wwPDB EM Validation Summary Report ⓘ

Mar 4, 2025 – 06:19 pm GMT

PDB ID	:	9EMA
EMDB ID	:	EMD-19815
Title	:	RUVBL1/2 in complex with ATP and CB-6644 inhibitor
Authors	:	Lopez-Perrote, A.; Llorca, O.; Garcia-Martin, C.
Deposited on	:	2024-03-07
Resolution	:	2.40 Å(reported)
Based on initial model	:	.

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 ⓘ 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 ⓘ) were used in the production of this report:

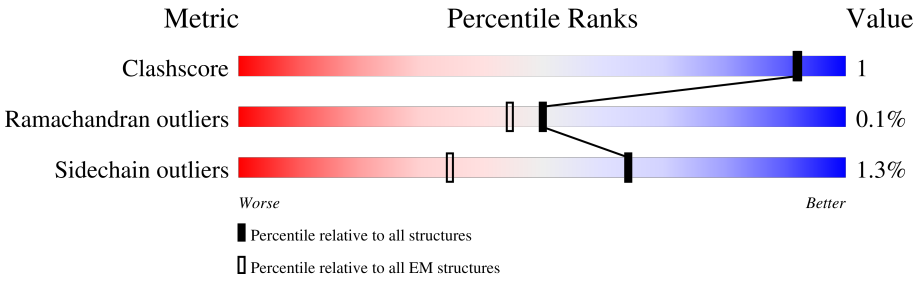
EMDB validation analysis	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

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 2.40 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	459	67% · 29%
1	B	459	67% · 29%
1	C	459	66% 5% 29%
2	D	481	67% · 31%
2	E	481	66% · 31%
2	F	481	66% · 31%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15562 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 RuvB-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	326	Total 2508	C 1583	N 437	O 474	S 14	0	0
1	B	326	Total 2508	C 1583	N 437	O 474	S 14	0	0
1	C	326	Total 2508	C 1583	N 437	O 474	S 14	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q9Y265
A	-1	SER	-	expression tag	UNP Q9Y265
A	0	HIS	-	expression tag	UNP Q9Y265
B	-2	GLY	-	expression tag	UNP Q9Y265
B	-1	SER	-	expression tag	UNP Q9Y265
B	0	HIS	-	expression tag	UNP Q9Y265
C	-2	GLY	-	expression tag	UNP Q9Y265
C	-1	SER	-	expression tag	UNP Q9Y265
C	0	HIS	-	expression tag	UNP Q9Y265

- Molecule 2 is a protein called RuvB-like 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	332	Total 2576	C 1613	N 457	O 494	S 12	0	0
2	E	332	Total 2576	C 1613	N 457	O 494	S 12	0	0
2	F	332	Total 2576	C 1613	N 457	O 494	S 12	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	MET	-	initiating methionine	UNP Q9Y230
D	-16	ALA	-	expression tag	UNP Q9Y230
D	-15	ASP	-	expression tag	UNP Q9Y230
D	-14	LEU	-	expression tag	UNP Q9Y230
D	-13	ASN	-	expression tag	UNP Q9Y230
D	-12	TRP	-	expression tag	UNP Q9Y230
D	-11	ILE	-	expression tag	UNP Q9Y230
D	-10	SER	-	expression tag	UNP Q9Y230
D	-9	ALA	-	expression tag	UNP Q9Y230
D	-8	GLY	-	expression tag	UNP Q9Y230
D	-7	HIS	-	expression tag	UNP Q9Y230
D	-6	ALA	-	expression tag	UNP Q9Y230
D	-5	ILE	-	expression tag	UNP Q9Y230
D	-4	ALA	-	expression tag	UNP Q9Y230
D	-3	ASP	-	expression tag	UNP Q9Y230
D	-2	VAL	-	expression tag	UNP Q9Y230
D	-1	GLY	-	expression tag	UNP Q9Y230
D	0	THR	-	expression tag	UNP Q9Y230
E	-17	MET	-	initiating methionine	UNP Q9Y230
E	-16	ALA	-	expression tag	UNP Q9Y230
E	-15	ASP	-	expression tag	UNP Q9Y230
E	-14	LEU	-	expression tag	UNP Q9Y230
E	-13	ASN	-	expression tag	UNP Q9Y230
E	-12	TRP	-	expression tag	UNP Q9Y230
E	-11	ILE	-	expression tag	UNP Q9Y230
E	-10	SER	-	expression tag	UNP Q9Y230
E	-9	ALA	-	expression tag	UNP Q9Y230
E	-8	GLY	-	expression tag	UNP Q9Y230
E	-7	HIS	-	expression tag	UNP Q9Y230
E	-6	ALA	-	expression tag	UNP Q9Y230
E	-5	ILE	-	expression tag	UNP Q9Y230
E	-4	ALA	-	expression tag	UNP Q9Y230
E	-3	ASP	-	expression tag	UNP Q9Y230
E	-2	VAL	-	expression tag	UNP Q9Y230
E	-1	GLY	-	expression tag	UNP Q9Y230
E	0	THR	-	expression tag	UNP Q9Y230
F	-17	MET	-	initiating methionine	UNP Q9Y230
F	-16	ALA	-	expression tag	UNP Q9Y230
F	-15	ASP	-	expression tag	UNP Q9Y230
F	-14	LEU	-	expression tag	UNP Q9Y230
F	-13	ASN	-	expression tag	UNP Q9Y230
F	-12	TRP	-	expression tag	UNP Q9Y230
F	-11	ILE	-	expression tag	UNP Q9Y230

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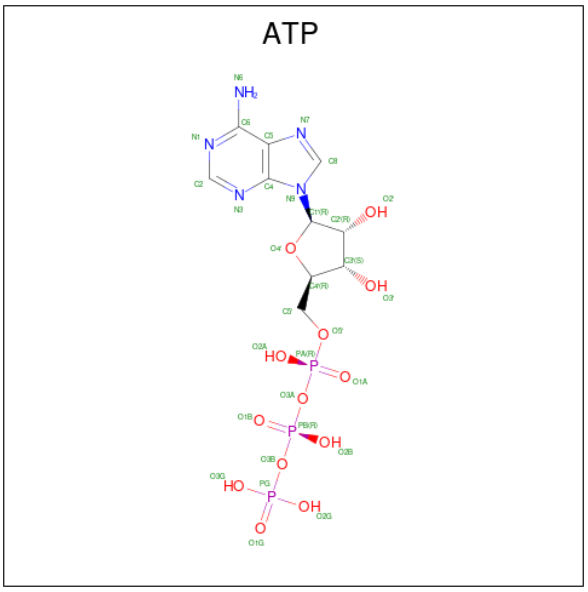
Chain	Residue	Modelled	Actual	Comment	Reference
F	-10	SER	-	expression tag	UNP Q9Y230
F	-9	ALA	-	expression tag	UNP Q9Y230
F	-8	GLY	-	expression tag	UNP Q9Y230
F	-7	HIS	-	expression tag	UNP Q9Y230
F	-6	ALA	-	expression tag	UNP Q9Y230
F	-5	ILE	-	expression tag	UNP Q9Y230
F	-4	ALA	-	expression tag	UNP Q9Y230
F	-3	ASP	-	expression tag	UNP Q9Y230
F	-2	VAL	-	expression tag	UNP Q9Y230
F	-1	GLY	-	expression tag	UNP Q9Y230
F	0	THR	-	expression tag	UNP Q9Y230

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

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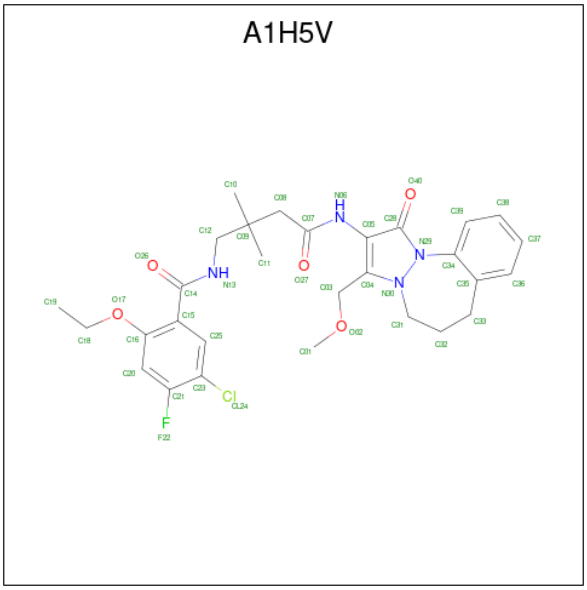
Mol	Chain	Residues	Atoms					AltConf
3	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is 5-chloranyl-2-ethoxy-4-fluoranyl- {N}-[4-[[3-(methoxymethyl)-1-oxidanylidene-6,7-dihydro-5 {H}-pyrazolo[1,2-a][1,2]benzodiazepin-2-yl]amino]-2,2-dimethyl-4-oxidanylidene-butyl]benzamide (three-letter code: A1H5V) (formula: $C_{29}H_{34}ClFN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	Cl	F	N	O	0
			40	29	1	1	4	5	
4	B	1	Total	C	Cl	F	N	O	0
			40	29	1	1	4	5	
4	C	1	Total	C	Cl	F	N	O	0
			40	29	1	1	4	5	

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

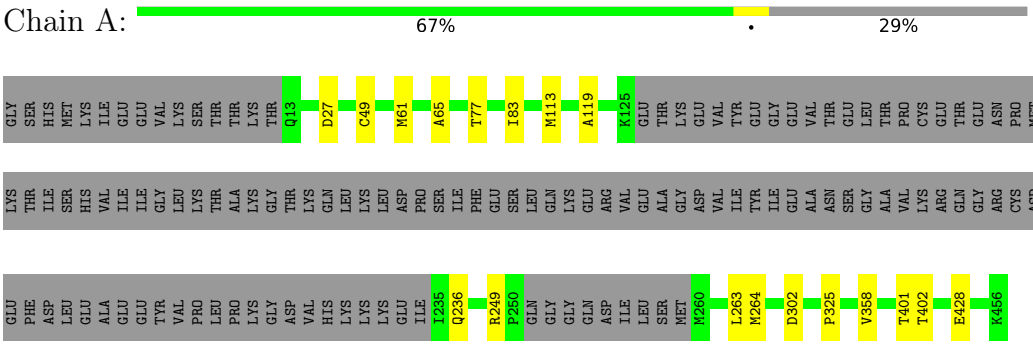
Mol	Chain	Residues	Atoms		AltConf
5	D	1	Total	Mg	0
			1	1	
5	E	1	Total	Mg	0
			1	1	
5	F	2	Total	Mg	0
			2	2	

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.

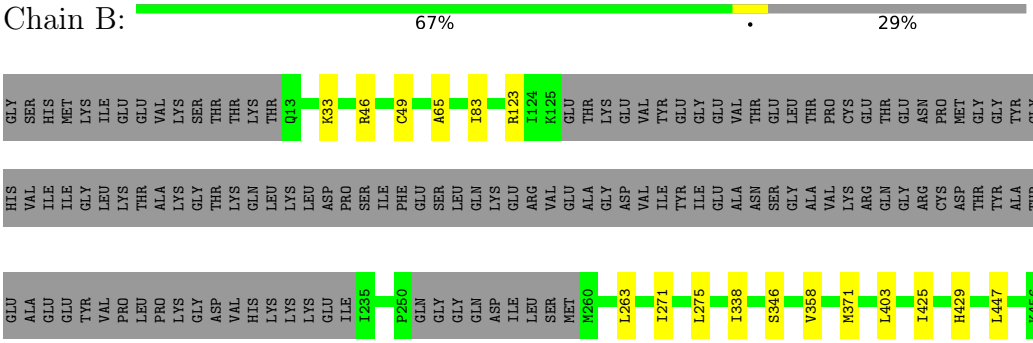
- Molecule 1: RuvB-like 1

Chain A:



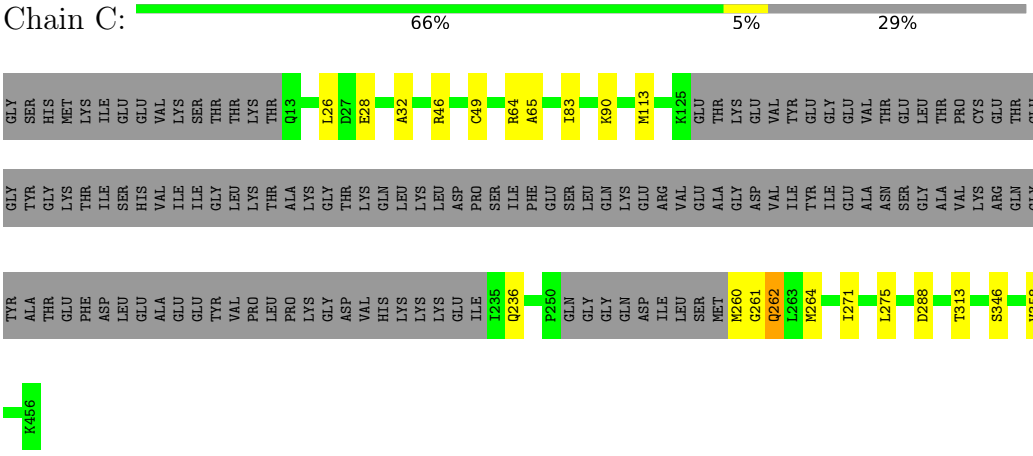
- Molecule 1: RuvB-like 1

Chain B:



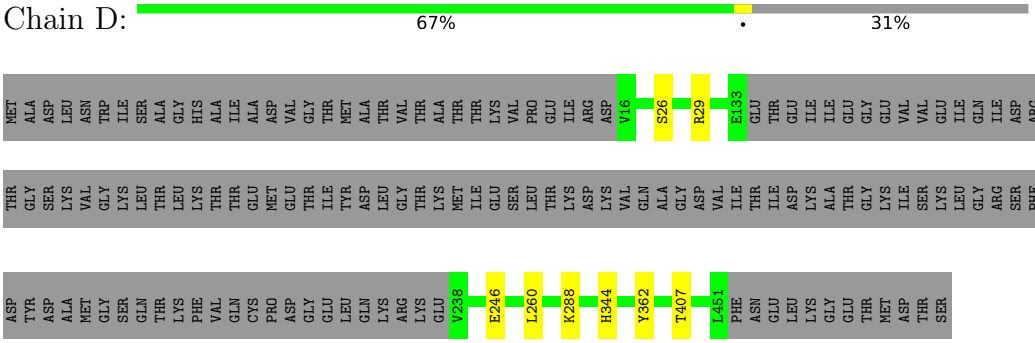
- Molecule 1: RuvB-like 1

Chain C:



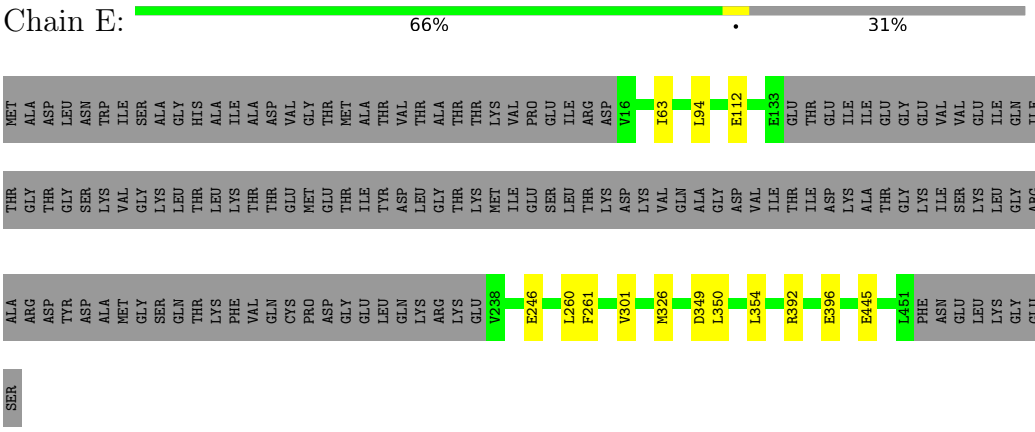
• Molecule 2: RuvB-like 2

Chain D:



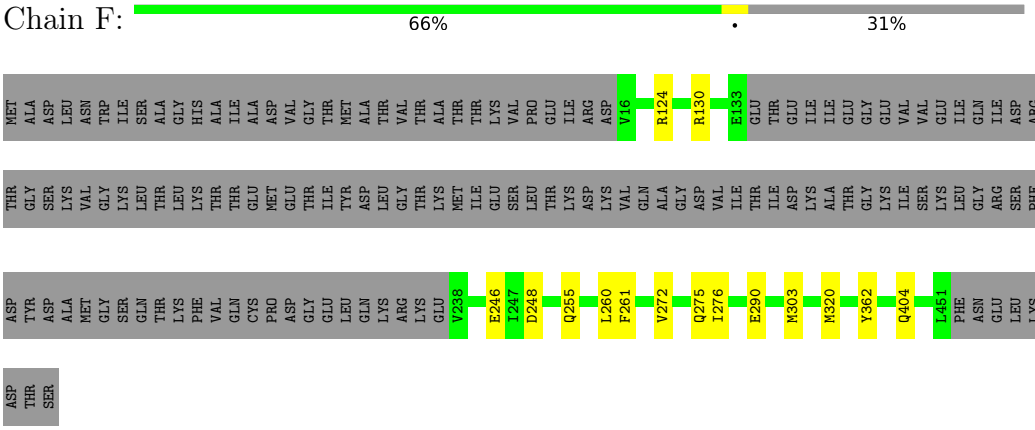
• Molecule 2: RuvB-like 2

Chain E:



• Molecule 2: RuvB-like 2

Chain F:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	393823	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 ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k 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: ATP, MG, A1H5V

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	0.34	0/2538	0.68	0/3417
1	B	0.34	0/2538	0.70	0/3417
1	C	0.35	0/2538	0.68	0/3417
2	D	0.33	0/2608	0.74	0/3515
2	E	0.36	0/2608	0.78	0/3515
2	F	0.33	0/2608	0.75	0/3515
All	All	0.34	0/15438	0.72	0/20796

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2508	0	2612	8	0
1	B	2508	0	2612	9	0
1	C	2508	0	2612	13	0
2	D	2576	0	2626	5	0
2	E	2576	0	2626	8	0
2	F	2576	0	2626	10	0
3	A	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	12	0	0
3	C	31	0	12	1	0
3	D	31	0	12	1	0
3	E	31	0	12	0	0
3	F	31	0	12	1	0
4	A	40	0	0	0	0
4	B	40	0	0	0	0
4	C	40	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	2	0	0	0	0
All	All	15562	0	15786	45	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 1.

The worst 5 of 45 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:F:124:ARG:NE	2:F:248:ASP:OD2	2.29	0.66
1:C:261:GLY:O	1:C:264:MET:N	2.34	0.60
1:A:263:LEU:O	2:F:255:GLN:NE2	2.37	0.57
1:C:64:ARG:NH2	2:F:404:GLN:O	2.37	0.57
2:D:26:SER:O	2:D:29:ARG:NH1	2.39	0.55

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	320/459 (70%)	318 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	320/459 (70%)	315 (98%)	5 (2%)	0	100 100
1	C	320/459 (70%)	310 (97%)	9 (3%)	1 (0%)	37 51
2	D	328/481 (68%)	325 (99%)	3 (1%)	0	100 100
2	E	328/481 (68%)	324 (99%)	4 (1%)	0	100 100
2	F	328/481 (68%)	325 (99%)	3 (1%)	0	100 100
All	All	1944/2820 (69%)	1917 (99%)	26 (1%)	1 (0%)	50 65

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	262	GLN

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	275/389 (71%)	269 (98%)	6 (2%)	47 67
1	B	275/389 (71%)	273 (99%)	2 (1%)	81 91
1	C	275/389 (71%)	267 (97%)	8 (3%)	37 58
2	D	277/402 (69%)	276 (100%)	1 (0%)	89 95
2	E	277/402 (69%)	275 (99%)	2 (1%)	81 91
2	F	277/402 (69%)	275 (99%)	2 (1%)	81 91
All	All	1656/2373 (70%)	1635 (99%)	21 (1%)	64 81

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	346	SER
2	E	112	GLU
2	F	320	MET
2	E	445	GLU
2	D	288	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 (i)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	A1H5V	A	502	-	42,43,43	2.85	11 (26%)	53,62,62	2.20	11 (20%)
3	ATP	A	501	5	26,33,33	0.64	0	31,52,52	1.06	1 (3%)
4	A1H5V	C	502	-	42,43,43	2.88	11 (26%)	53,62,62	2.26	9 (16%)
3	ATP	D	801	5	26,33,33	0.68	1 (3%)	31,52,52	1.04	2 (6%)
3	ATP	C	501	-	26,33,33	0.63	0	31,52,52	1.06	1 (3%)
3	ATP	E	801	5	26,33,33	0.67	1 (3%)	31,52,52	1.04	2 (6%)
4	A1H5V	B	501	-	42,43,43	2.88	11 (26%)	53,62,62	2.25	10 (18%)
3	ATP	F	802	5	26,33,33	0.68	1 (3%)	31,52,52	1.05	3 (9%)
3	ATP	B	500	-	26,33,33	0.62	0	31,52,52	1.05	1 (3%)

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
4	A1H5V	A	502	-	-	3/25/35/35	0/3/4/4
3	ATP	A	501	5	-	5/18/38/38	0/3/3/3
4	A1H5V	C	502	-	-	2/25/35/35	0/3/4/4
3	ATP	D	801	5	-	3/18/38/38	0/3/3/3
3	ATP	C	501	-	-	9/18/38/38	0/3/3/3
3	ATP	E	801	5	-	3/18/38/38	0/3/3/3
4	A1H5V	B	501	-	-	5/25/35/35	0/3/4/4
3	ATP	F	802	5	-	4/18/38/38	0/3/3/3
3	ATP	B	500	-	-	1/18/38/38	0/3/3/3

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	A1H5V	C05-C04	14.40	1.56	1.36
4	C	502	A1H5V	C05-C04	14.27	1.55	1.36
4	A	502	A1H5V	C05-C04	14.25	1.55	1.36
4	C	502	A1H5V	C34-N29	5.94	1.49	1.43
4	A	502	A1H5V	C34-N29	5.92	1.49	1.43

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	502	A1H5V	C31-N30-C04	-8.65	113.52	128.24
4	B	501	A1H5V	C31-N30-C04	-7.82	114.92	128.24
4	A	502	A1H5V	C31-N30-C04	-7.76	115.02	128.24
4	C	502	A1H5V	C28-C05-C04	-6.69	105.03	108.98
4	A	502	A1H5V	C28-C05-C04	-6.17	105.34	108.98

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	ATP	C5'-O5'-PA-O1A
3	C	501	ATP	C5'-O5'-PA-O1A
3	E	801	ATP	O4'-C4'-C5'-O5'
3	F	802	ATP	O4'-C4'-C5'-O5'
4	A	502	A1H5V	O02-C03-C04-C05

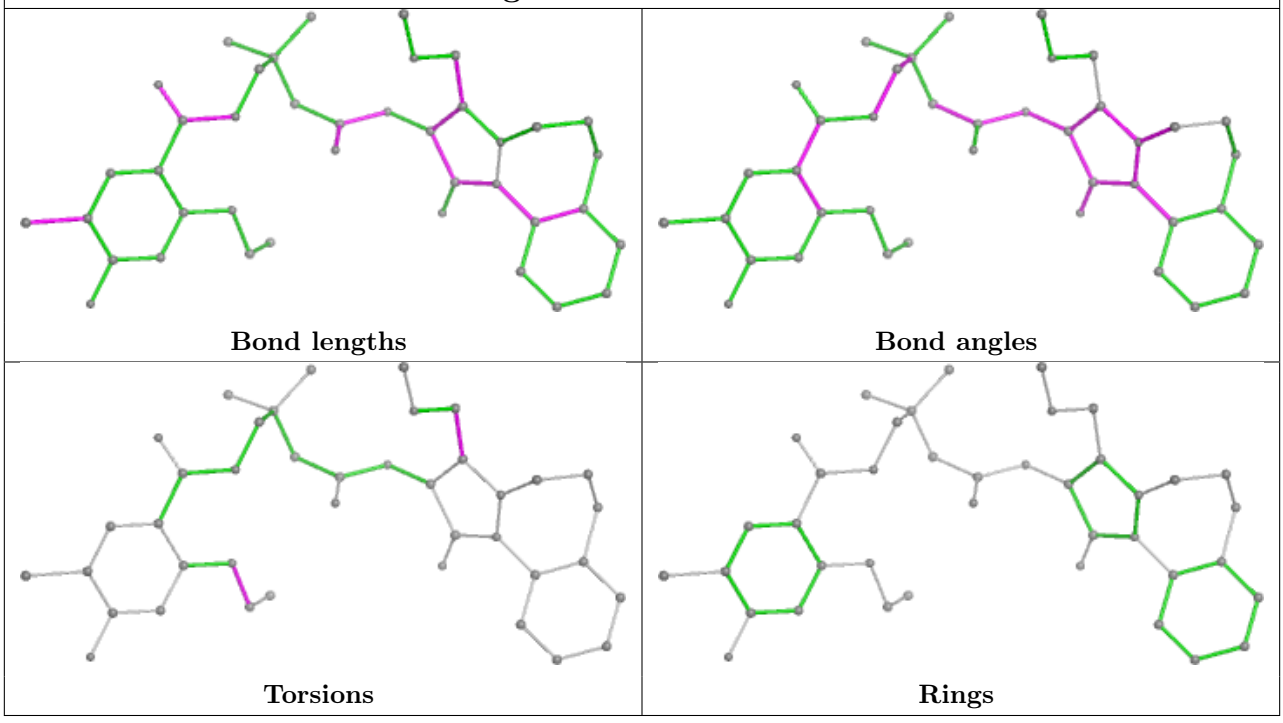
There are no ring outliers.

3 monomers are involved in 3 short contacts:

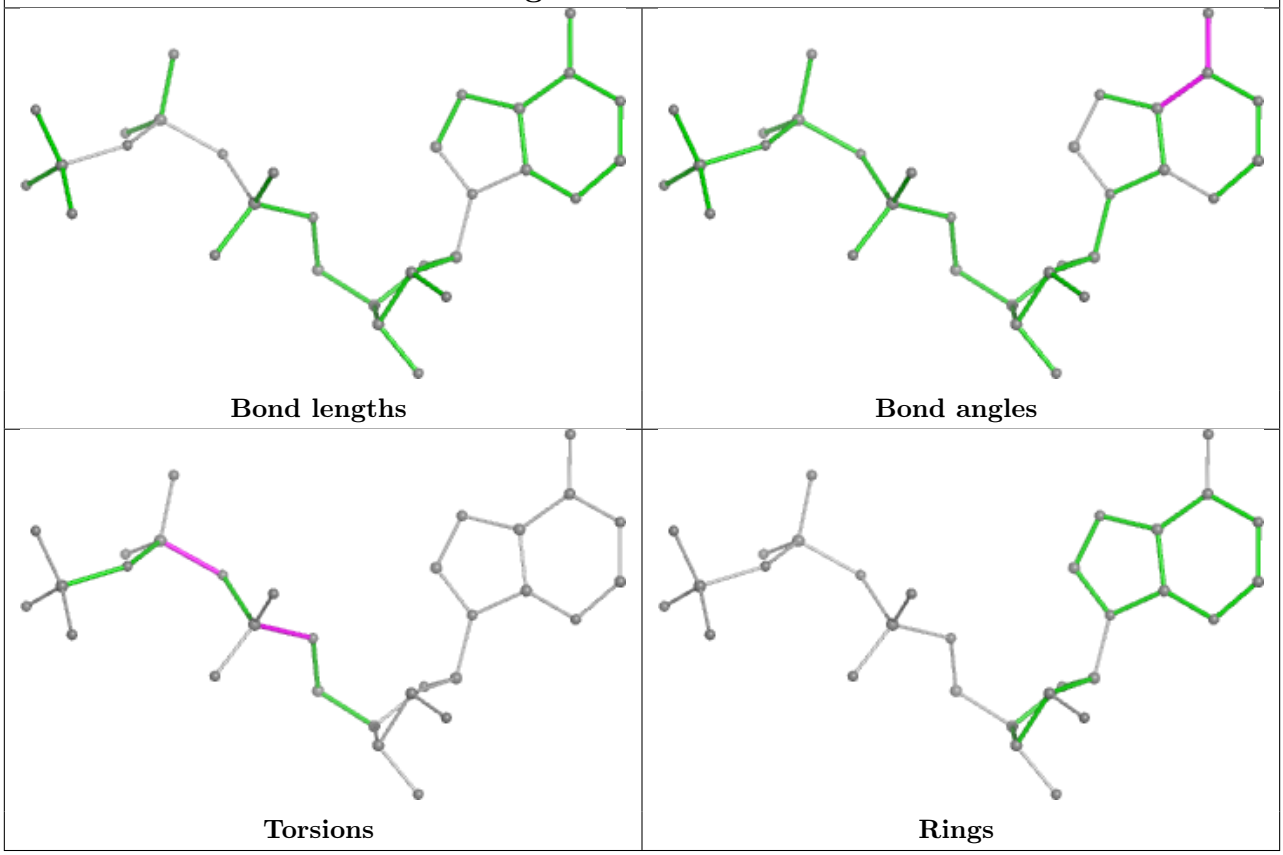
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	801	ATP	1	0
3	C	501	ATP	1	0
3	F	802	ATP	1	0

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 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.

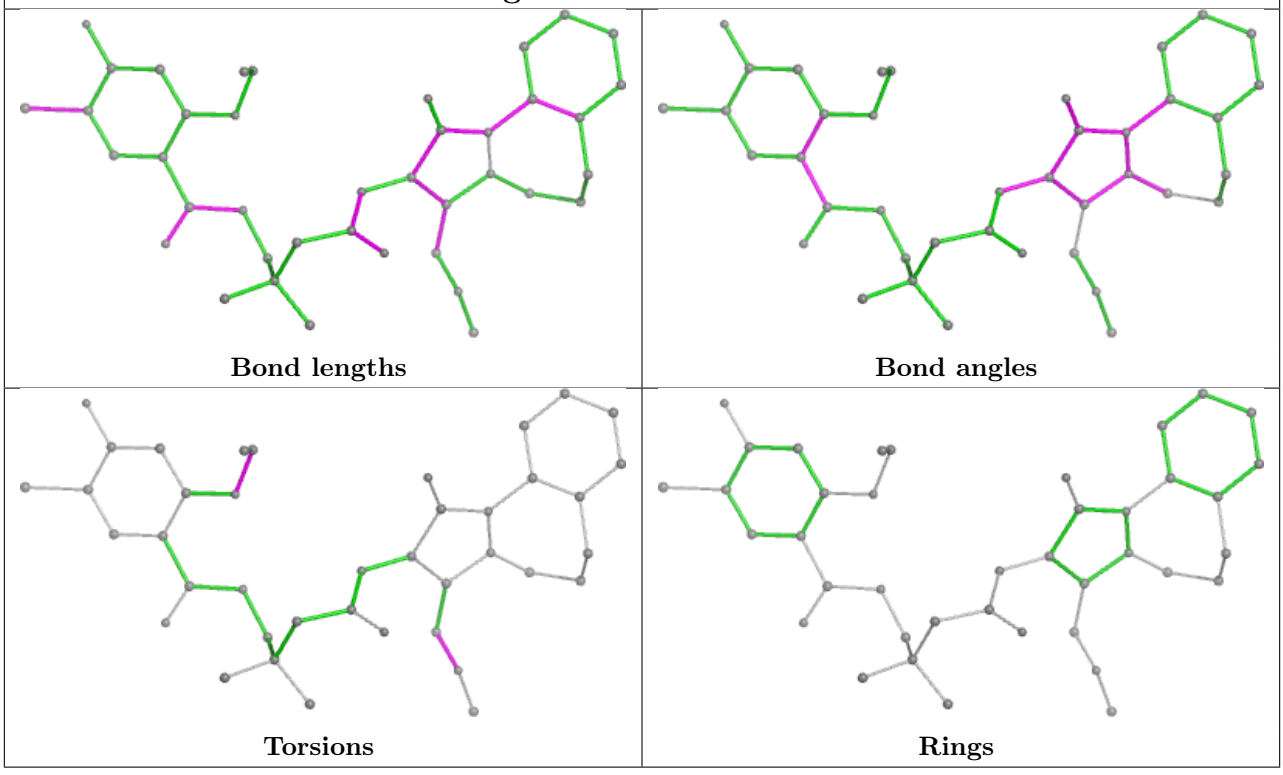
Ligand A1H5V A 502



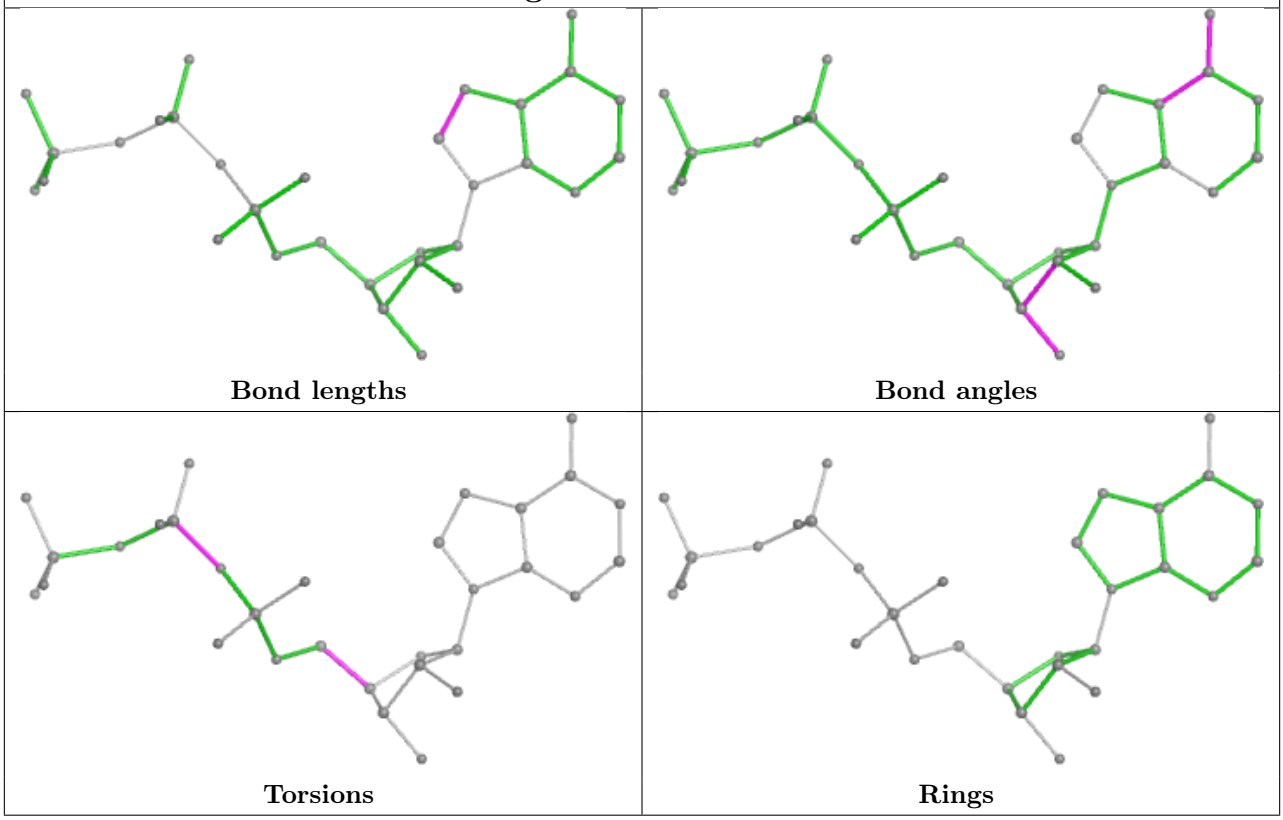
Ligand ATP A 501



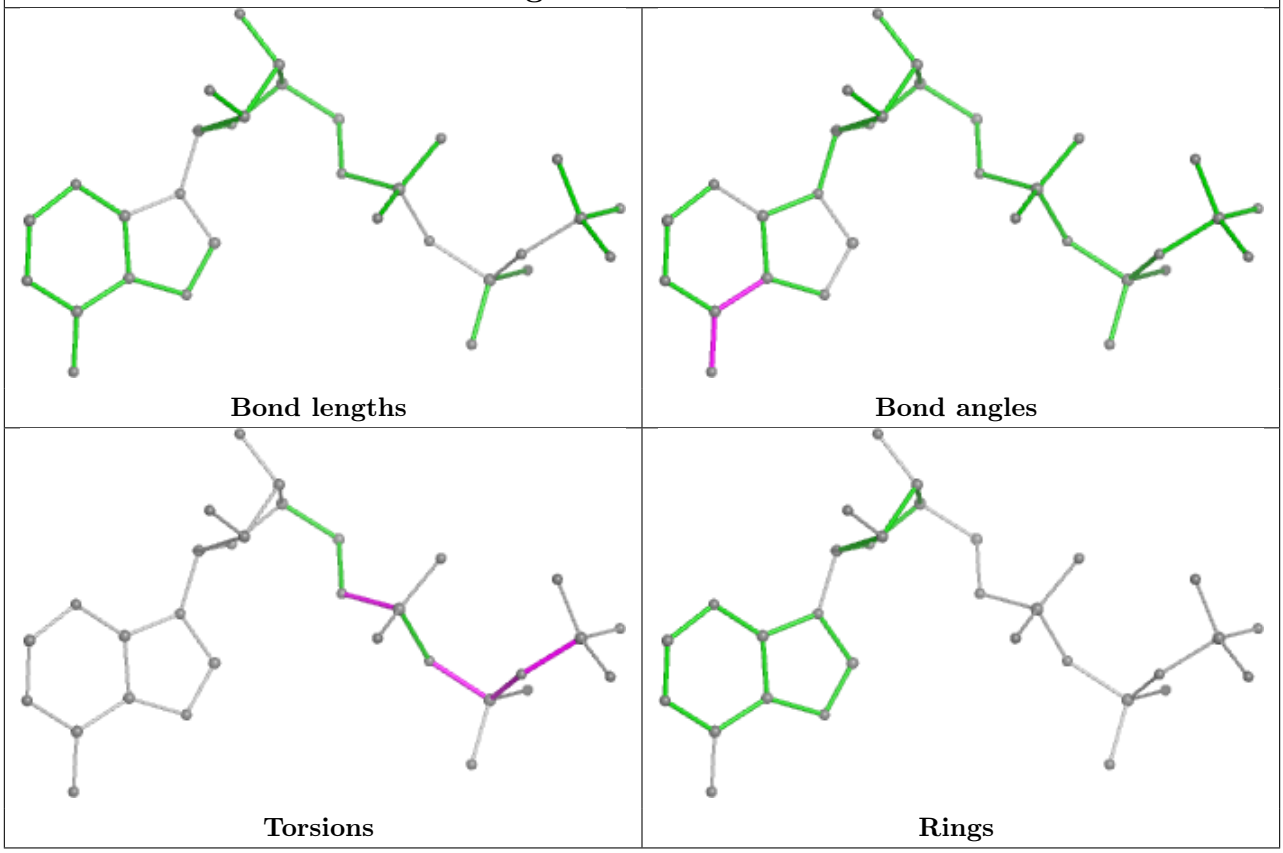
Ligand A1H5V C 502



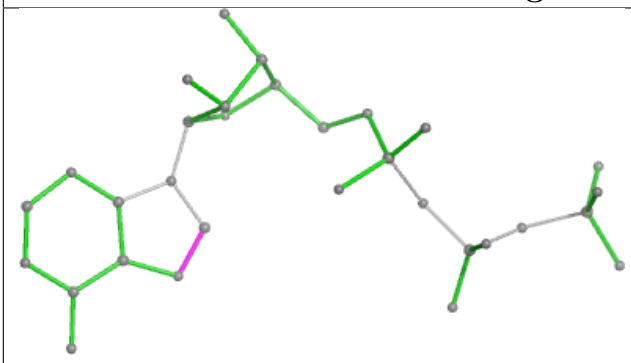
Ligand ATP D 801



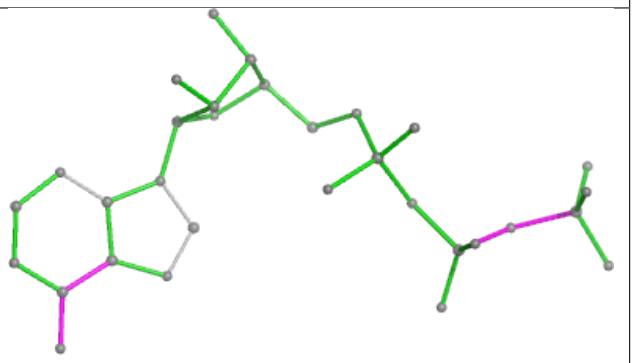
Ligand ATP C 501



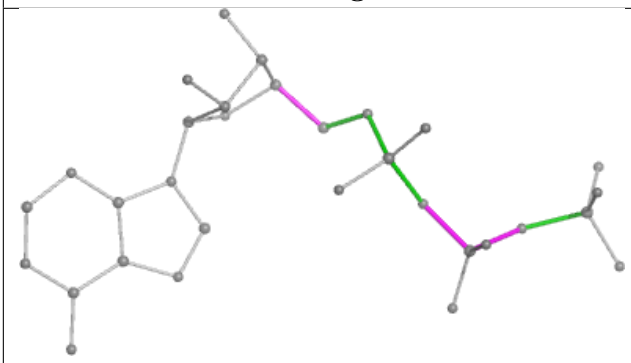
Ligand ATP E 801



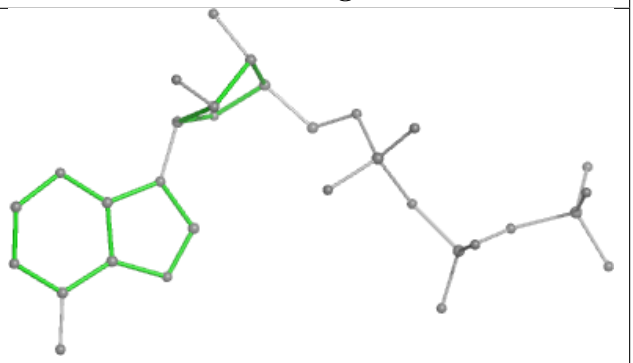
Bond lengths



Bond angles

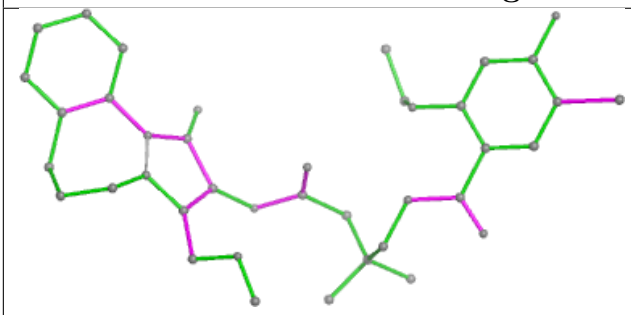


Torsions

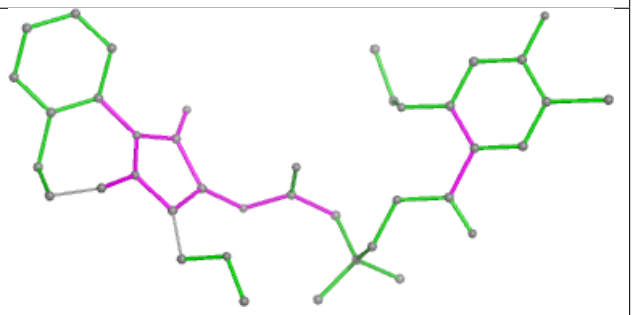


Rings

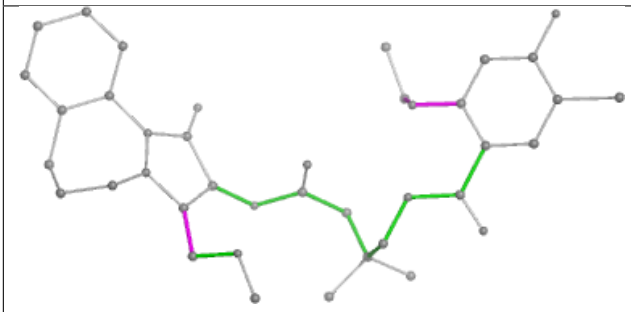
Ligand A1H5V B 501



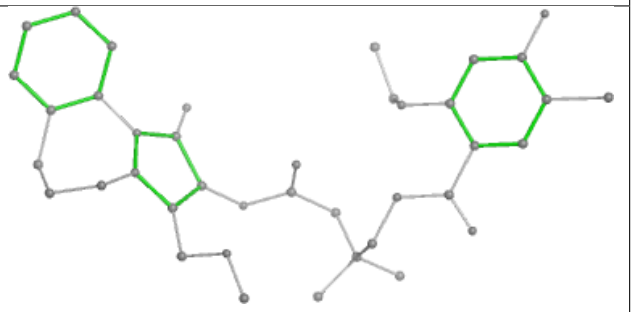
Bond lengths



Bond angles

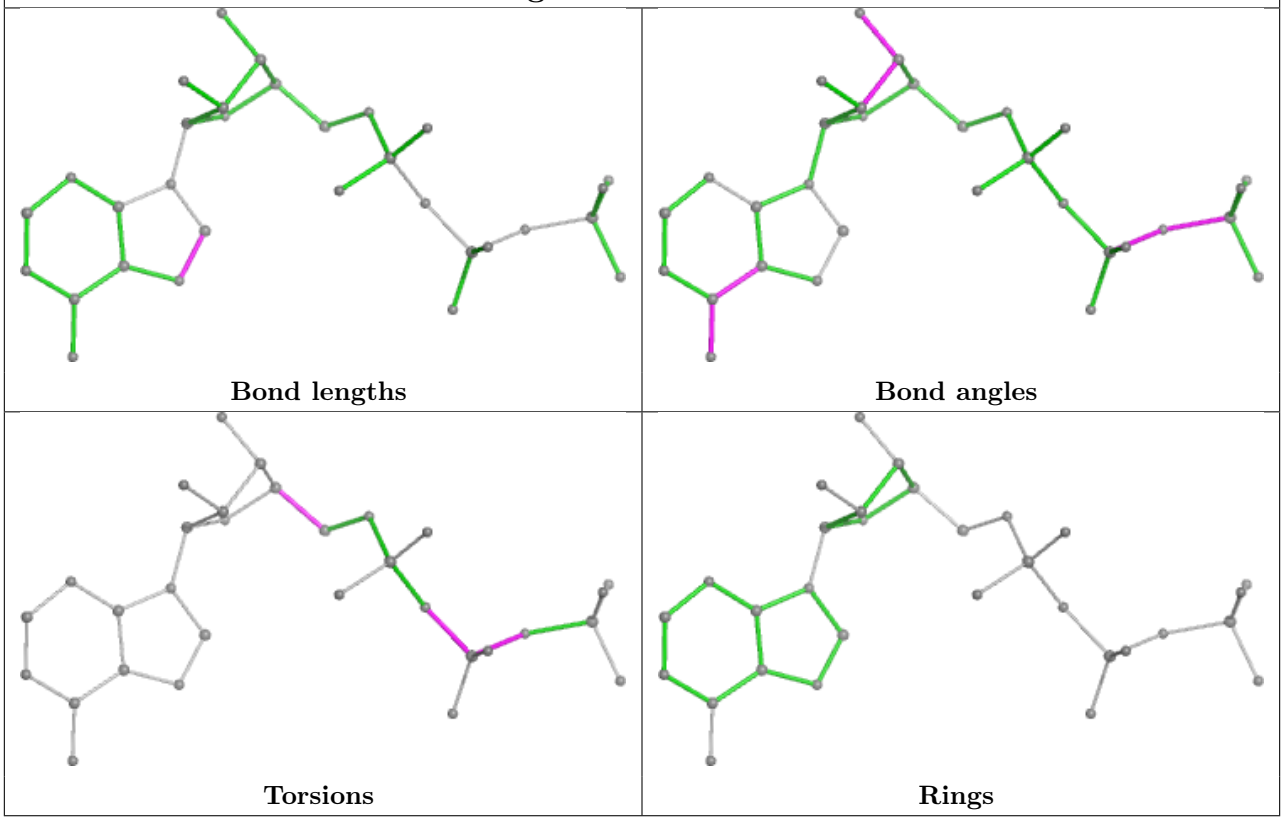


Torsions

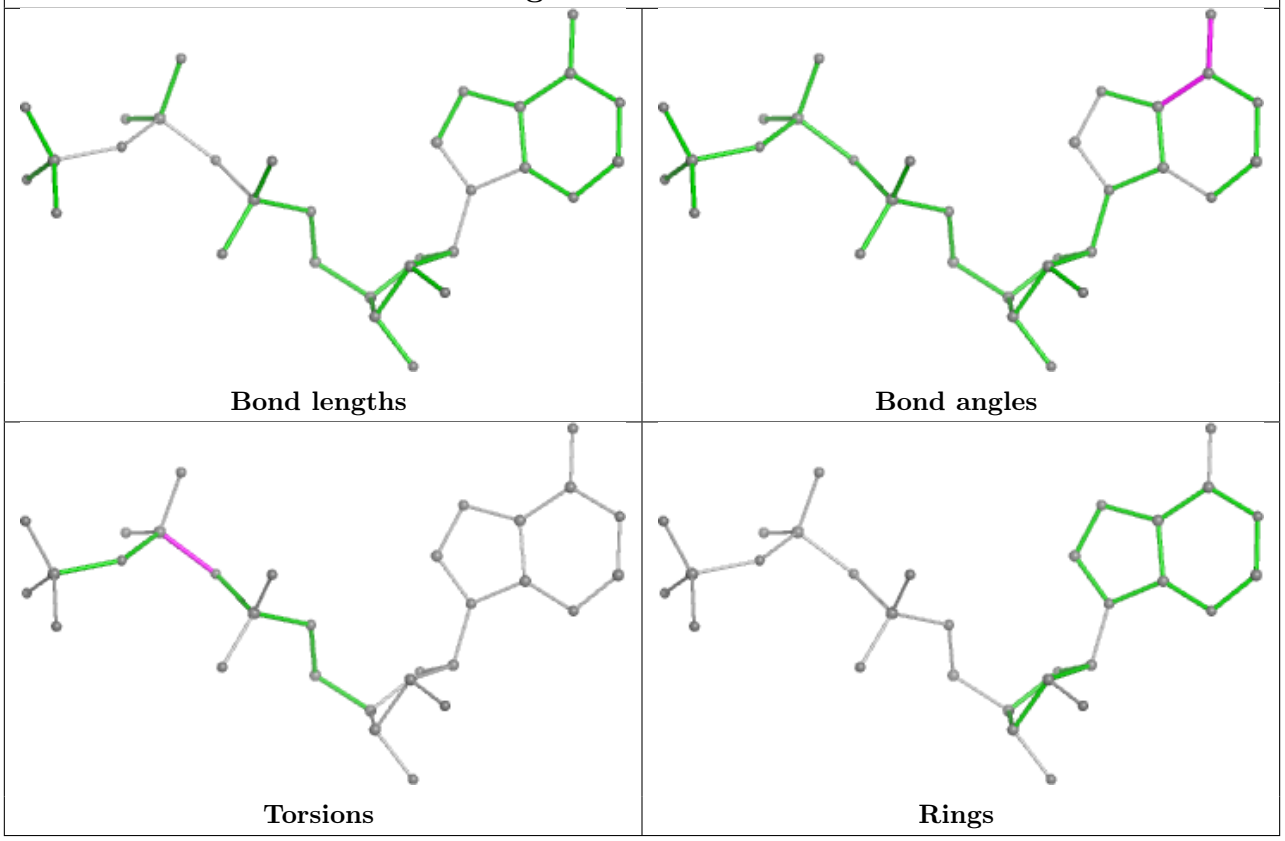


Rings

Ligand ATP F 802



Ligand ATP B 500



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.