

Chain M:

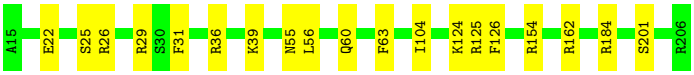
• Molecule 2: ATP-dependent Clp protease proteolytic subunit

Chain N:

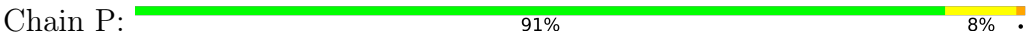


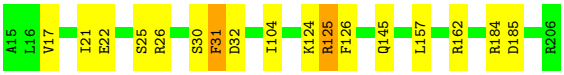
• Molecule 2: ATP-dependent Clp protease proteolytic subunit

Chain O:

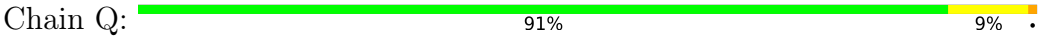


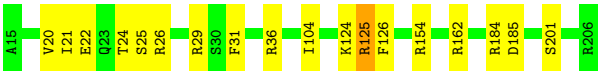
• Molecule 2: ATP-dependent Clp protease proteolytic subunit



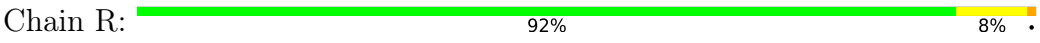


• Molecule 2: ATP-dependent Clp protease proteolytic subunit

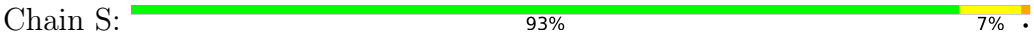




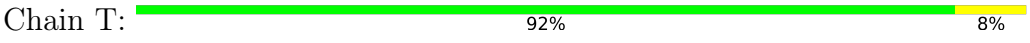
• Molecule 2: ATP-dependent Clp protease proteolytic subunit



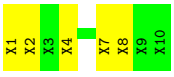
• Molecule 2: ATP-dependent Clp protease proteolytic subunit



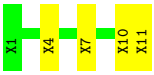
• Molecule 2: ATP-dependent Clp protease proteolytic subunit



• Molecule 3: RepA-GFP



• Molecule 4: RepA-GFP


X1
X4
X7
X10
X11

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	169000	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 ($e^-/Å^2$)	69	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	58616	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k 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: 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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.08	1/4441 (0.0%)	0.96	14/5991 (0.2%)
1	B	1.04	0/4577	0.93	10/6175 (0.2%)
1	C	1.17	1/4577 (0.0%)	0.91	6/6175 (0.1%)
1	D	1.14	2/4576 (0.0%)	0.89	4/6175 (0.1%)
1	E	1.11	15/4577 (0.3%)	0.95	10/6175 (0.2%)
1	F	1.04	12/4576 (0.3%)	0.92	9/6172 (0.1%)
2	G	1.35	4/1525 (0.3%)	0.91	3/2054 (0.1%)
2	H	1.34	10/1525 (0.7%)	1.09	12/2054 (0.6%)
2	I	1.19	0/1525	0.86	1/2054 (0.0%)
2	J	1.27	0/1525	0.90	4/2054 (0.2%)
2	K	1.25	1/1525 (0.1%)	0.92	6/2054 (0.3%)
2	L	1.25	0/1525	0.93	6/2054 (0.3%)
2	M	1.34	1/1525 (0.1%)	0.89	2/2054 (0.1%)
2	N	1.21	0/1525	0.93	5/2054 (0.2%)
2	O	1.21	0/1525	0.93	5/2054 (0.2%)
2	P	1.28	0/1525	0.92	4/2054 (0.2%)
2	Q	1.33	0/1525	0.95	5/2054 (0.2%)
2	R	1.29	0/1525	0.89	3/2054 (0.1%)
2	S	1.29	1/1525 (0.1%)	0.96	5/2054 (0.2%)
2	T	1.24	0/1525	0.90	2/2054 (0.1%)
All	All	1.18	48/48674 (0.1%)	0.93	116/65619 (0.2%)

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	1	1
1	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	3
2	H	0	3
All	All	1	11

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	437	PRO	N-CA	13.68	1.70	1.47
1	E	536	ALA	C-N	8.59	1.50	1.34
1	C	565	GLU	CG-CD	-8.56	1.39	1.51
2	S	32	ASP	CB-CG	-7.87	1.35	1.51
1	E	741	GLU	CD-OE1	-7.04	1.18	1.25

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	436	ILE	C-N-CD	-14.59	88.51	120.60
2	S	31	PHE	CB-CA-C	-13.37	83.66	110.40
1	B	633	LYS	CB-CA-C	-10.54	89.31	110.40
1	C	592	ARG	NE-CZ-NH2	-9.83	115.39	120.30
2	K	184	ARG	NE-CZ-NH1	9.66	125.13	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	629	MET	CA

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	300	GLN	Peptide
1	A	313	SER	Peptide
1	A	417	ARG	Mainchain
1	B	627	ASP	Mainchain
1	E	484	GLU	Mainchain

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	A	4377	0	4468	131	0
1	B	4511	0	4609	188	0
1	C	4511	0	4609	113	0
1	D	4510	0	4609	97	0
1	E	4511	0	4609	127	0
1	F	4511	0	4608	56	0
2	G	1501	0	1512	36	0
2	H	1501	0	1512	87	0
2	I	1501	0	1512	83	0
2	J	1501	0	1512	40	0
2	K	1501	0	1512	36	0
2	L	1501	0	1512	29	0
2	M	1501	0	1512	32	0
2	N	1501	0	1512	34	0
2	O	1501	0	1512	26	0
2	P	1501	0	1512	26	0
2	Q	1501	0	1512	18	0
2	R	1501	0	1512	17	0
2	S	1501	0	1512	15	0
2	T	1501	0	1512	15	0
3	X	50	0	13	19	0
4	Y	55	0	15	6	0
5	A	54	0	23	1	0
5	E	54	0	22	19	0
5	F	27	0	11	1	0
6	B	62	0	24	4	0
6	C	62	0	22	1	0
6	D	62	0	22	1	0
6	E	31	0	11	9	0
All	All	48402	0	48843	1052	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 1052 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)
2:I:29:ARG:HD3	2:I:31:PHE:CE1	1.15	1.66
2:J:31:PHE:CZ	2:K:21:ILE:HD11	1.43	1.50
2:J:31:PHE:CE2	2:K:21:ILE:HD11	1.47	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:TYR:CD2	3:X:2:UNK:O	1.69	1.45
1:C:263:PHE:CZ	1:C:293:ALA:CB	2.04	1.39

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	558/578 (96%)	537 (96%)	18 (3%)	3 (0%)	29 68
1	B	576/578 (100%)	545 (95%)	24 (4%)	7 (1%)	13 48
1	C	576/578 (100%)	553 (96%)	21 (4%)	2 (0%)	41 76
1	D	576/578 (100%)	555 (96%)	17 (3%)	4 (1%)	22 60
1	E	576/578 (100%)	554 (96%)	15 (3%)	7 (1%)	13 48
1	F	574/578 (99%)	559 (97%)	12 (2%)	3 (0%)	29 68
2	G	190/192 (99%)	177 (93%)	13 (7%)	0	100 100
2	H	190/192 (99%)	171 (90%)	15 (8%)	4 (2%)	7 33
2	I	190/192 (99%)	180 (95%)	8 (4%)	2 (1%)	14 50
2	J	190/192 (99%)	184 (97%)	6 (3%)	0	100 100
2	K	190/192 (99%)	180 (95%)	10 (5%)	0	100 100
2	L	190/192 (99%)	181 (95%)	9 (5%)	0	100 100
2	M	190/192 (99%)	180 (95%)	9 (5%)	1 (0%)	29 68
2	N	190/192 (99%)	182 (96%)	7 (4%)	1 (0%)	29 68
2	O	190/192 (99%)	184 (97%)	6 (3%)	0	100 100
2	P	190/192 (99%)	183 (96%)	7 (4%)	0	100 100
2	Q	190/192 (99%)	184 (97%)	6 (3%)	0	100 100
2	R	190/192 (99%)	183 (96%)	7 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	S	190/192 (99%)	184 (97%)	6 (3%)	0	100 100
2	T	190/192 (99%)	183 (96%)	7 (4%)	0	100 100
All	All	6096/6156 (99%)	5839 (96%)	223 (4%)	34 (1%)	29 64

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	308	LYS
1	B	293	ALA
1	B	637	THR
1	E	438	GLU
1	E	442	SER

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 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	469/485 (97%)	457 (97%)	12 (3%)	46 78
1	B	485/485 (100%)	465 (96%)	20 (4%)	30 67
1	C	485/485 (100%)	478 (99%)	7 (1%)	67 88
1	D	485/485 (100%)	473 (98%)	12 (2%)	47 79
1	E	485/485 (100%)	478 (99%)	7 (1%)	67 88
1	F	485/485 (100%)	483 (100%)	2 (0%)	91 97
2	G	162/162 (100%)	159 (98%)	3 (2%)	57 84
2	H	162/162 (100%)	147 (91%)	15 (9%)	9 33
2	I	162/162 (100%)	157 (97%)	5 (3%)	40 75
2	J	162/162 (100%)	160 (99%)	2 (1%)	71 90
2	K	162/162 (100%)	158 (98%)	4 (2%)	47 79
2	L	162/162 (100%)	156 (96%)	6 (4%)	34 70
2	M	162/162 (100%)	156 (96%)	6 (4%)	34 70
2	N	162/162 (100%)	160 (99%)	2 (1%)	71 90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	O	162/162 (100%)	162 (100%)	0	100 100
2	P	162/162 (100%)	160 (99%)	2 (1%)	71 90
2	Q	162/162 (100%)	161 (99%)	1 (1%)	86 95
2	R	162/162 (100%)	160 (99%)	2 (1%)	71 90
2	S	162/162 (100%)	162 (100%)	0	100 100
2	T	162/162 (100%)	161 (99%)	1 (1%)	86 95
All	All	5162/5178 (100%)	5053 (98%)	109 (2%)	56 82

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	722	PHE
2	H	85	THR
2	M	125	ARG
1	F	339	ARG
2	H	29	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	579	GLN
2	I	137	GLN
1	F	621	HIS
2	R	55	ASN
2	I	55	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
5	ADP	E	802	1	24,29,29	4.37	5 (20%)	29,45,45	1.43	4 (13%)
5	ADP	F	801	-	24,29,29	4.53	9 (37%)	29,45,45	1.84	8 (27%)
5	ADP	E	801	-	24,29,29	4.56	9 (37%)	29,45,45	1.78	6 (20%)
5	ADP	A	802	-	24,29,29	4.25	8 (33%)	29,45,45	1.79	6 (20%)
6	AGS	D	802	-	26,33,33	4.02	12 (46%)	26,52,52	2.10	9 (34%)
5	ADP	A	801	-	24,29,29	4.31	9 (37%)	29,45,45	1.90	6 (20%)
6	AGS	C	802	-	26,33,33	3.85	12 (46%)	26,52,52	1.99	5 (19%)
6	AGS	C	801	-	26,33,33	4.06	11 (42%)	26,52,52	1.86	5 (19%)
6	AGS	D	801	-	26,33,33	3.71	11 (42%)	26,52,52	1.80	4 (15%)
6	AGS	B	802	-	26,33,33	3.79	11 (42%)	26,52,52	1.86	6 (23%)
6	AGS	E	803	-	26,33,33	3.99	10 (38%)	26,52,52	1.74	5 (19%)
6	AGS	B	801	-	26,33,33	3.83	12 (46%)	26,52,52	2.06	7 (26%)

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
5	ADP	E	802	1	2/2/6/6	5/12/32/32	0/3/3/3
5	ADP	F	801	-	2/2/6/6	0/12/32/32	0/3/3/3
5	ADP	E	801	-	2/2/6/6	4/12/32/32	0/3/3/3
5	ADP	A	802	-	1/1/6/6	1/12/32/32	0/3/3/3
6	AGS	D	802	-	3/3/7/7	4/17/38/38	0/3/3/3
5	ADP	A	801	-	2/2/6/6	5/12/32/32	0/3/3/3
6	AGS	C	802	-	2/2/7/7	6/17/38/38	0/3/3/3
6	AGS	C	801	-	2/2/7/7	2/17/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	AGS	D	801	-	2/2/7/7	4/17/38/38	0/3/3/3
6	AGS	B	802	-	3/3/7/7	1/17/38/38	0/3/3/3
6	AGS	E	803	-	2/2/7/7	2/17/38/38	0/3/3/3
6	AGS	B	801	-	2/2/7/7	3/17/38/38	0/3/3/3

The worst 5 of 119 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	801	ADP	O4'-C1'	17.04	1.64	1.41
5	E	801	ADP	O4'-C1'	16.63	1.64	1.41
5	A	802	ADP	O4'-C1'	16.03	1.63	1.41
5	A	801	ADP	O4'-C1'	15.56	1.62	1.41
5	E	802	ADP	O4'-C1'	15.04	1.62	1.41

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	801	ADP	O4'-C1'-C2'	-5.63	98.70	106.93
6	C	802	AGS	PA-O3A-PB	-5.25	114.81	132.83
6	B	801	AGS	PA-O3A-PB	-5.03	115.58	132.83
6	C	802	AGS	N3-C2-N1	-5.00	120.87	128.68
5	F	801	ADP	N3-C2-N1	-4.96	120.92	128.68

5 of 25 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	801	ADP	C3'
5	A	801	ADP	C1'
5	A	802	ADP	C1'
5	E	801	ADP	C3'
5	E	801	ADP	C1'

5 of 37 torsion outliers are listed below:

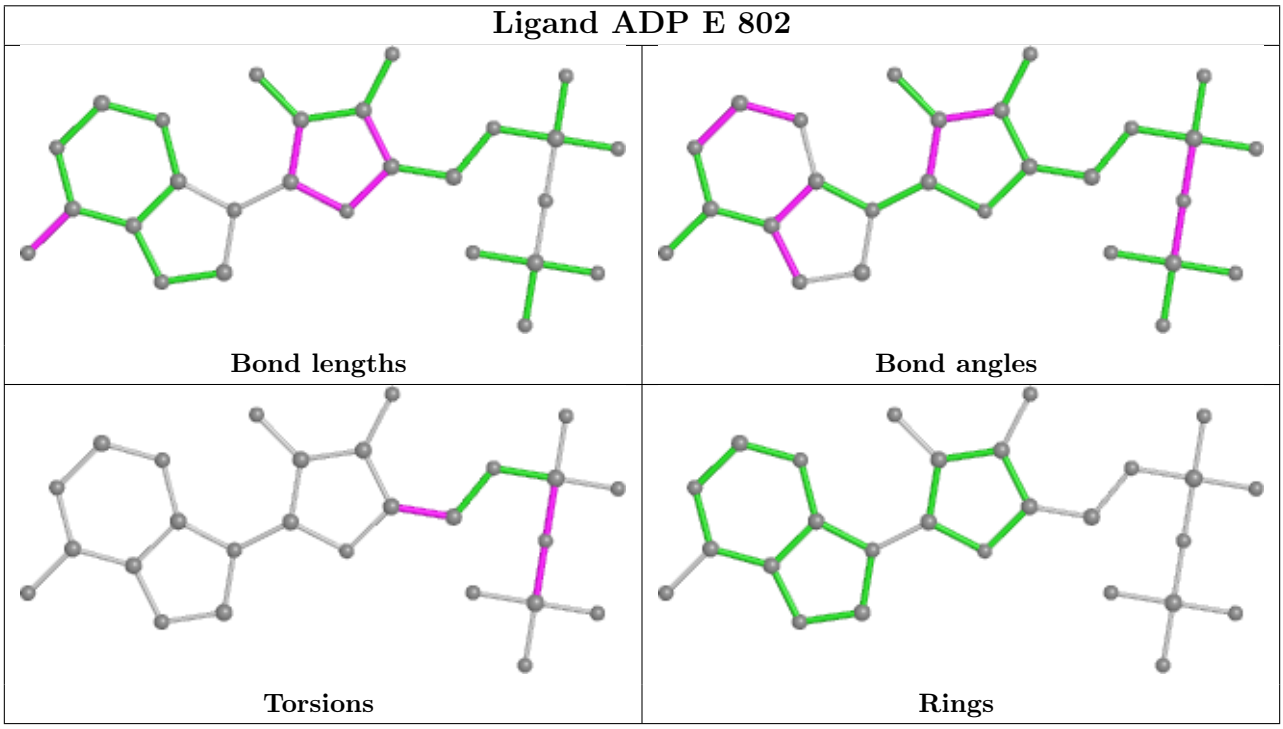
Mol	Chain	Res	Type	Atoms
5	A	801	ADP	C5'-O5'-PA-O3A
5	A	801	ADP	C4'-C5'-O5'-PA
5	A	802	ADP	C5'-O5'-PA-O1A
5	E	801	ADP	C5'-O5'-PA-O3A
6	B	801	AGS	C5'-O5'-PA-O1A

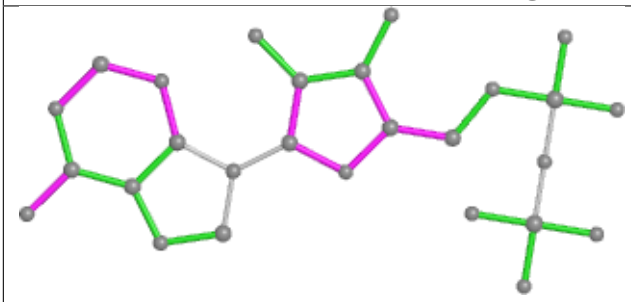
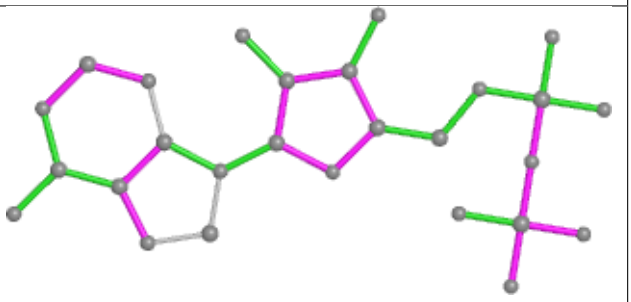
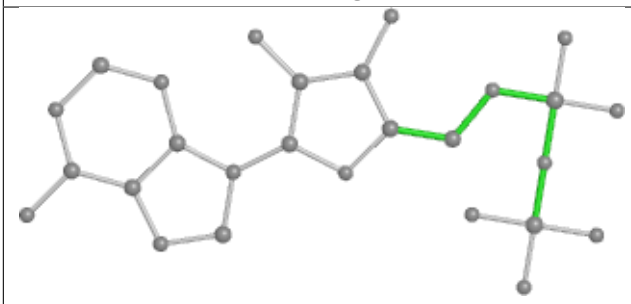
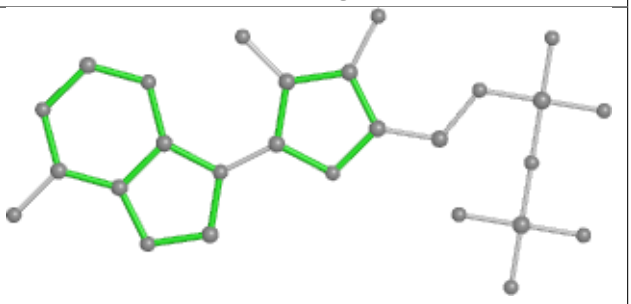
There are no ring outliers.

8 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	802	ADP	17	0
5	F	801	ADP	1	0
5	E	801	ADP	2	0
5	A	802	ADP	1	0
6	D	802	AGS	1	0
6	C	802	AGS	1	0
6	B	802	AGS	4	0
6	E	803	AGS	9	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 then 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 ADP F 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

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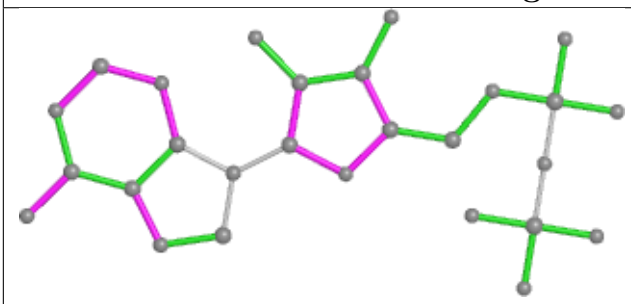
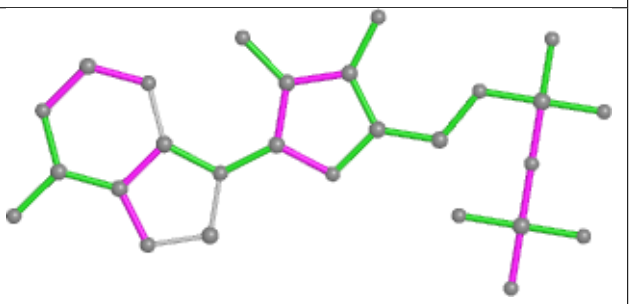
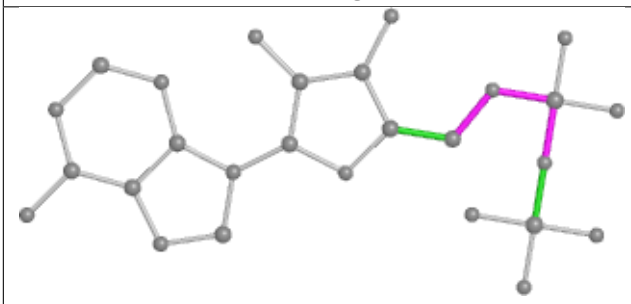
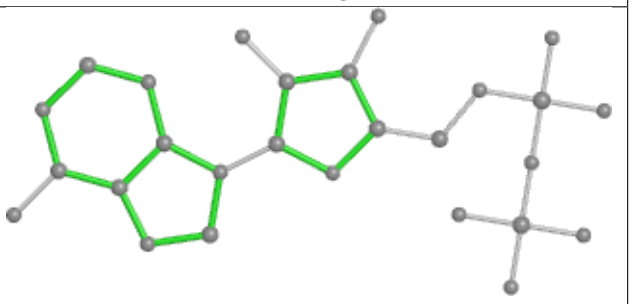
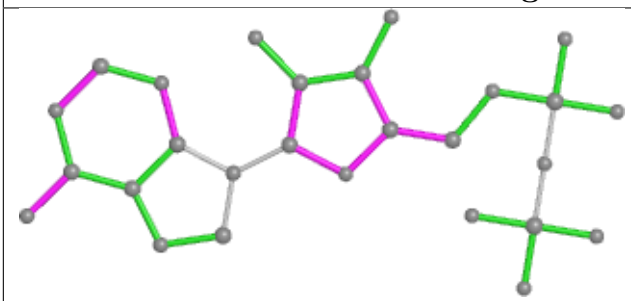
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP A 802



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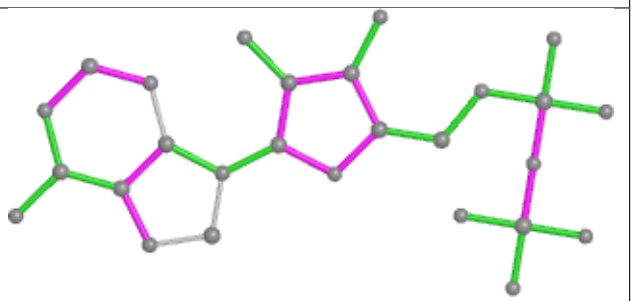

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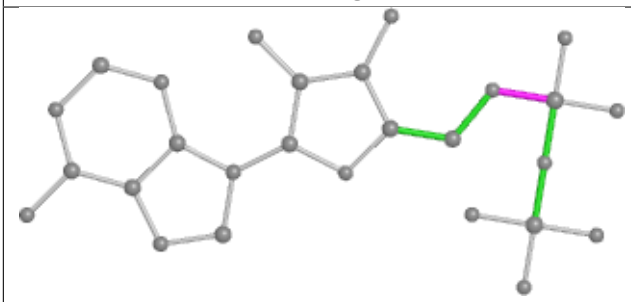

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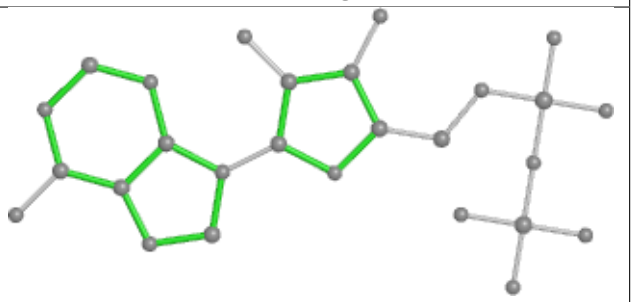
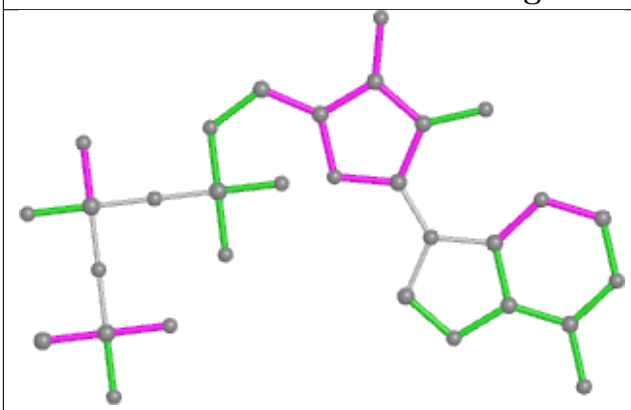


Rings

Ligand AGS D 802



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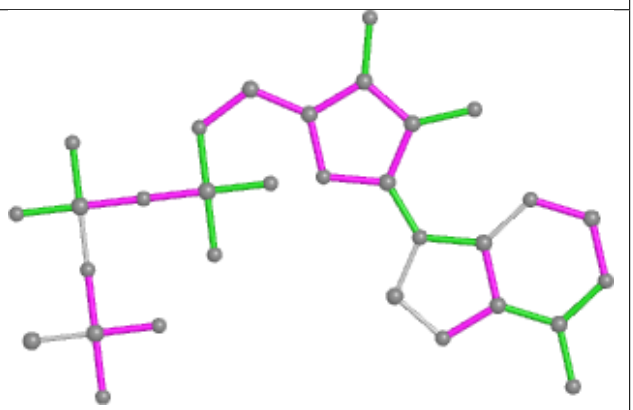

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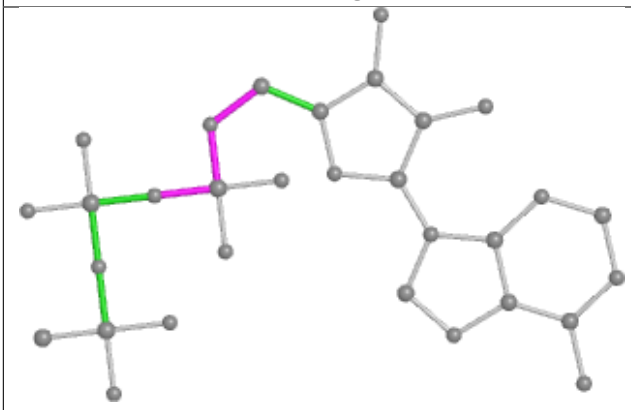

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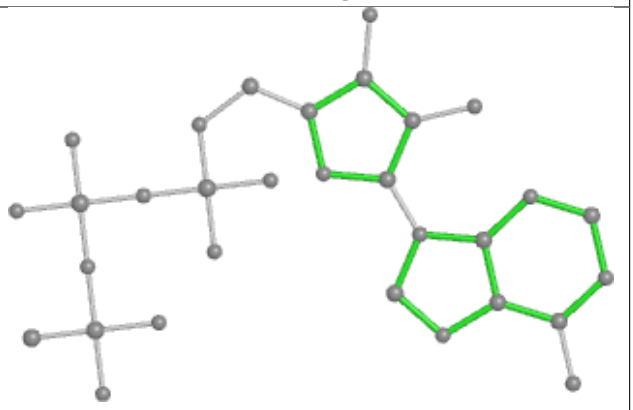
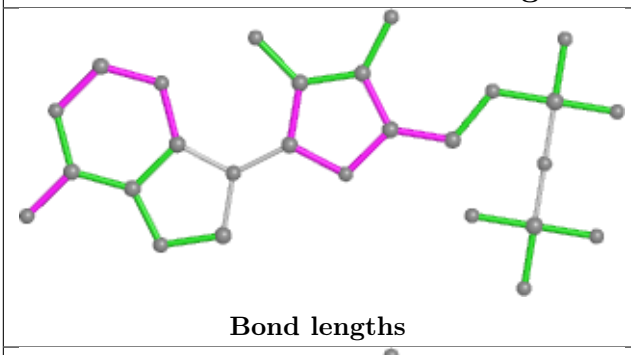


Rings

Ligand ADP A 801



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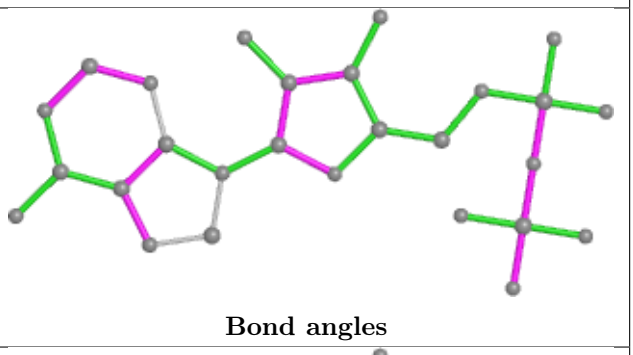
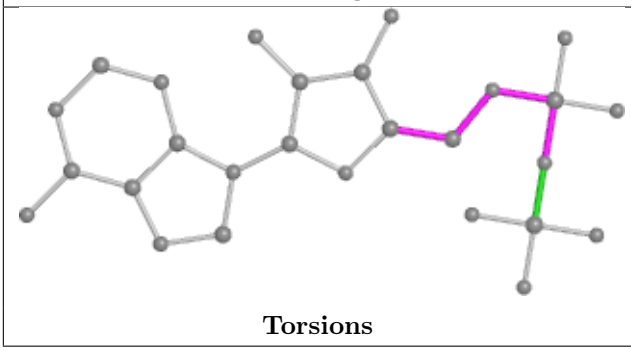


Bond angles



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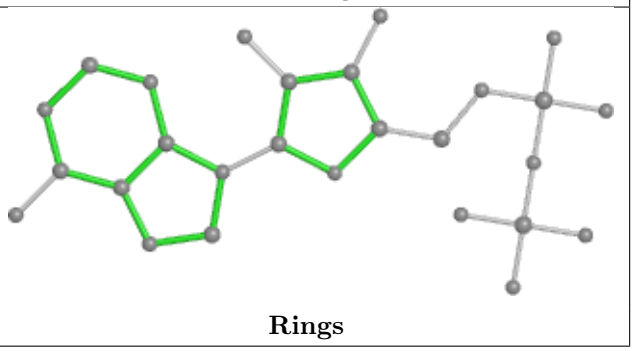

Rings

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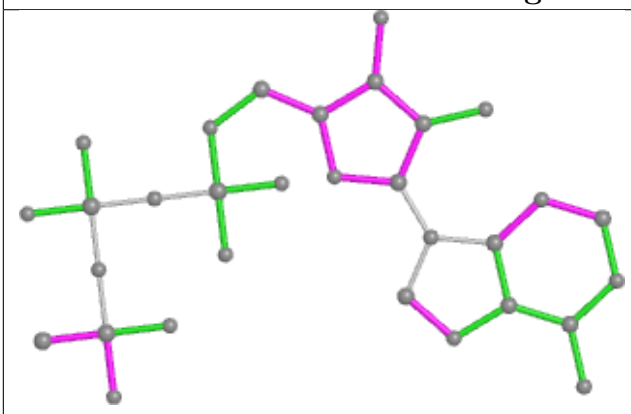
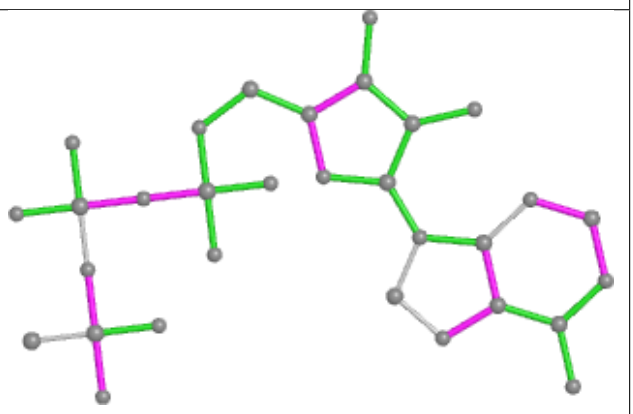
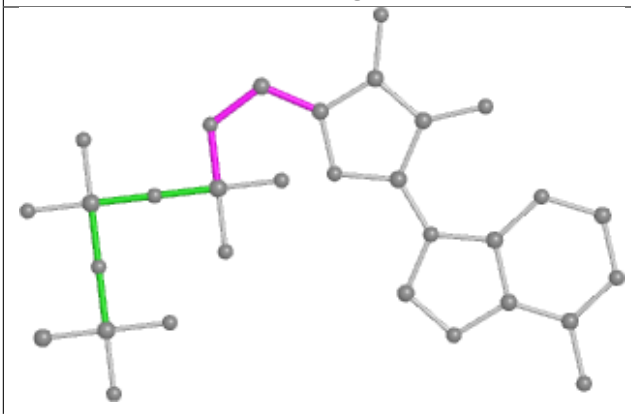


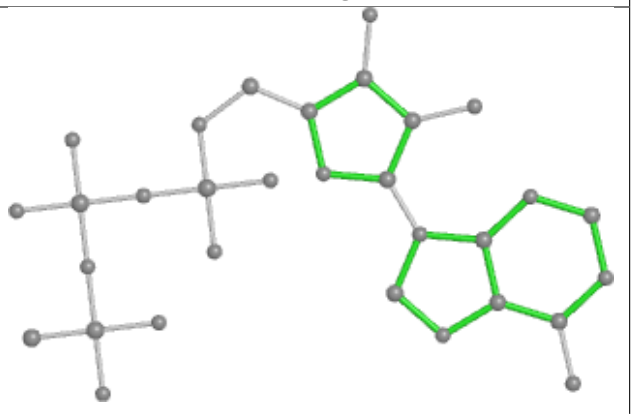
Bond lengths



Bond angles

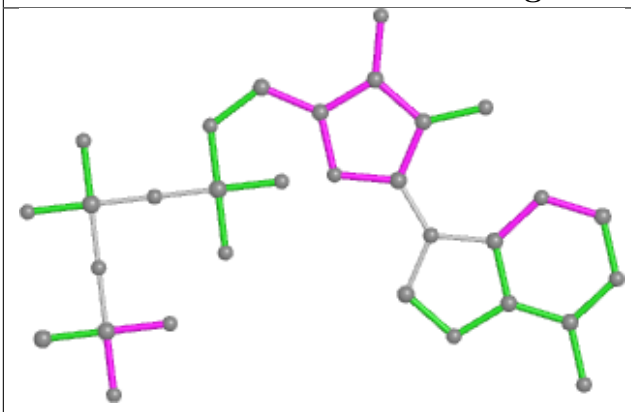


Torsions



Rings

Ligand AGS C 801



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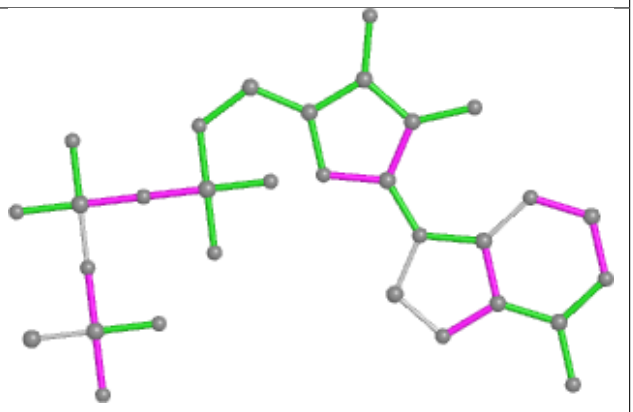
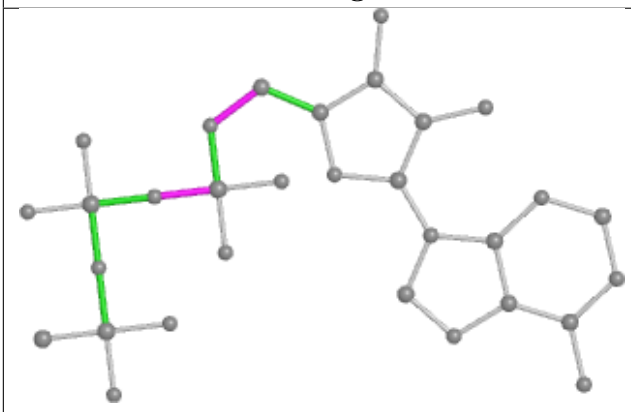
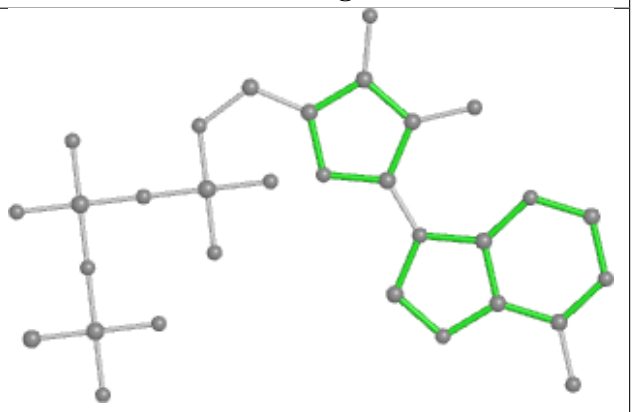


Bond angles

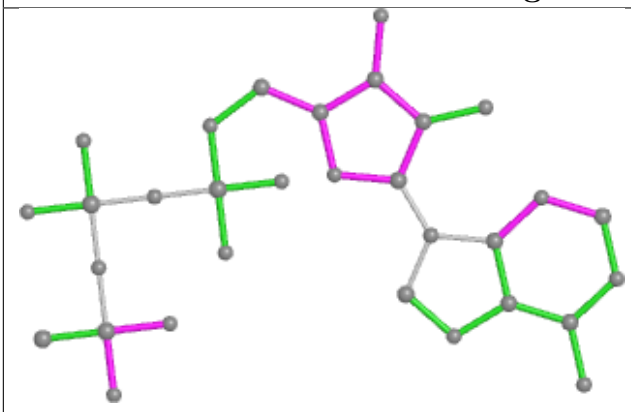


Torsions

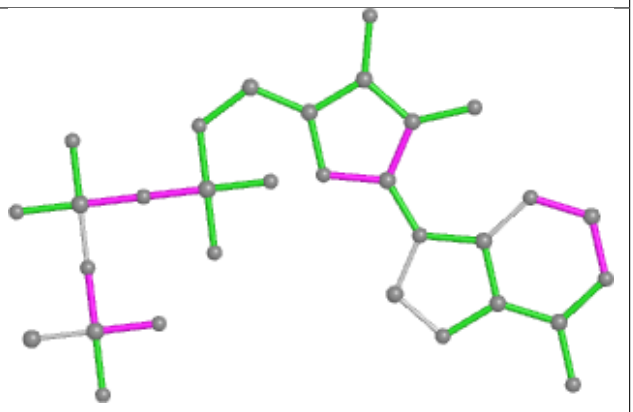


Rings

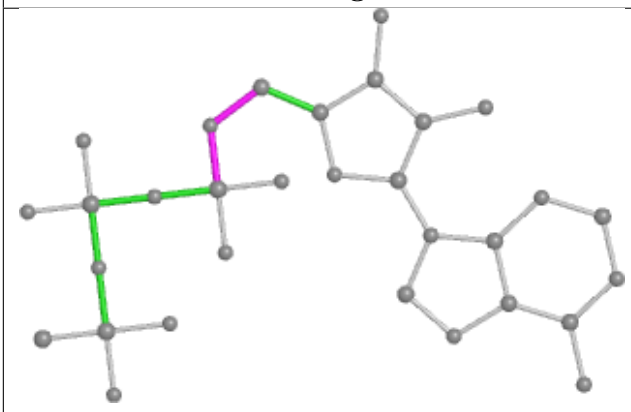
Ligand AGS D 801



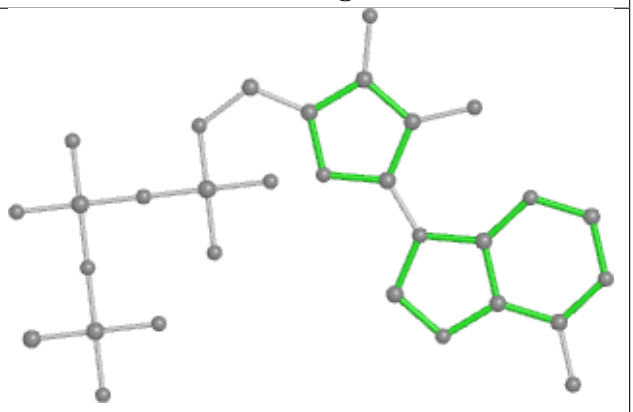
Bond lengths



Bond angles

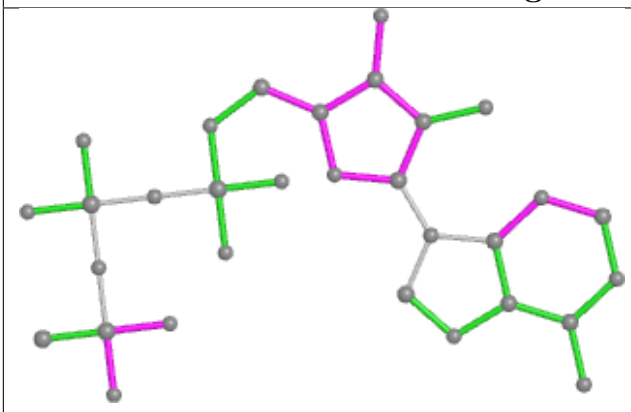


Torsions

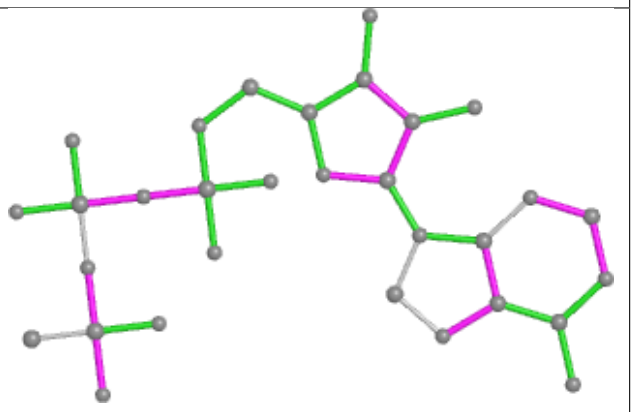


Rings

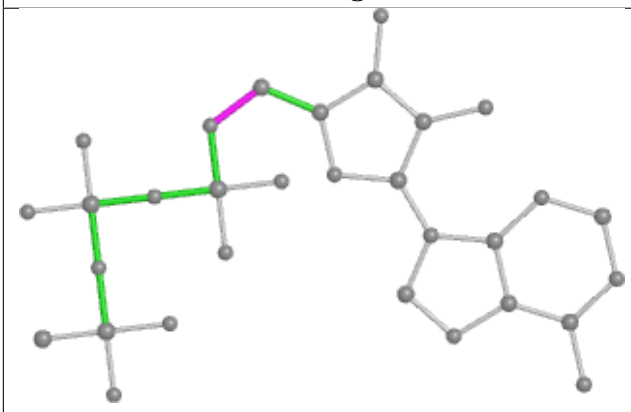
Ligand AGS B 802



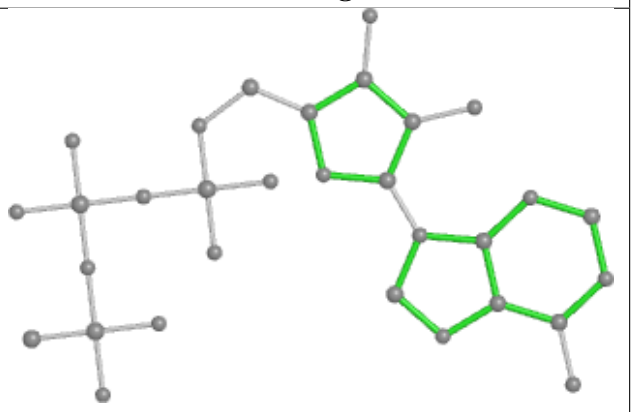
Bond lengths



Bond angles

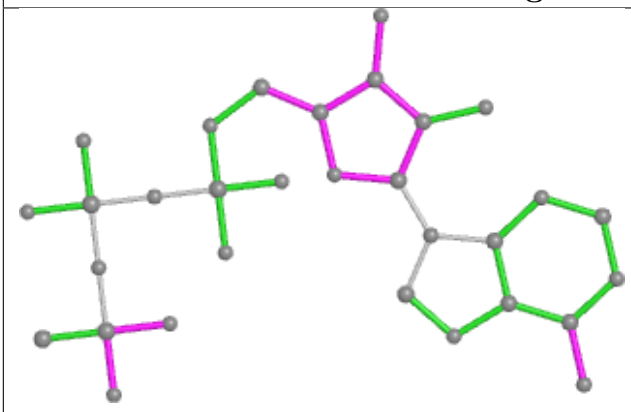


Torsions

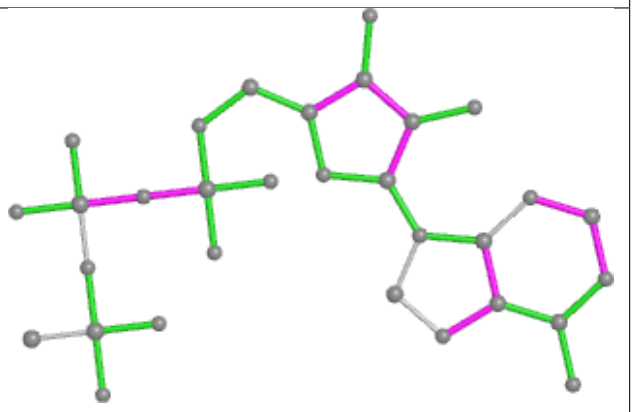


Rings

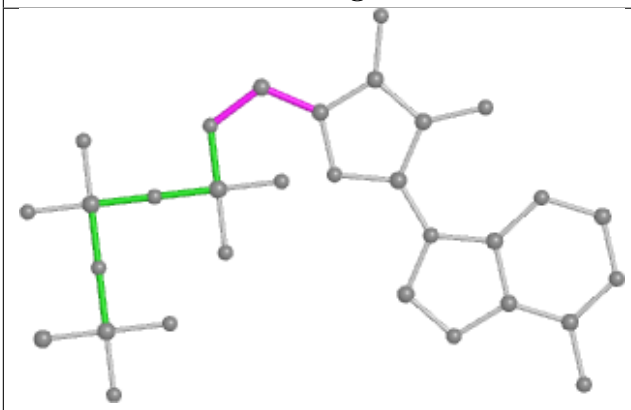
Ligand AGS E 803



Bond lengths



Bond angles



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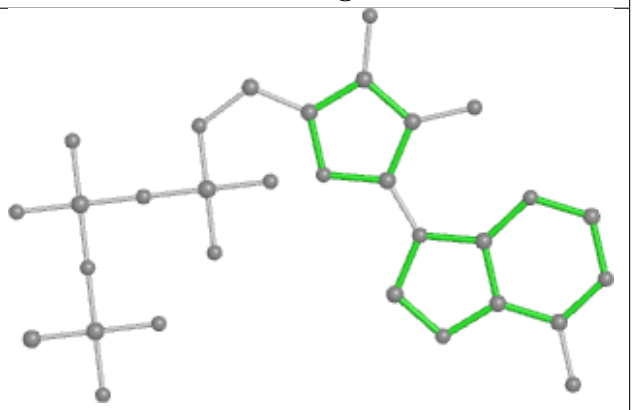
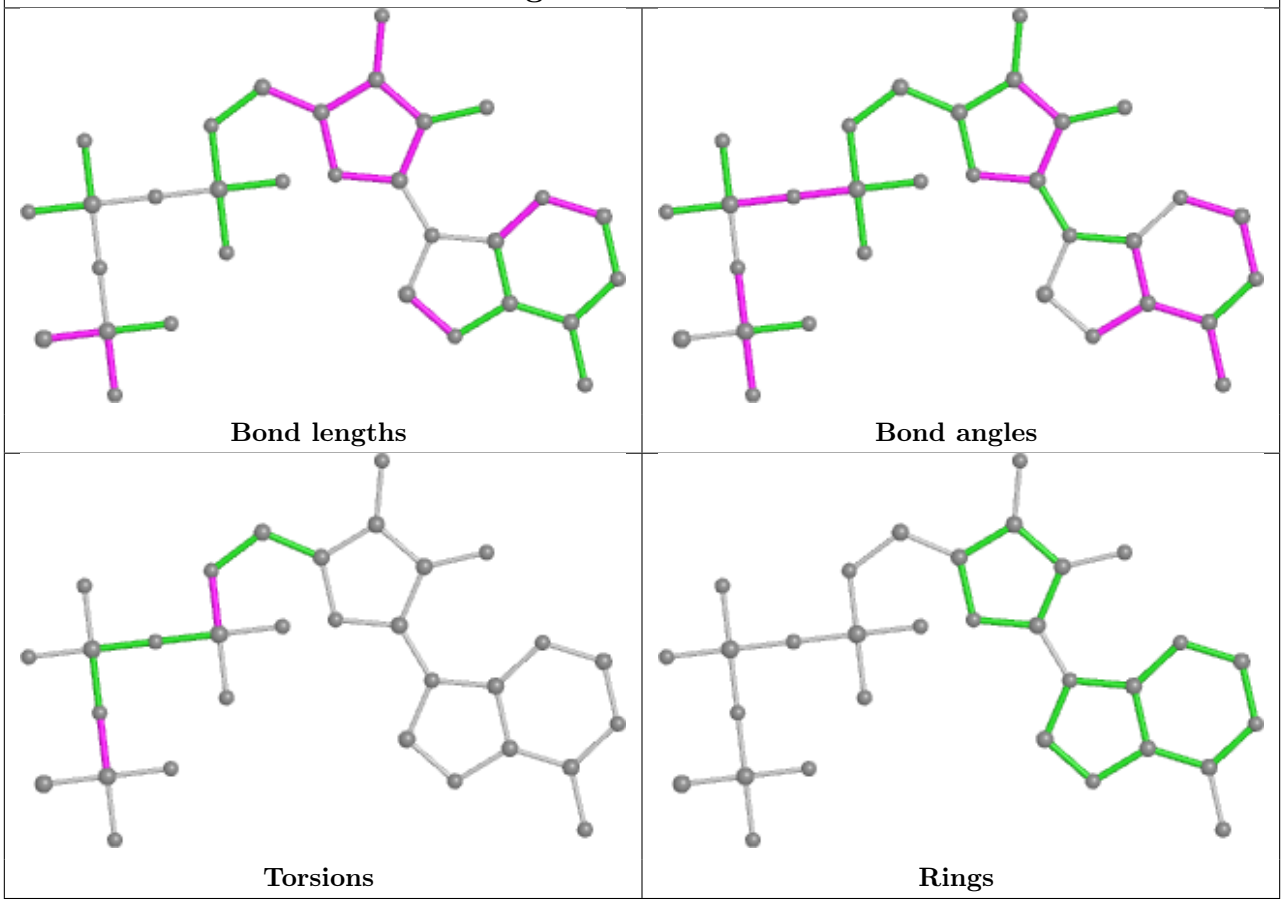


Rings

Ligand AGS B 801



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	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	214:GLY	C	215:GLU	N	3.06