wwPDB EM Validation Summary Report

Nov 21, 2022 – 03:08 AM EST

PDB ID	:	7TZC
EMDB ID	:	EMD-26205
Title	:	A drug and ATP binding site in type 1 ryanodine receptor
Authors	:	Melville, Z.; Dridi, H.; Yuan, Q.; Reiken, S.; Anetta, W.; Liu, Y.; Clarke, O.B.; Marks, A.R.
Deposited on	:	2022-02-15
Resolution	:	2.45 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 ⓘ 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:

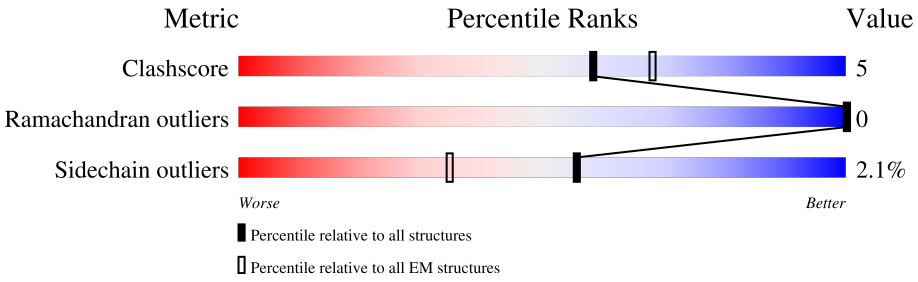
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.45 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	C	150	77% 22% ••
1	D	150	79% 20% ••
1	E	150	79% 20% ••
1	K	150	78% 20% ••
2	F	107	86% 14%
2	H	107	85% 15%
2	J	107	88% 11% •
2	O	107	86% 13% •
3	A	5037	75% 12% 13%

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Mol	Chain	Length	Quality of chain
3	B	5037	
3	G	5037	
3	I	5037	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 149472 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 Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	149	Total	C	N	O	S	0	0
			1174	719	190	255	10		
1	D	149	Total	C	N	O	S	0	0
			1174	719	190	255	10		
1	E	149	Total	C	N	O	S	0	0
			1174	719	190	255	10		
1	C	149	Total	C	N	O	S	0	0
			1174	719	190	255	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	HIS	-	expression tag	UNP P0DP23
D	-1	HIS	-	expression tag	UNP P0DP23
E	-1	HIS	-	expression tag	UNP P0DP23
C	-1	HIS	-	expression tag	UNP P0DP23

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	H	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	J	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	O	107	Total	C	N	O	S	0	0
			831	527	146	154	4		

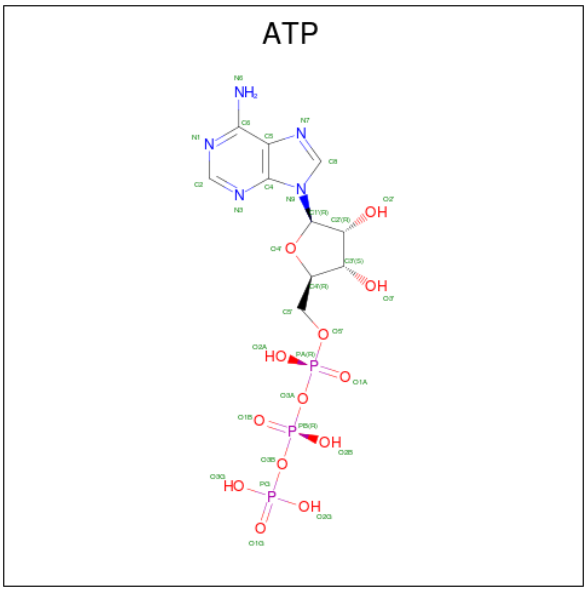
- Molecule 3 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	4404	Total 35150	C 22365	N 6063	O 6485	S 237	9	0
3	B	4404	Total 35150	C 22365	N 6063	O 6485	S 237	9	0
3	G	4404	Total 35150	C 22365	N 6063	O 6485	S 237	9	0
3	I	4404	Total 35150	C 22365	N 6063	O 6485	S 237	9	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	K	4	Total 4	Ca 4	0
4	D	4	Total 4	Ca 4	0
4	E	4	Total 4	Ca 4	0
4	C	4	Total 4	Ca 4	0
4	A	1	Total 1	Ca 1	0
4	B	1	Total 1	Ca 1	0
4	G	1	Total 1	Ca 1	0
4	I	1	Total 1	Ca 1	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

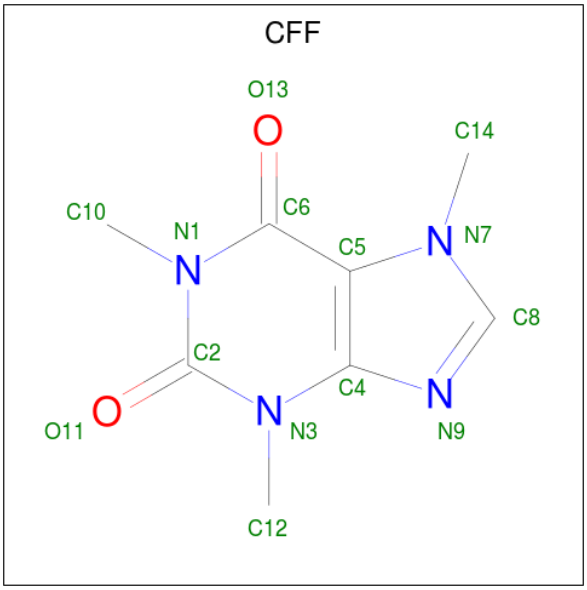


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	B	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	B	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	G	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	G	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	I	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	I	1	Total	C	N	O	P	0
			62	20	10	26	6	

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

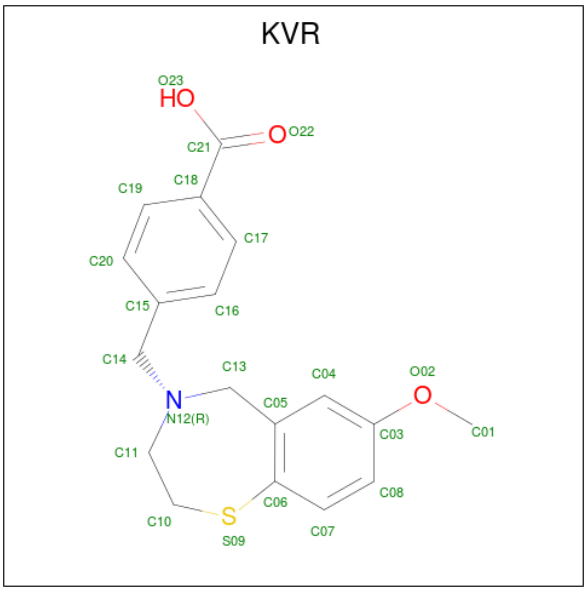
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Zn	0
			1	1	
6	B	1	Total	Zn	0
			1	1	
6	G	1	Total	Zn	0
			1	1	
6	I	1	Total	Zn	0
			1	1	

- Molecule 7 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$).



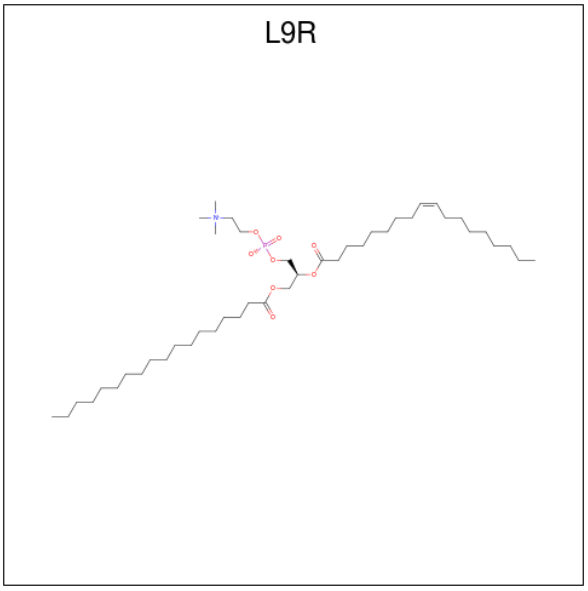
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	4	2	
7	B	1	Total	C	N	O	0
			14	8	4	2	
7	G	1	Total	C	N	O	0
			14	8	4	2	
7	I	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 8 is 4-[(7-methoxy-2,3-dihydro-1,4-benzothiazepin-4(5H)-yl)methyl]benzoic acid (three-letter code: KVR) (formula: $C_{18}H_{19}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	S	0
			23	18	1	3	1	
8	B	1	Total	C	N	O	S	0
			23	18	1	3	1	
8	G	1	Total	C	N	O	S	0
			23	18	1	3	1	
8	I	1	Total	C	N	O	S	0
			23	18	1	3	1	

- Molecule 9 is (2S)-3-(octadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: L9R) (formula: $C_{44}H_{86}NO_8P$).



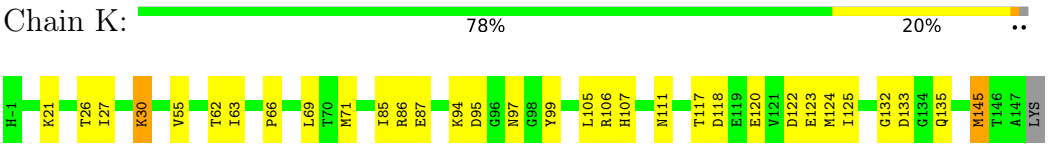
Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			108	88	2	16	2	
9	A	1	Total	C	N	O	P	0
			108	88	2	16	2	
9	B	1	Total	C	N	O	P	0
			108	88	2	16	2	
9	B	1	Total	C	N	O	P	0
			108	88	2	16	2	
9	G	1	Total	C	N	O	P	0
			108	88	2	16	2	
9	G	1	Total	C	N	O	P	0
			108	88	2	16	2	
9	I	1	Total	C	N	O	P	0
			108	88	2	16	2	
9	I	1	Total	C	N	O	P	0
			108	88	2	16	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.

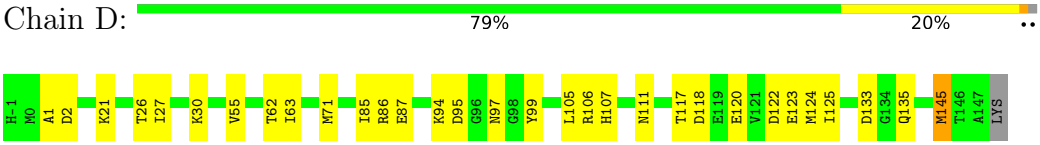
- Molecule 1: Calmodulin-1

Chain K:



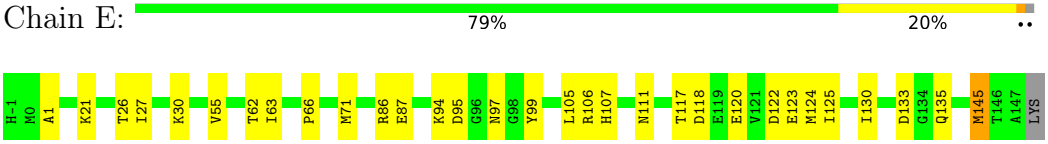
- Molecule 1: Calmodulin-1

Chain D:



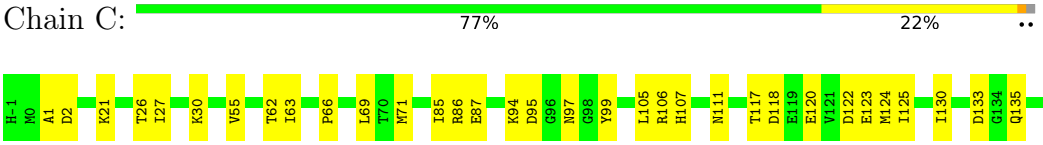
- Molecule 1: Calmodulin-1

Chain E:



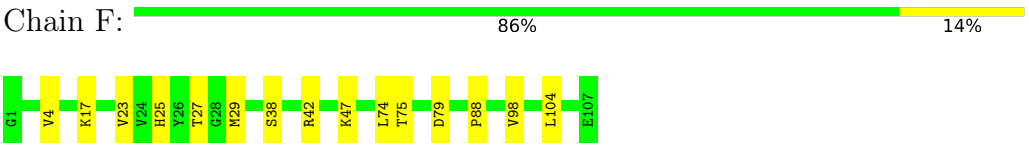
- Molecule 1: Calmodulin-1

Chain C:



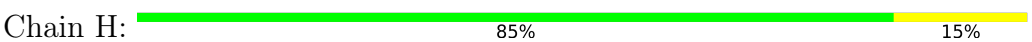
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

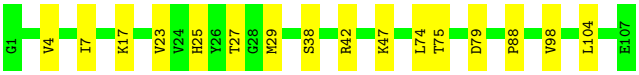
Chain F:



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain H:





• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

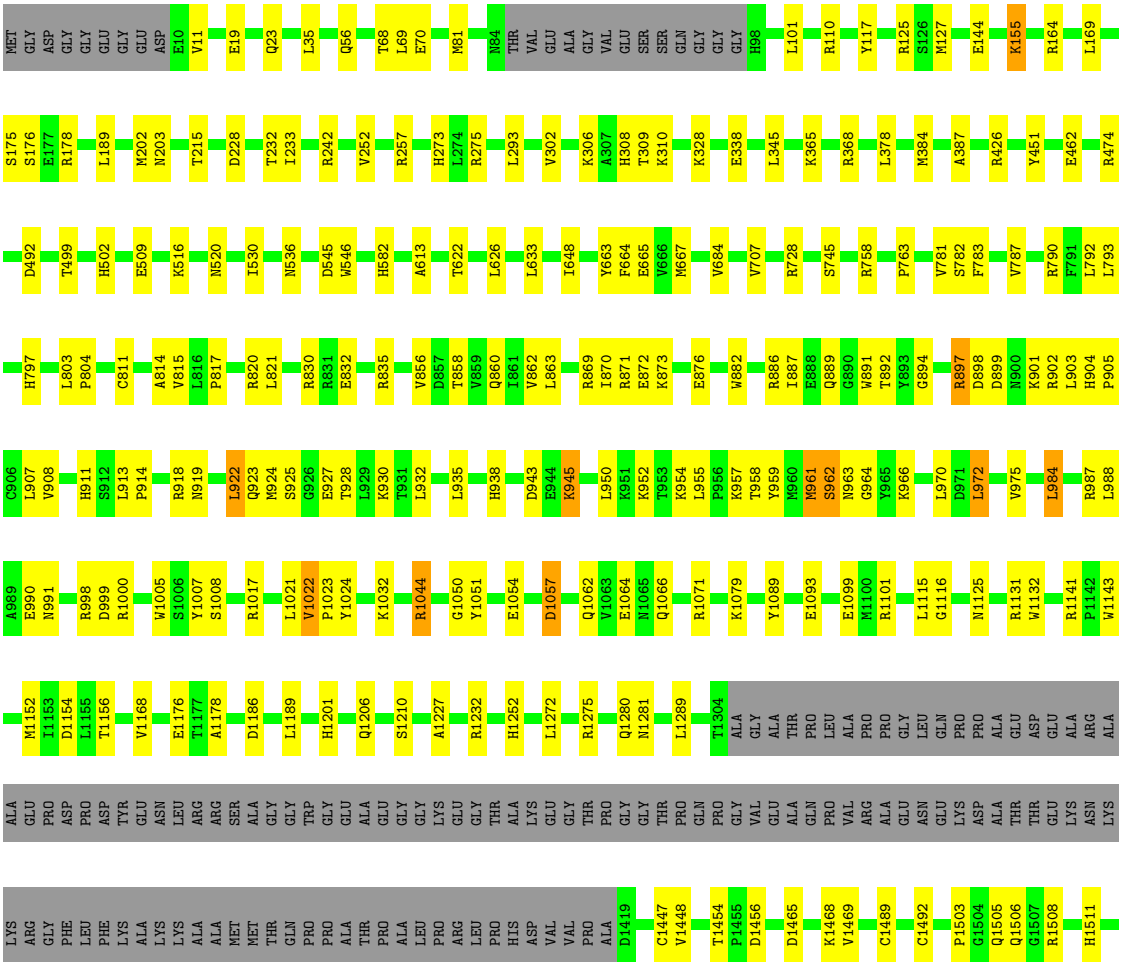
Chain J:

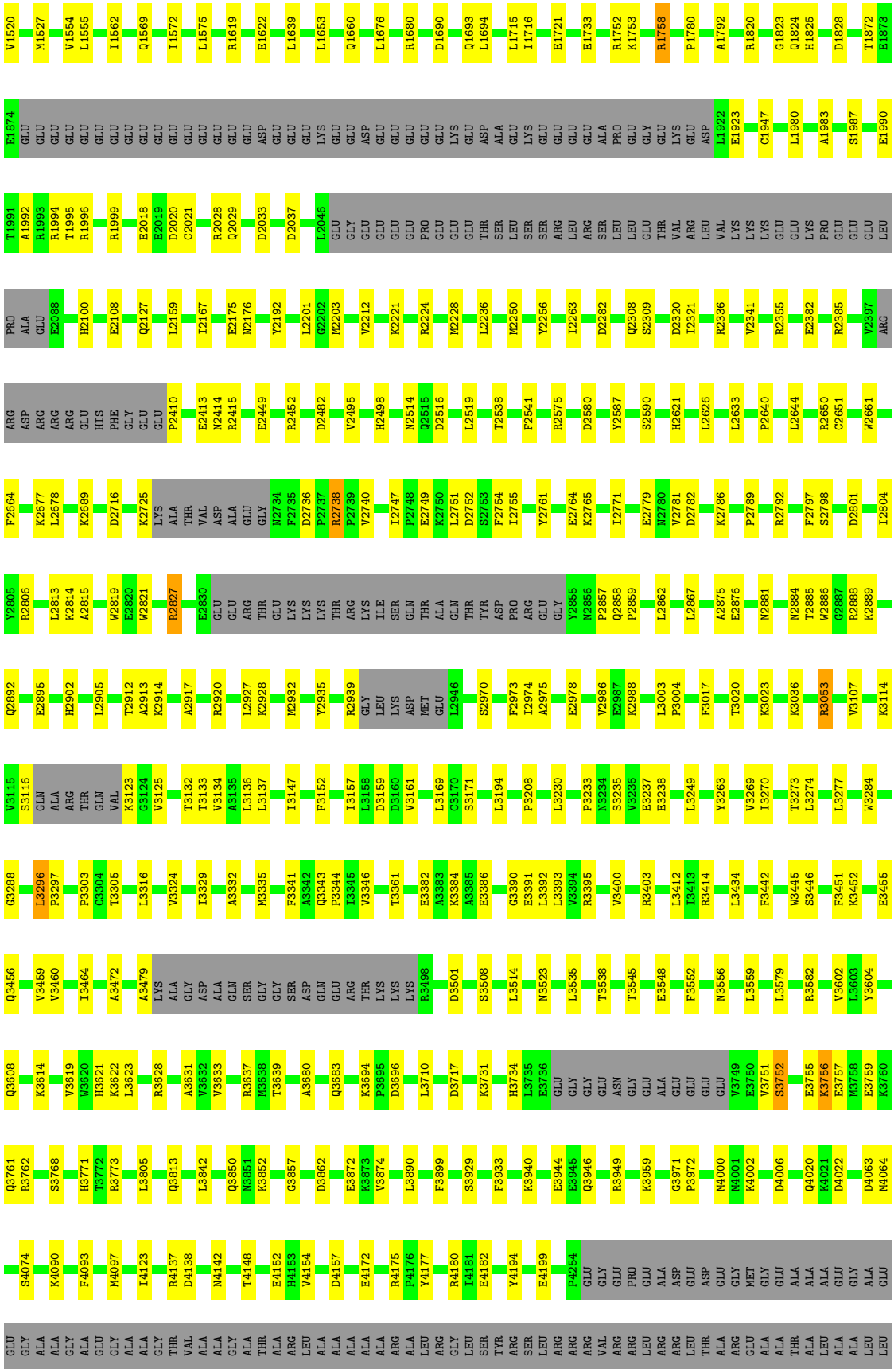
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

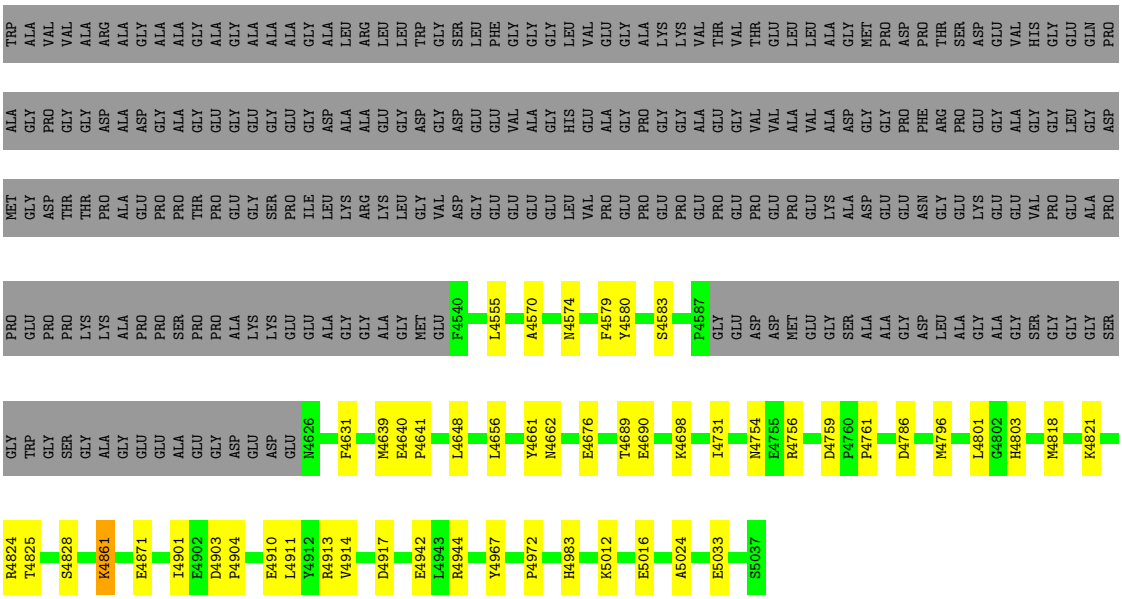
Chain O:

• Molecule 3: Ryanodine receptor 1

Chain A:

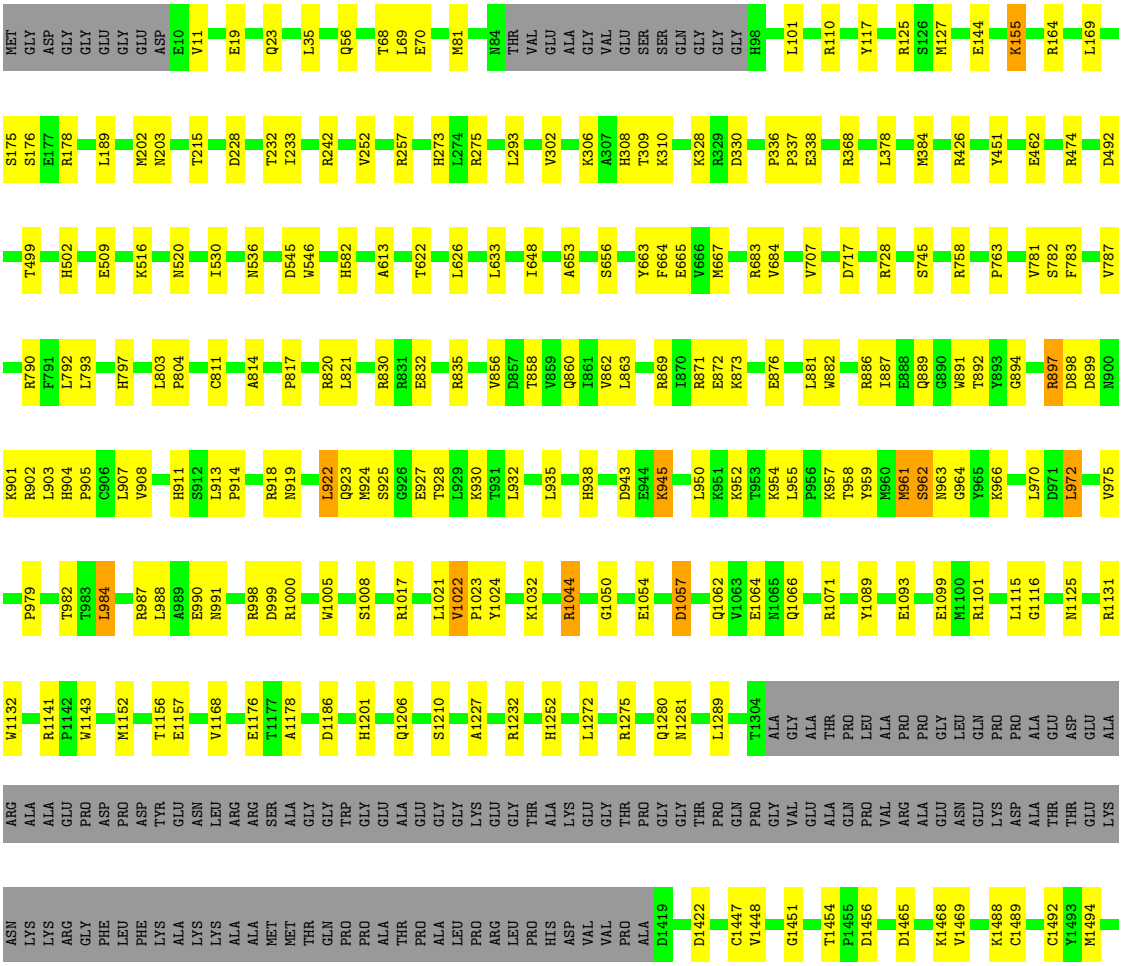


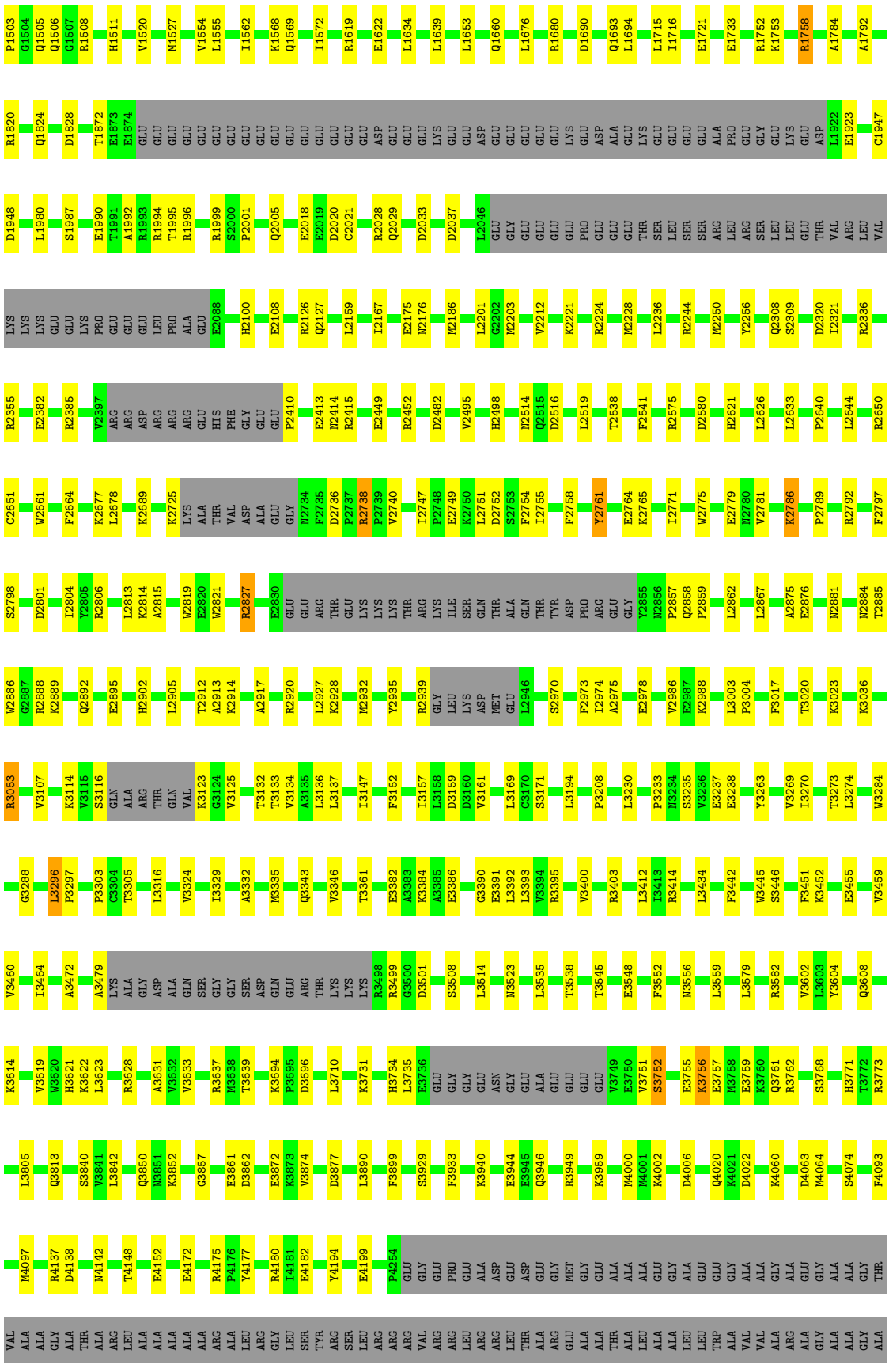


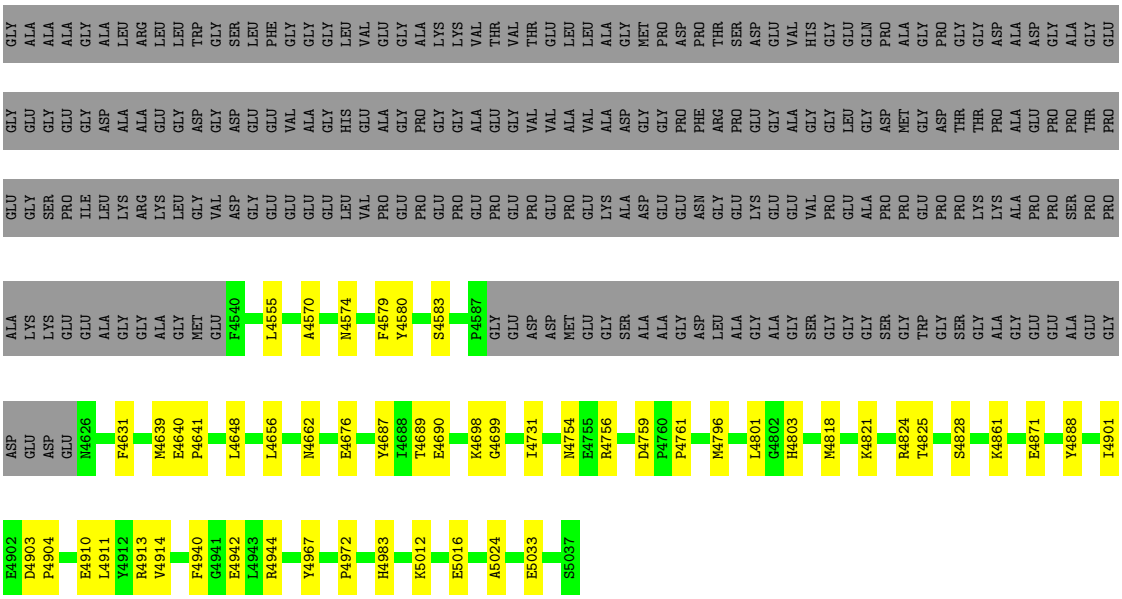


• Molecule 3: Ryanodine receptor 1

Chain B:

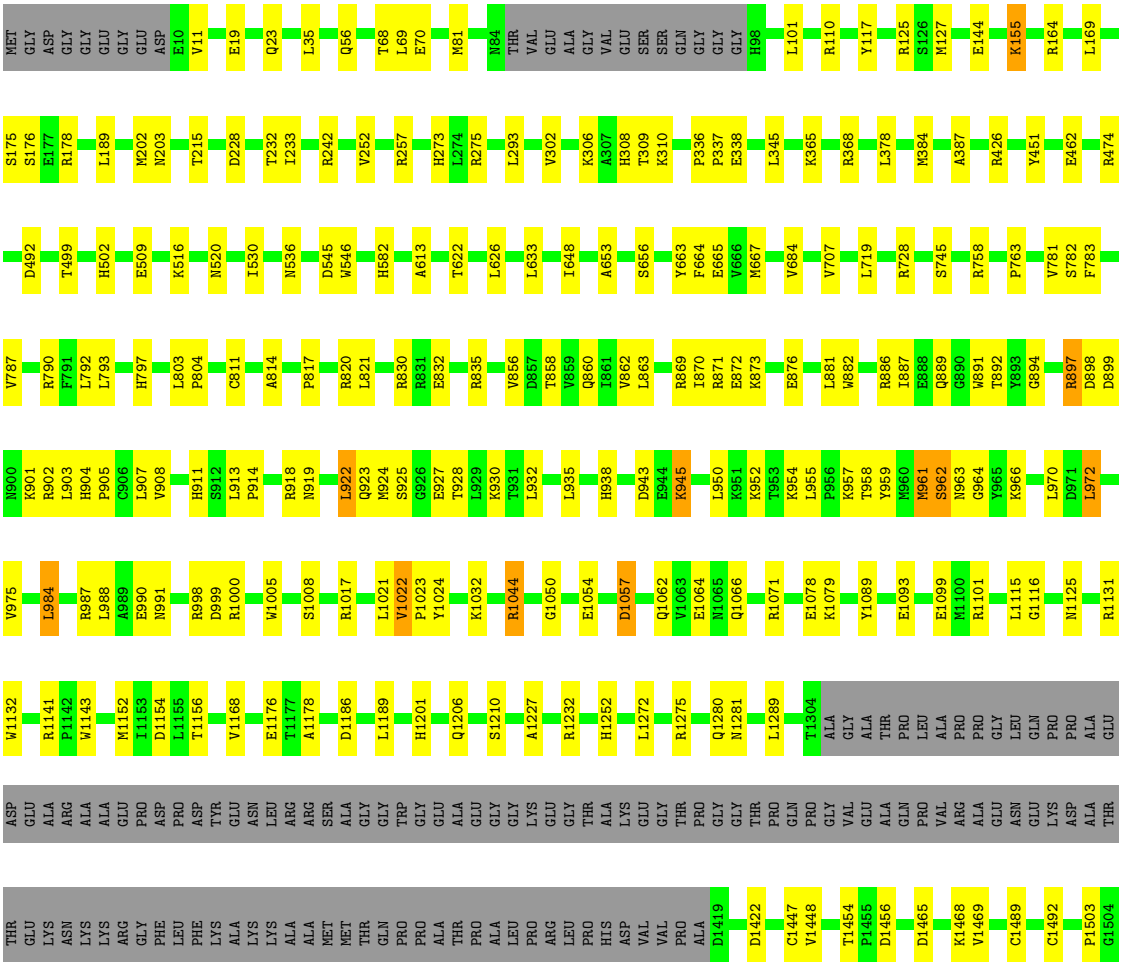


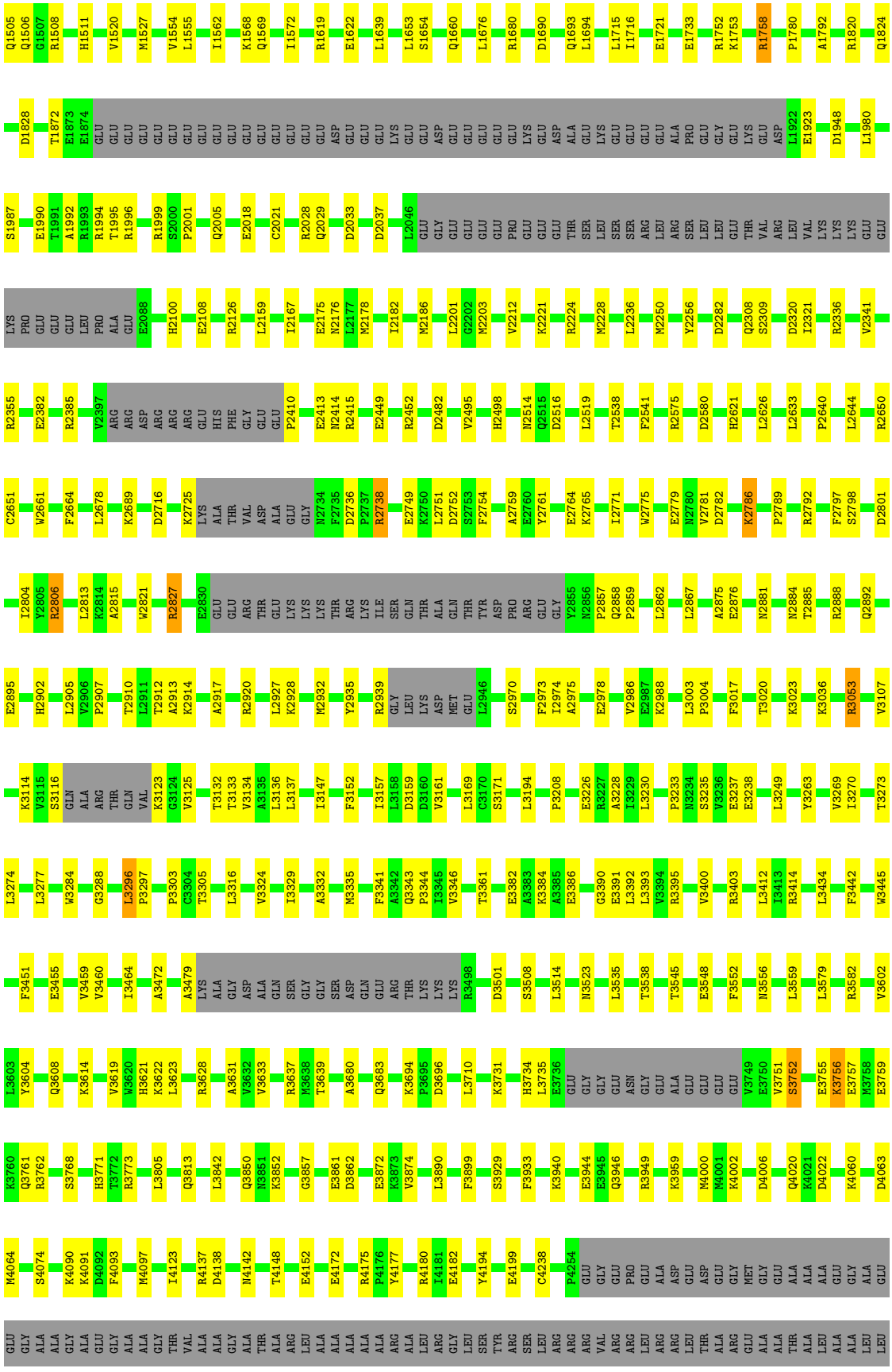


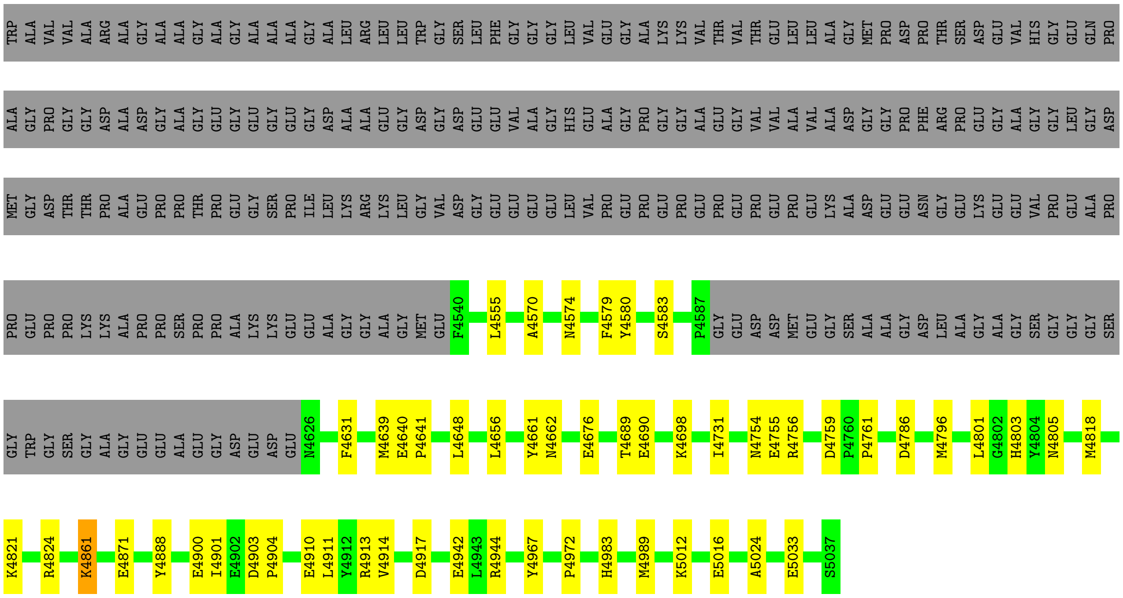


• Molecule 3: Ryanodine receptor 1

Chain G:

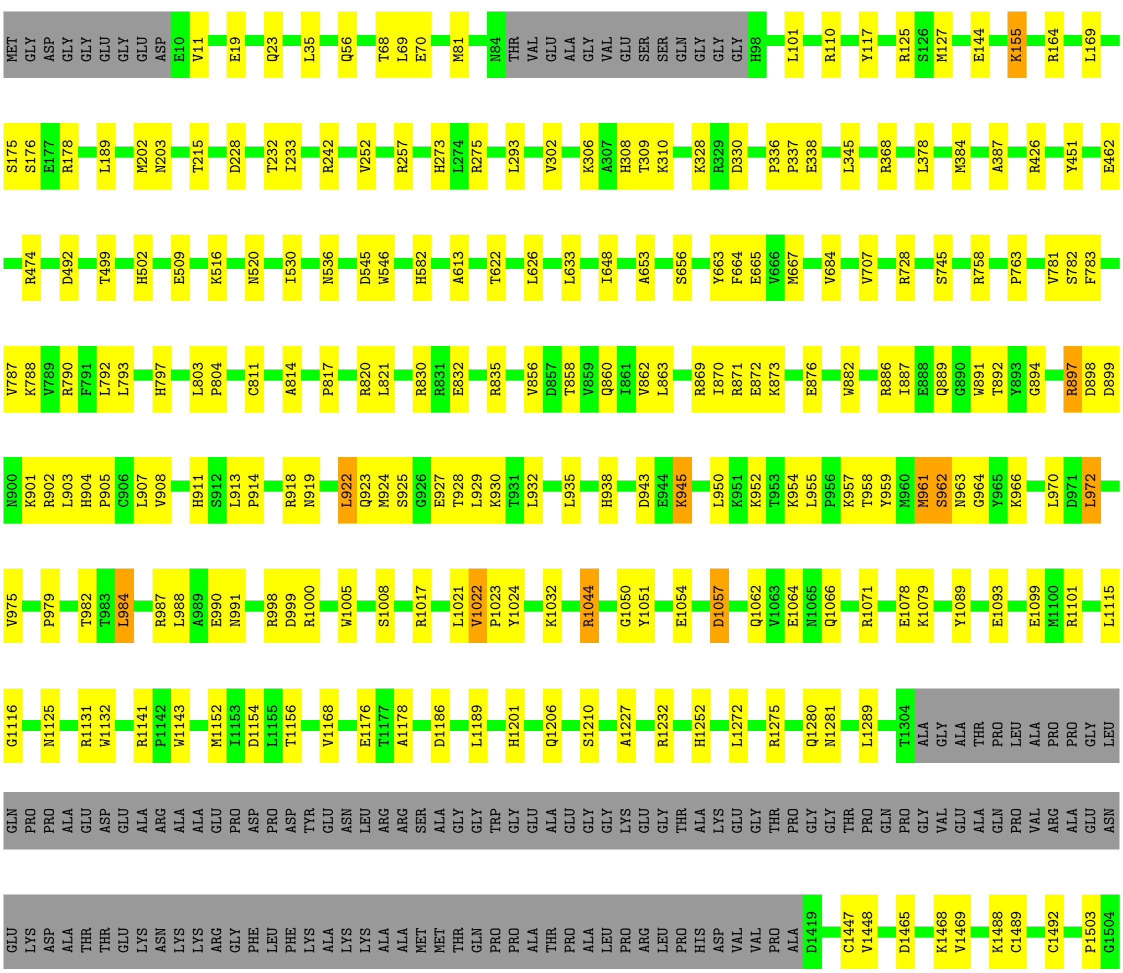


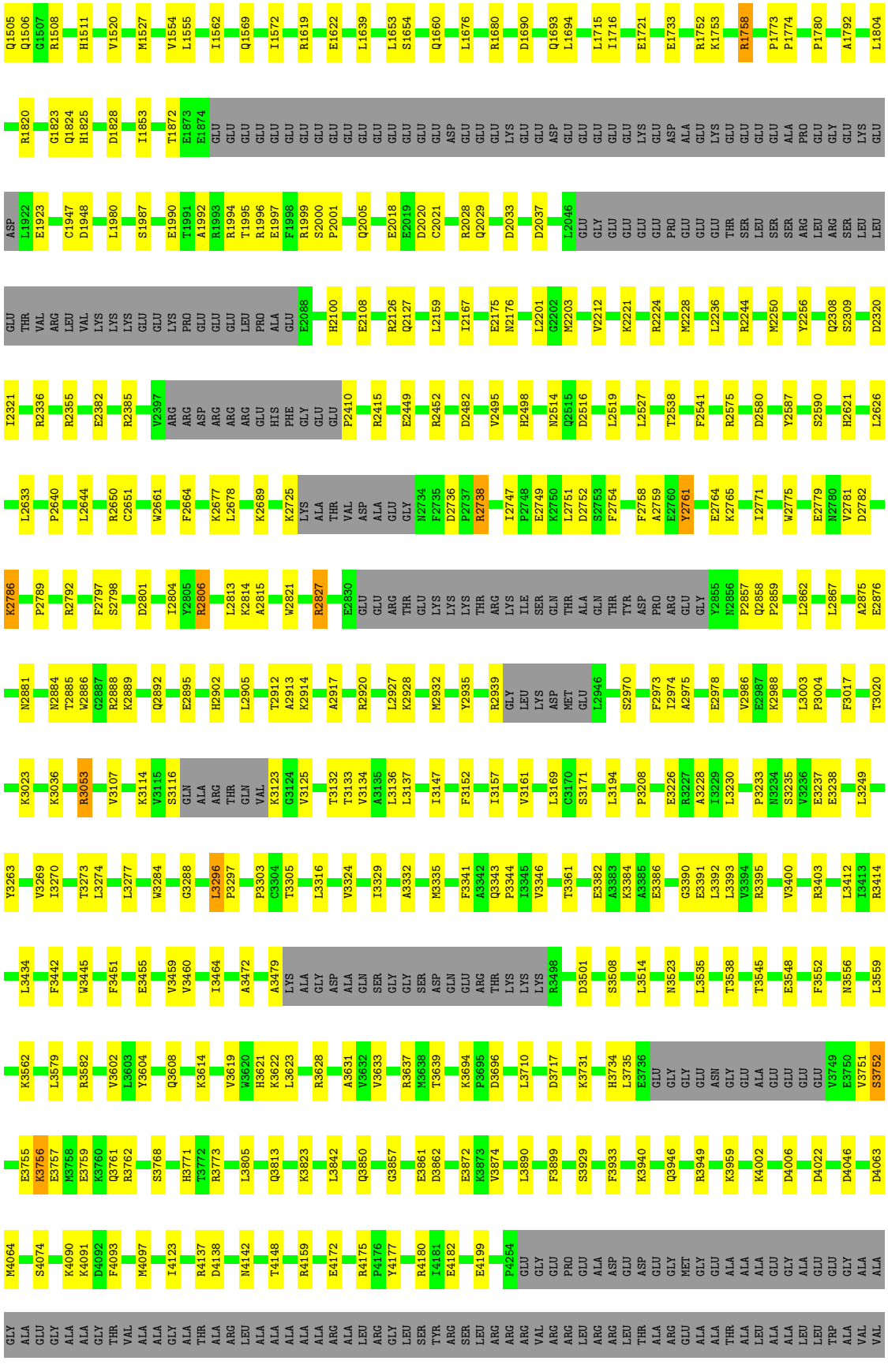


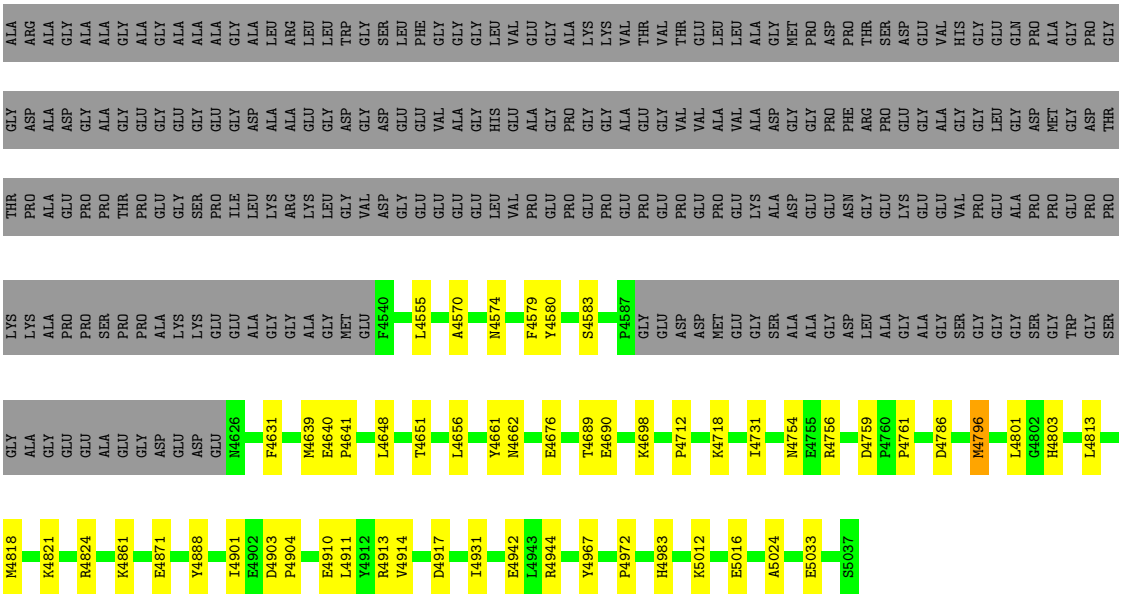


• Molecule 3: Ryanodine receptor 1

Chain I: 75% 12% 13%






ALA ARG ALA GLY ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU GLY VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY
GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY ASP GLY ASP GLU GLU VAL ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL ALA VAL ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY ALA GLY GLY LEU GLY ASP MET GLY THR
THR PRO ALA GLU PRO PRO THR PRO GLU GLY GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU LEU VAL PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU LYS ALA ASP GLU GLY GLU GLY ASN GLY GLU LYS GLU GLU ALA GLU GLY ALA PRO PRO PRO
LYS LYS ALA PRO PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA GLY MET GLU F4540 L4555 A4570 N4574 F4579 Y4580 S4583 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER GLY TRP GLY SER
GLY ALA GLY GLU GLU ALA GLY GLU ASP GLU GLY ASP GLU N4626 F4631 M4639 E4640 P4641 L4648 T4651 L4656 Y4661 N4662 E4676 T4689 E4690 K4698 P4712 K4718 I4731 N4754 E4755 R4756 D4759 P4760 P4761 D4786 M4796 L4801 G4802 H4803 L4813
M4818 K4821 R4824 K4861 E4871 Y4888 I4901 E4902 D4903 P4904 E4910 L4911 Y4912 R4913 V4914 D4917 I4931 E4942 L4943 R4944 Y4967 P4972 H4983 K5012 E5016 A5024 E5033 S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	153840	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 ($e^-/Å^2$)	57.65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (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: CA, CFF, ZN, ATP, KVR, L9R

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	C	0.24	0/1187	0.44	0/1594
1	D	0.24	0/1187	0.44	0/1594
1	E	0.24	0/1187	0.44	0/1594
1	K	0.24	0/1187	0.44	0/1594
2	F	0.32	0/850	0.52	0/1146
2	H	0.32	0/850	0.52	0/1146
2	J	0.32	0/850	0.52	0/1146
2	O	0.32	0/850	0.52	0/1146
3	A	0.25	0/35977	0.46	0/48726
3	B	0.25	0/35977	0.46	0/48726
3	G	0.25	0/35977	0.46	0/48726
3	I	0.25	0/35977	0.46	0/48726
All	All	0.25	0/152056	0.46	0/205864

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	C	1174	0	1099	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1174	0	1099	17	0
1	E	1174	0	1099	17	0
1	K	1174	0	1099	19	0
2	F	831	0	831	7	0
2	H	831	0	831	8	0
2	J	831	0	831	7	0
2	O	831	0	831	8	0
3	A	35150	0	34797	347	0
3	B	35150	0	34797	347	0
3	G	35150	0	34797	347	0
3	I	35150	0	34797	353	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
4	E	4	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	4	0	0	0	0
5	A	62	0	24	2	0
5	B	62	0	24	2	0
5	G	62	0	24	2	0
5	I	62	0	24	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
7	A	14	0	10	0	0
7	B	14	0	10	0	0
7	G	14	0	10	0	0
7	I	14	0	10	0	0
8	A	23	0	0	0	0
8	B	23	0	0	0	0
8	G	23	0	0	0	0
8	I	23	0	0	0	0
9	A	108	0	172	9	0
9	B	108	0	172	6	0
9	G	108	0	172	9	0
9	I	108	0	172	8	0
All	All	149472	0	147732	1461	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 5.

The worst 5 of 1461 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)
3:I:4904:PRO:HB3	3:I:4913:ARG:HG2	1.57	0.86
3:G:4904:PRO:HB3	3:G:4913:ARG:HG2	1.57	0.86
3:A:4904:PRO:HB3	3:A:4913:ARG:HG2	1.57	0.84
3:B:4904:PRO:HB3	3:B:4913:ARG:HG2	1.57	0.83
3:A:2779:GLU:HG3	3:A:2792:ARG:HG2	1.66	0.78

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	C	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
1	D	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
1	E	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
1	K	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
2	F	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
2	H	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
2	J	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
2	O	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
3	A	4385/5037 (87%)	4273 (97%)	112 (3%)	0	100	100
3	B	4385/5037 (87%)	4273 (97%)	112 (3%)	0	100	100
3	G	4385/5037 (87%)	4274 (98%)	111 (2%)	0	100	100
3	I	4385/5037 (87%)	4273 (97%)	112 (3%)	0	100	100
All	All	18548/21176 (88%)	18089 (98%)	459 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	C	127/128 (99%)	122 (96%)	5 (4%)	32	42
1	D	127/128 (99%)	122 (96%)	5 (4%)	32	42
1	E	127/128 (99%)	122 (96%)	5 (4%)	32	42
1	K	127/128 (99%)	122 (96%)	5 (4%)	32	42
2	F	89/89 (100%)	86 (97%)	3 (3%)	37	48
2	H	89/89 (100%)	86 (97%)	3 (3%)	37	48
2	J	89/89 (100%)	86 (97%)	3 (3%)	37	48
2	O	89/89 (100%)	86 (97%)	3 (3%)	37	48
3	A	3836/4276 (90%)	3760 (98%)	76 (2%)	55	67
3	B	3836/4276 (90%)	3760 (98%)	76 (2%)	55	67
3	G	3836/4276 (90%)	3760 (98%)	76 (2%)	55	67
3	I	3836/4276 (90%)	3760 (98%)	76 (2%)	55	67
All	All	16208/17972 (90%)	15872 (98%)	336 (2%)	56	66

5 of 336 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	3053	ARG
3	I	1758	ARG
3	G	3639	THR
3	I	897	ARG
3	I	2797	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	3761	GLN
3	G	991	ASN
3	I	2881	ASN
3	I	991	ASN

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Mol	Chain	Res	Type
3	I	2180	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 48 ligands modelled in this entry, 24 are monoatomic - leaving 24 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	$\#\|Z\| > 2$
8	KVR	G	5107	-	24,25,25	1.38	3 (12%)	32,34,34	1.54	4 (12%)
8	KVR	B	5306	-	24,25,25	1.39	3 (12%)	32,34,34	1.54	4 (12%)
9	L9R	B	5308	-	53,53,53	1.18	4 (7%)	59,61,61	1.11	2 (3%)
9	L9R	A	5307	-	53,53,53	1.22	5 (9%)	59,61,61	1.11	3 (5%)
5	ATP	B	5301	-	26,33,33	0.60	0	31,52,52	0.82	2 (6%)
5	ATP	G	5102	-	26,33,33	0.58	0	31,52,52	0.82	2 (6%)
5	ATP	I	5106	-	26,33,33	0.60	0	31,52,52	0.74	2 (6%)
8	KVR	A	5306	-	24,25,25	1.38	3 (12%)	32,34,34	1.54	4 (12%)
9	L9R	B	5307	-	53,53,53	1.22	5 (9%)	59,61,61	1.11	3 (5%)
7	CFF	B	5304	-	8,15,15	2.35	3 (37%)	8,23,23	1.42	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	CFF	A	5304	-	8,15,15	2.35	3 (37%)	8,23,23	1.42	1 (12%)
9	L9R	I	5101	-	53,53,53	1.18	4 (7%)	59,61,61	1.11	2 (3%)
5	ATP	G	5106	-	26,33,33	0.59	0	31,52,52	0.75	2 (6%)
9	L9R	I	5108	-	53,53,53	1.21	4 (7%)	59,61,61	1.11	3 (5%)
9	L9R	G	5108	-	53,53,53	1.22	4 (7%)	59,61,61	1.11	3 (5%)
7	CFF	I	5105	-	8,15,15	2.35	3 (37%)	8,23,23	1.43	1 (12%)
7	CFF	G	5105	-	8,15,15	2.35	3 (37%)	8,23,23	1.43	1 (12%)
9	L9R	G	5101	-	53,53,53	1.18	4 (7%)	59,61,61	1.11	2 (3%)
5	ATP	B	5305	-	26,33,33	0.60	0	31,52,52	0.74	2 (6%)
5	ATP	I	5102	-	26,33,33	0.61	0	31,52,52	0.82	2 (6%)
9	L9R	A	5308	-	53,53,53	1.18	4 (7%)	59,61,61	1.11	2 (3%)
5	ATP	A	5301	-	26,33,33	0.59	0	31,52,52	0.82	2 (6%)
8	KVR	I	5107	-	24,25,25	1.38	3 (12%)	32,34,34	1.54	4 (12%)
5	ATP	A	5305	-	26,33,33	0.59	0	31,52,52	0.74	2 (6%)

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
8	KVR	G	5107	-	-	2/10/20/20	0/2/3/3
8	KVR	B	5306	-	-	2/10/20/20	0/2/3/3
9	L9R	B	5308	-	-	34/57/57/57	-
9	L9R	A	5307	-	-	31/57/57/57	-
5	ATP	B	5301	-	-	8/18/38/38	0/3/3/3
5	ATP	G	5102	-	-	8/18/38/38	0/3/3/3
5	ATP	I	5106	-	-	6/18/38/38	0/3/3/3
8	KVR	A	5306	-	-	2/10/20/20	0/2/3/3
9	L9R	B	5307	-	-	31/57/57/57	-
7	CFF	B	5304	-	-	-	0/2/2/2
7	CFF	A	5304	-	-	-	0/2/2/2
9	L9R	I	5101	-	-	34/57/57/57	-
5	ATP	G	5106	-	-	6/18/38/38	0/3/3/3
9	L9R	I	5108	-	-	31/57/57/57	-
9	L9R	G	5108	-	-	31/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CFF	I	5105	-	-	-	0/2/2/2
9	L9R	G	5101	-	-	34/57/57/57	-
7	CFF	G	5105	-	-	-	0/2/2/2
5	ATP	B	5305	-	-	6/18/38/38	0/3/3/3
5	ATP	I	5102	-	-	8/18/38/38	0/3/3/3
9	L9R	A	5308	-	-	34/57/57/57	-
5	ATP	A	5301	-	-	8/18/38/38	0/3/3/3
8	KVR	I	5107	-	-	2/10/20/20	0/2/3/3
5	ATP	A	5305	-	-	6/18/38/38	0/3/3/3

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	5306	KVR	C06-S09	4.85	1.82	1.77
8	I	5107	KVR	C06-S09	4.84	1.82	1.77
8	A	5306	KVR	C06-S09	4.82	1.82	1.77
8	G	5107	KVR	C06-S09	4.80	1.82	1.77
7	G	5105	CFF	C5-C4	-4.24	1.33	1.39

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	G	5107	KVR	C10-S09-C06	5.26	110.17	102.71
8	A	5306	KVR	C10-S09-C06	5.26	110.16	102.71
8	B	5306	KVR	C10-S09-C06	5.24	110.14	102.71
8	I	5107	KVR	C10-S09-C06	5.24	110.13	102.71
9	B	5308	L9R	O2-C31-C32	4.04	120.20	111.50

There are no chirality outliers.

5 of 324 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	5301	ATP	C5'-O5'-PA-O1A
5	A	5301	ATP	C5'-O5'-PA-O2A
5	A	5305	ATP	C5'-O5'-PA-O2A
5	A	5305	ATP	C5'-O5'-PA-O3A
5	B	5301	ATP	C5'-O5'-PA-O1A

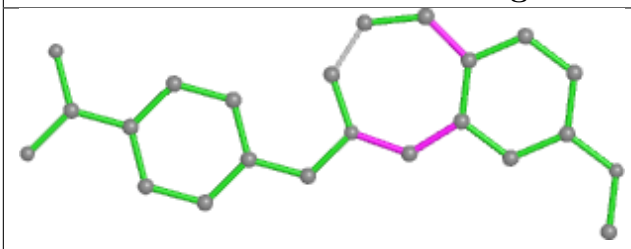
There are no ring outliers.

16 monomers are involved in 36 short contacts:

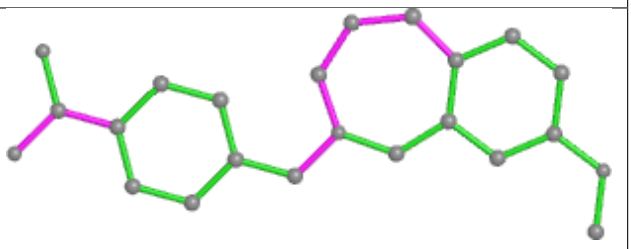
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	5308	L9R	4	0
9	A	5307	L9R	3	0
5	B	5301	ATP	1	0
5	G	5102	ATP	1	0
5	I	5106	ATP	1	0
9	B	5307	L9R	2	0
9	I	5101	L9R	5	0
5	G	5106	ATP	1	0
9	I	5108	L9R	3	0
9	G	5108	L9R	3	0
9	G	5101	L9R	6	0
5	B	5305	ATP	1	0
5	I	5102	ATP	1	0
9	A	5308	L9R	6	0
5	A	5301	ATP	1	0
5	A	5305	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.

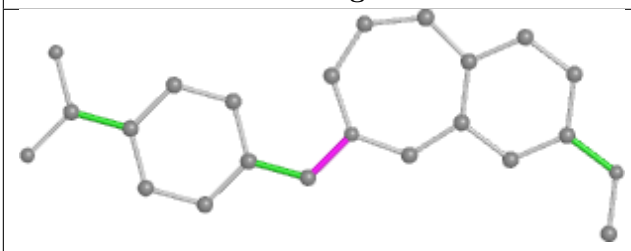
Ligand KVR G 5107



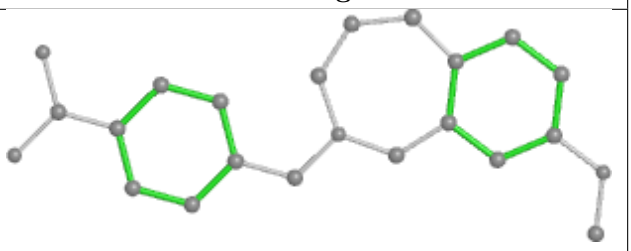
Bond lengths



Bond angles

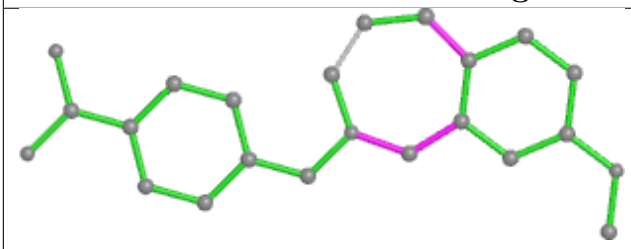


Torsions

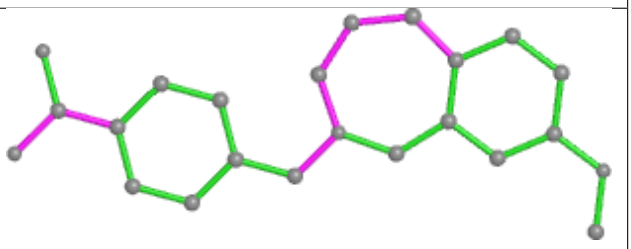


Rings

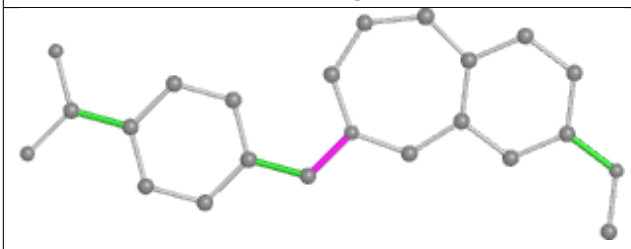
Ligand KVR B 5306



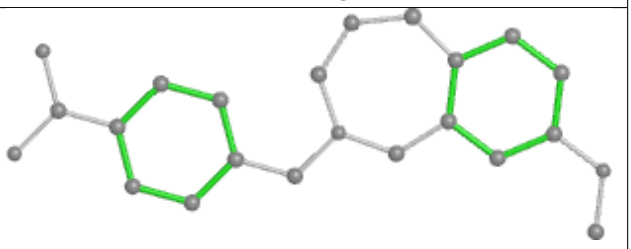
Bond lengths



Bond angles

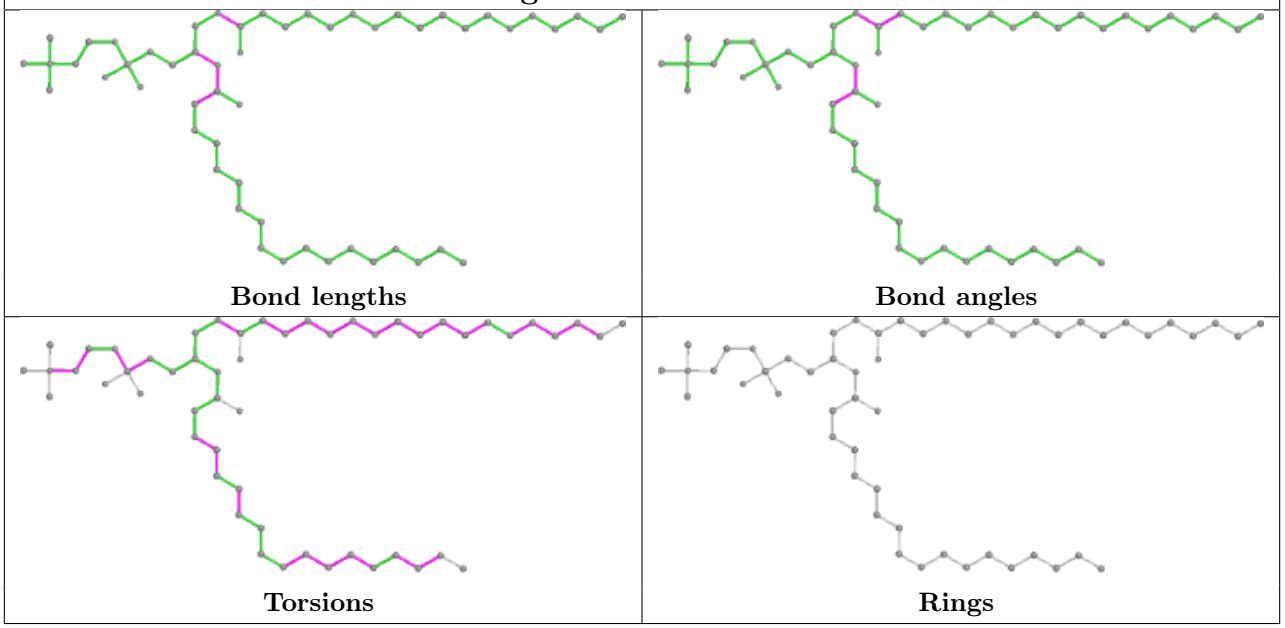


Torsions

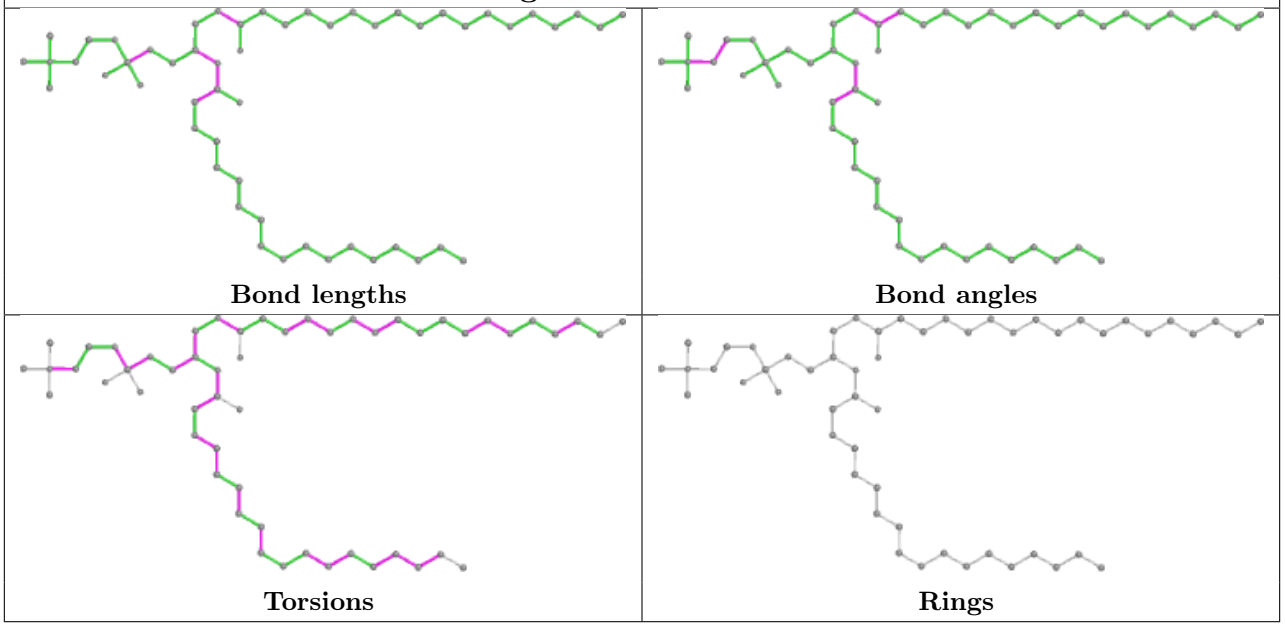


Rings

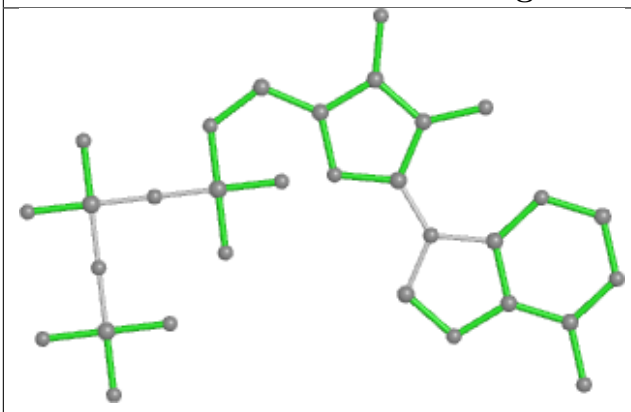
Ligand L9R B 5308



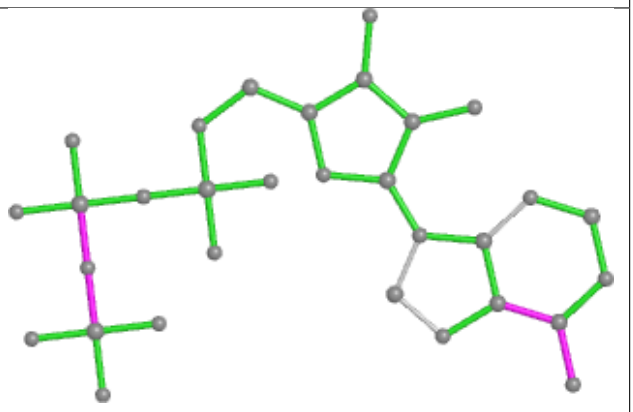
Ligand L9R A 5307



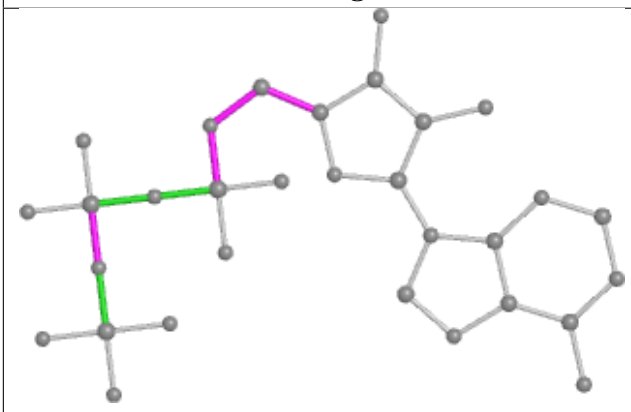
Ligand ATP B 5301



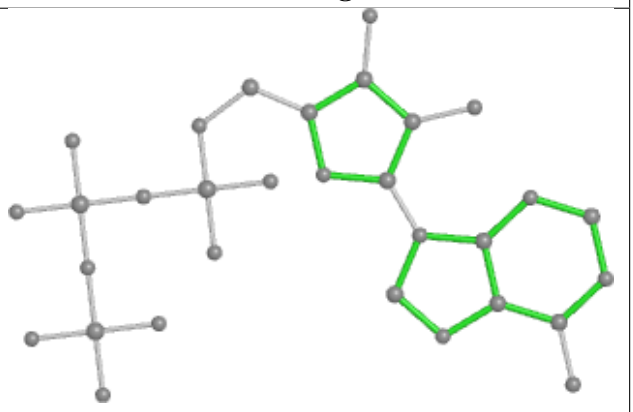
Bond lengths



Bond angles

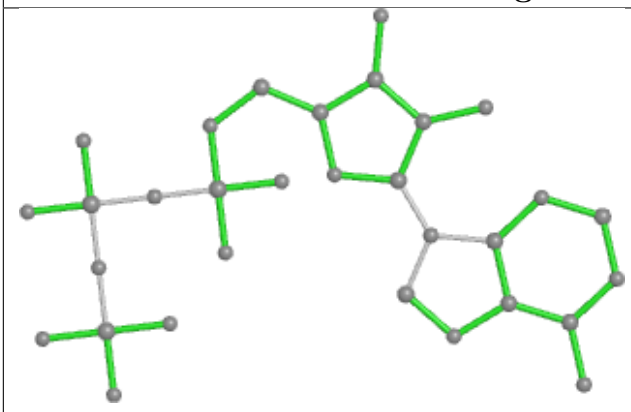


Torsions

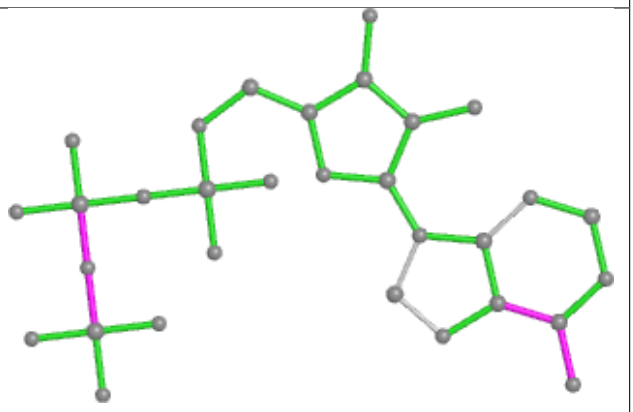


Rings

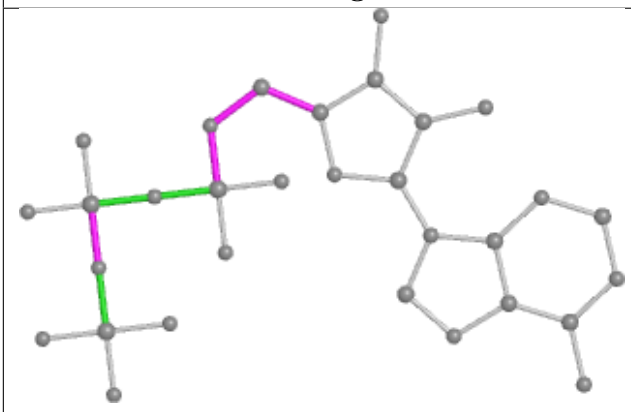
Ligand ATP G 5102



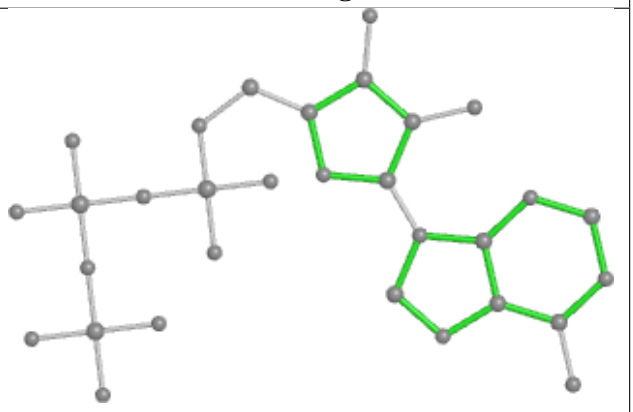
Bond lengths



Bond angles

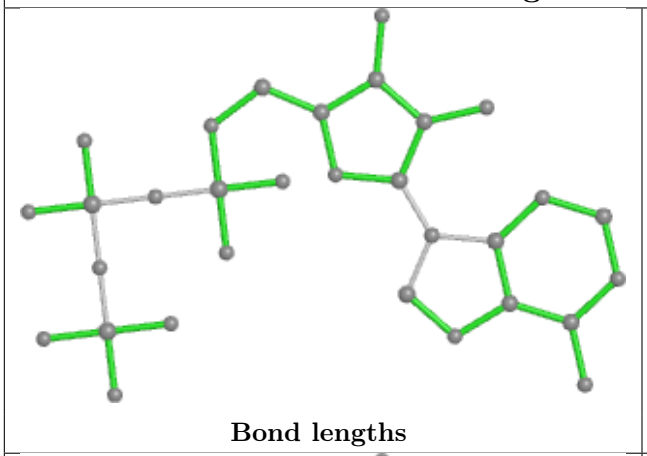


Torsions

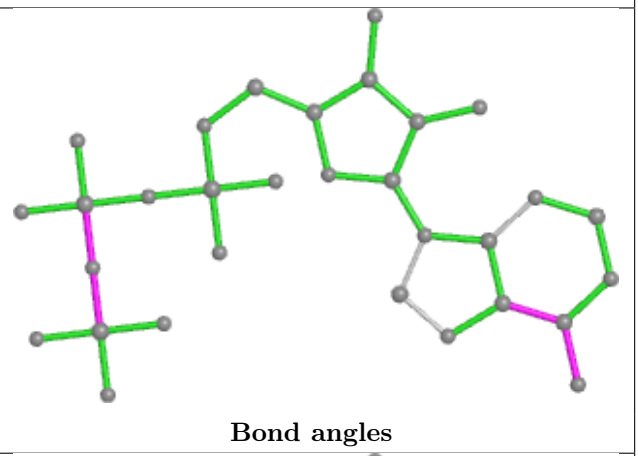


Rings

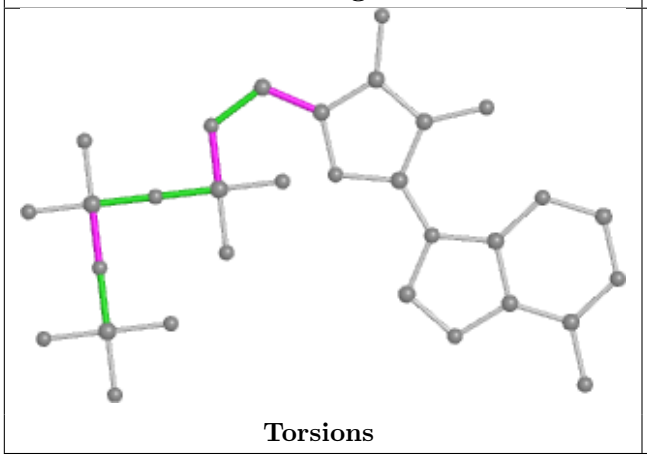
Ligand ATP I 5106



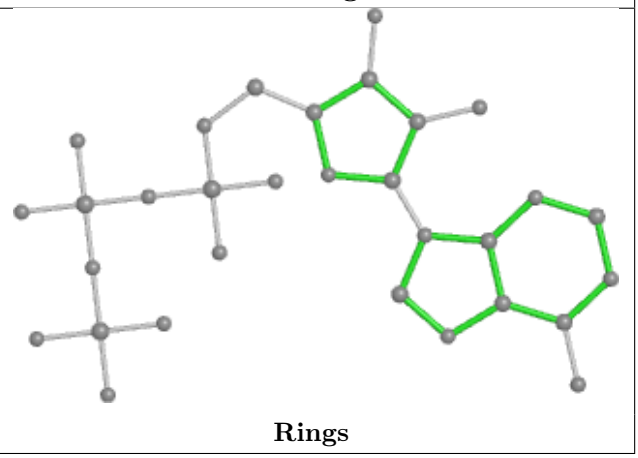
Bond lengths



Bond angles

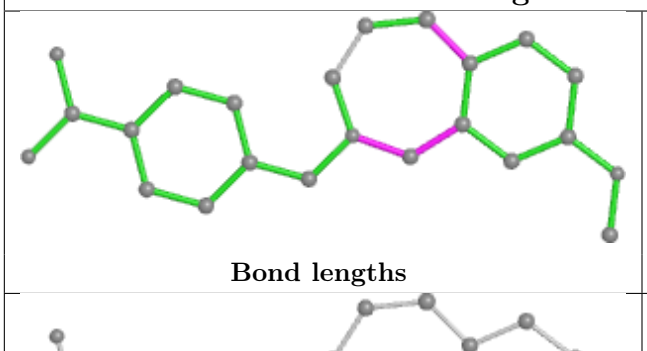


Torsions

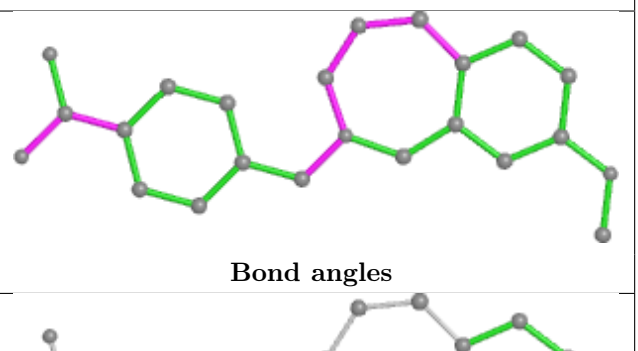


Rings

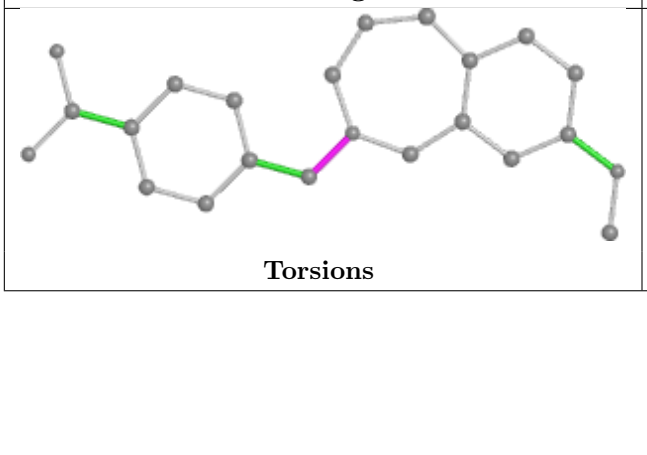
Ligand KVR A 5306



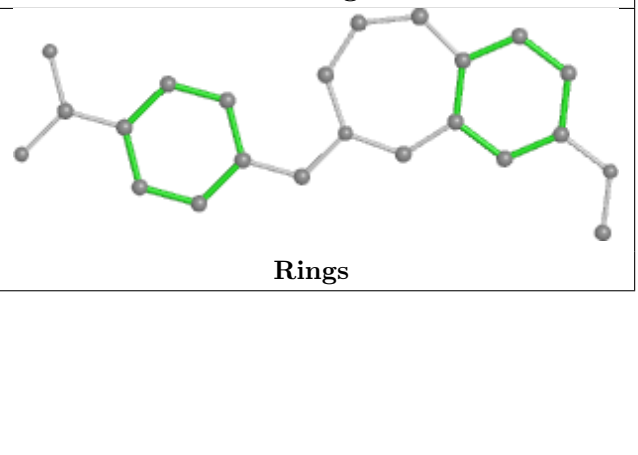
Bond lengths



Bond angles

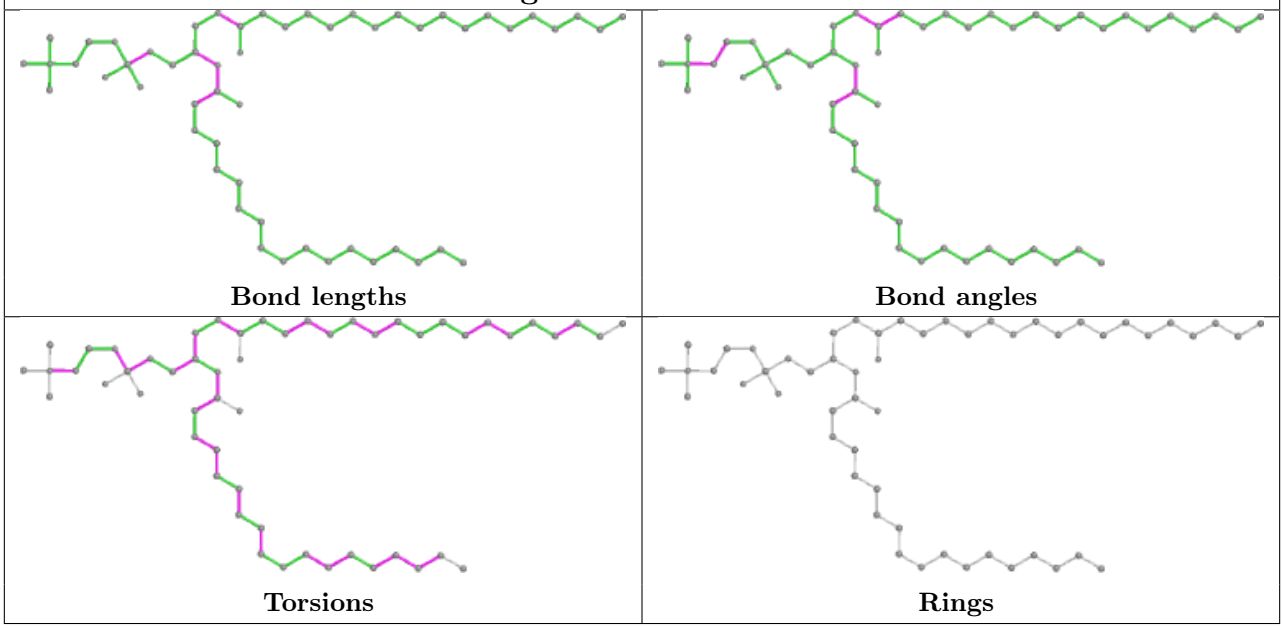


Torsions

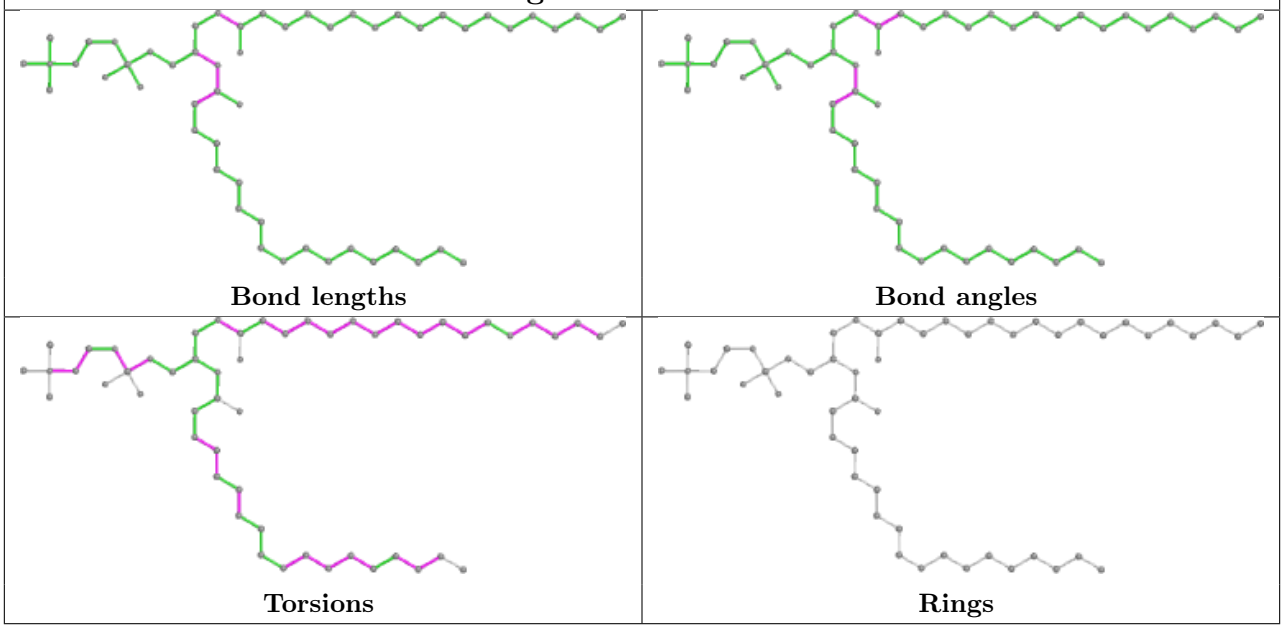


Rings

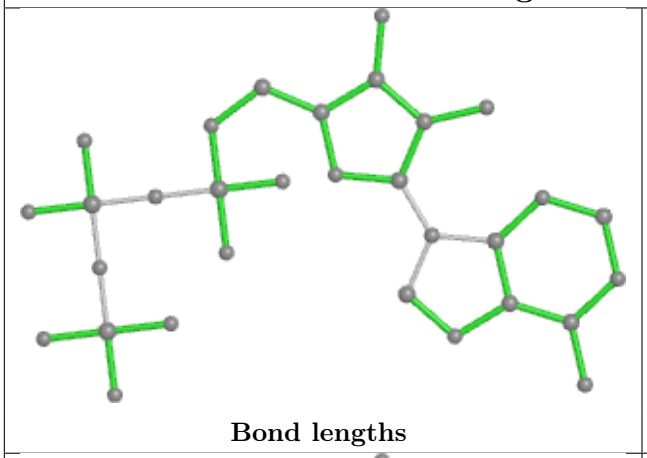
Ligand L9R B 5307



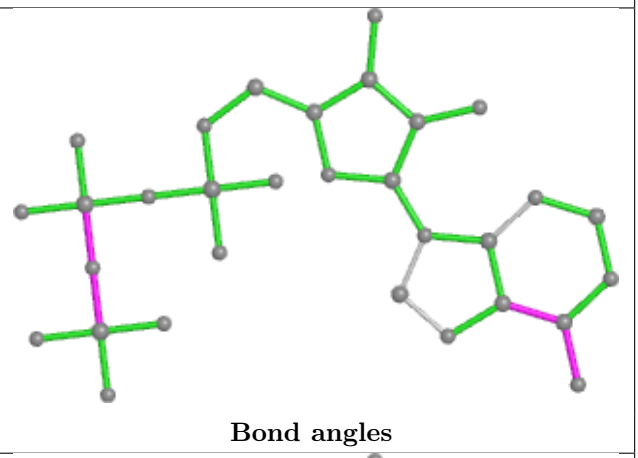
Ligand L9R I 5101



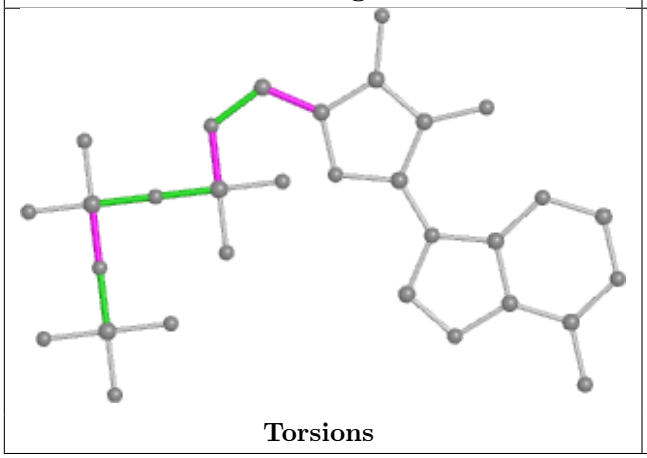
Ligand ATP G 5106



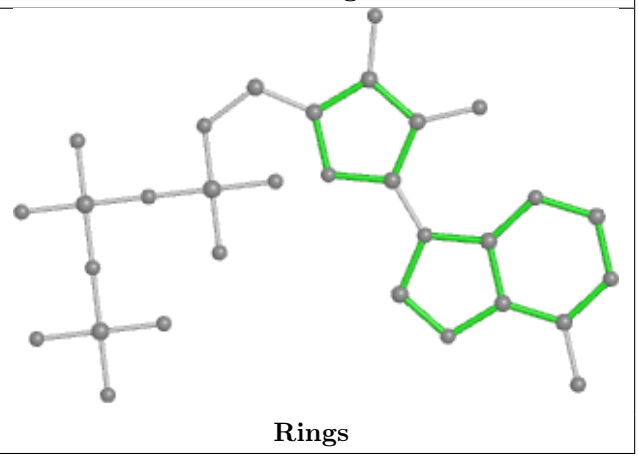
Bond lengths



Bond angles

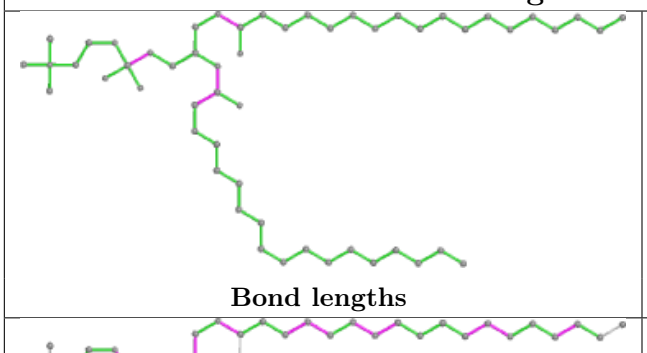


Torsions

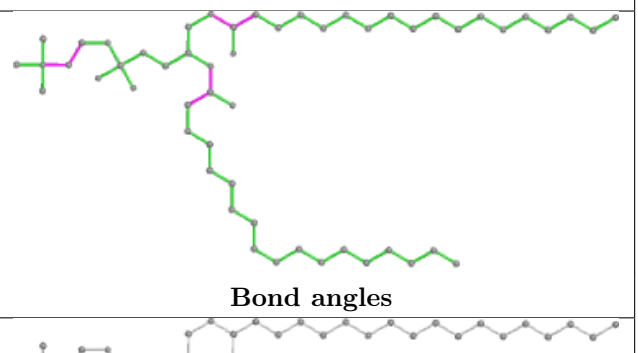


Rings

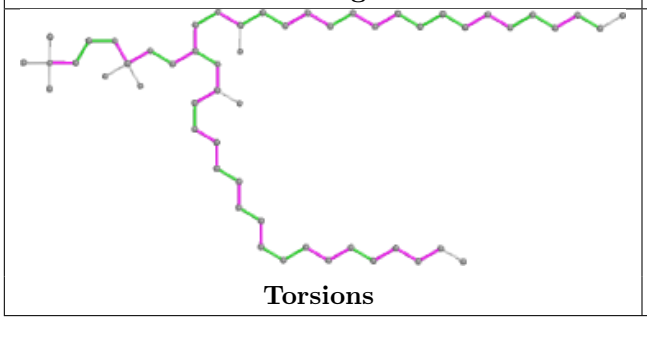
Ligand L9R I 5108



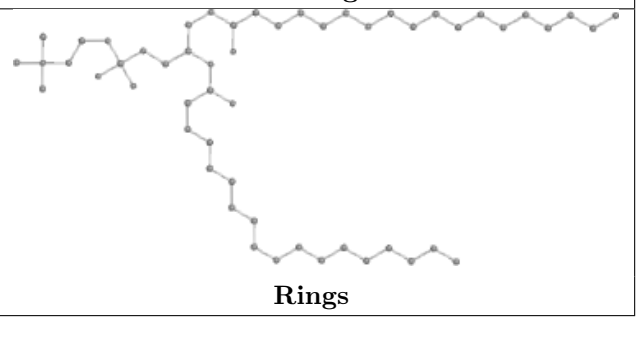
Bond lengths



Bond angles

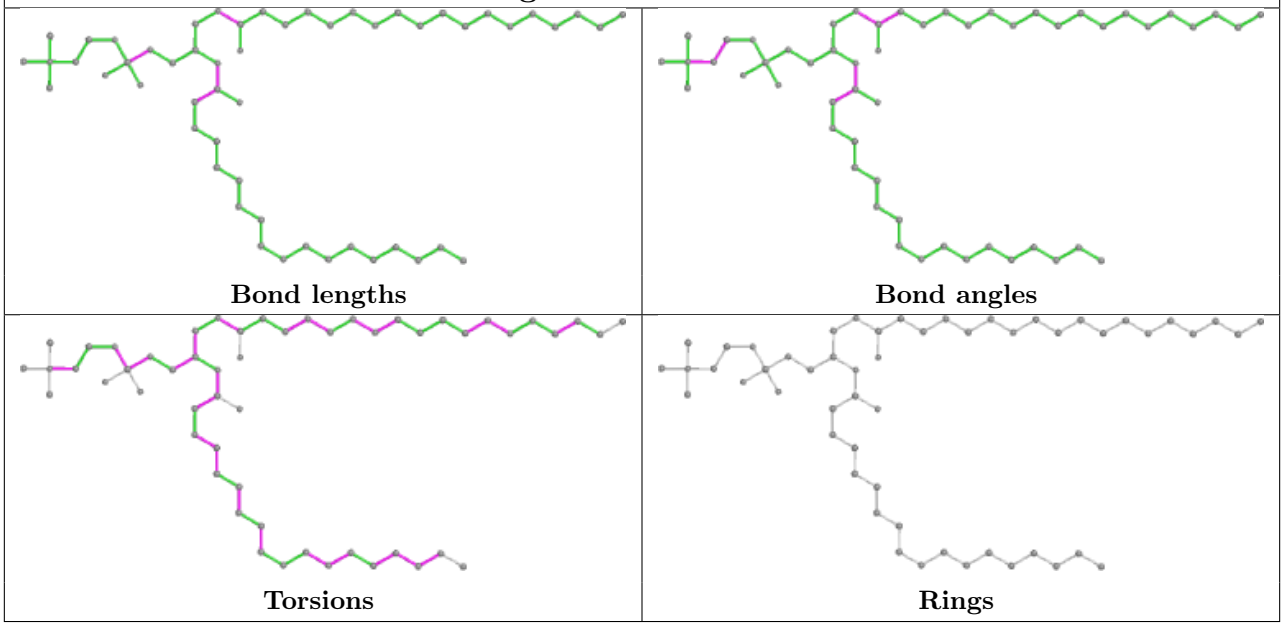


Torsions

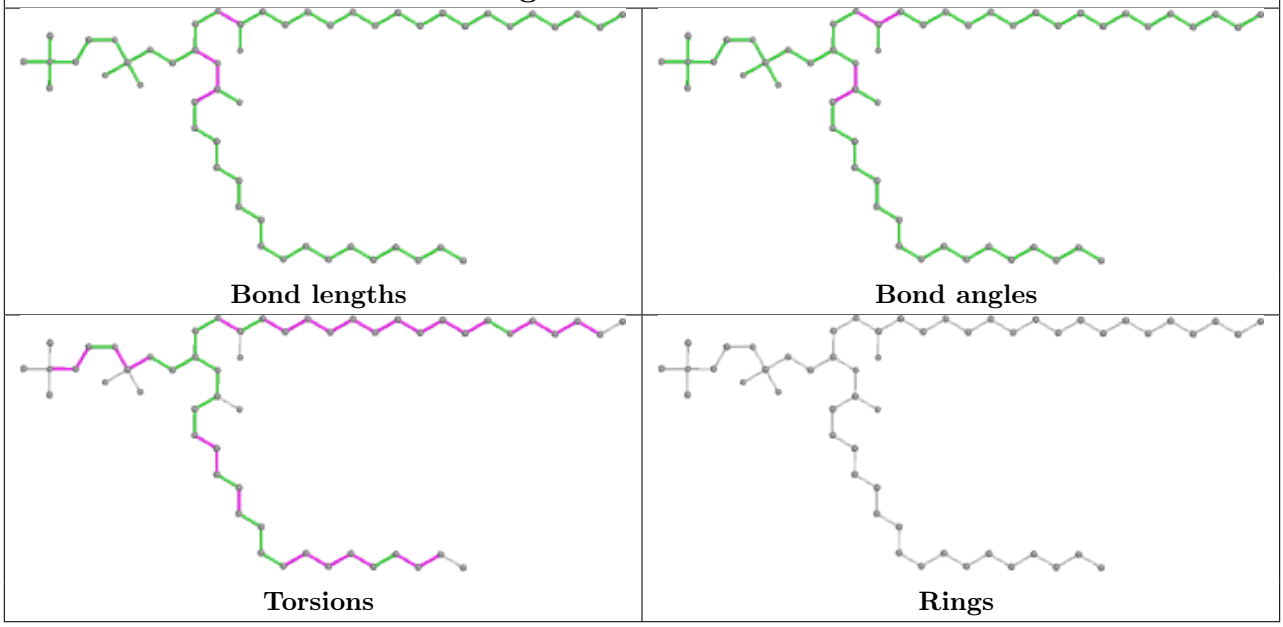


Rings

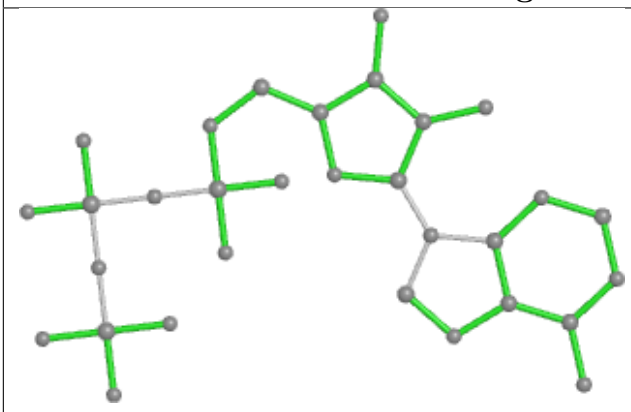
Ligand L9R G 5108



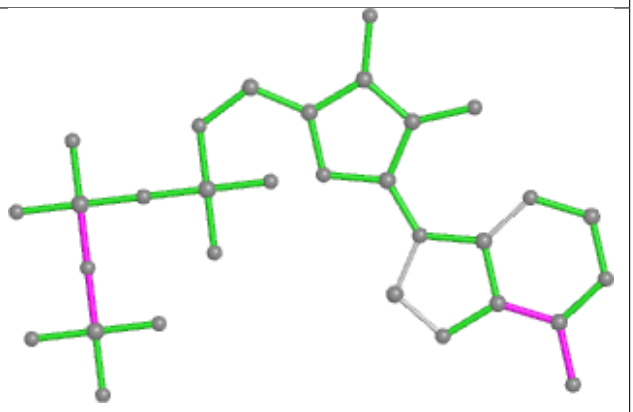
Ligand L9R G 5101



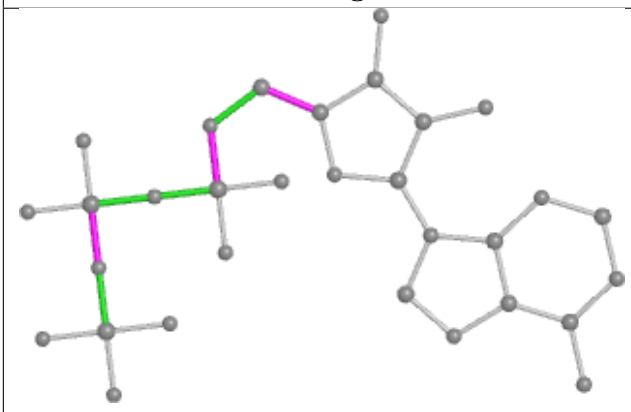
Ligand ATP B 5305



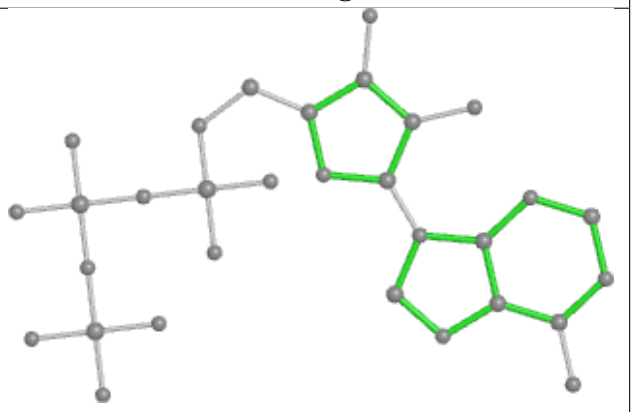
Bond lengths



Bond angles

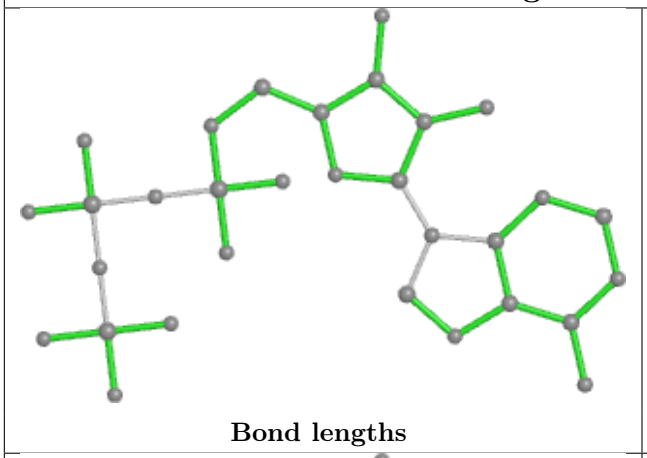


Torsions

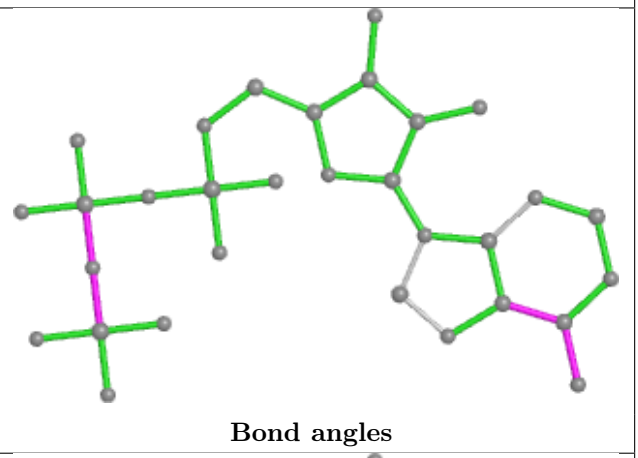


Rings

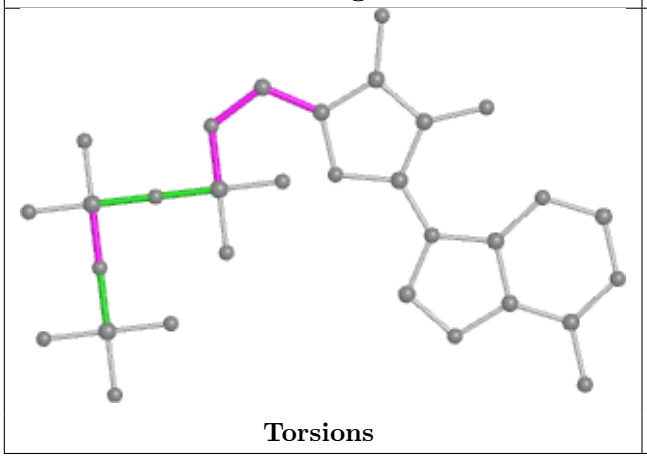
Ligand ATP I 5102



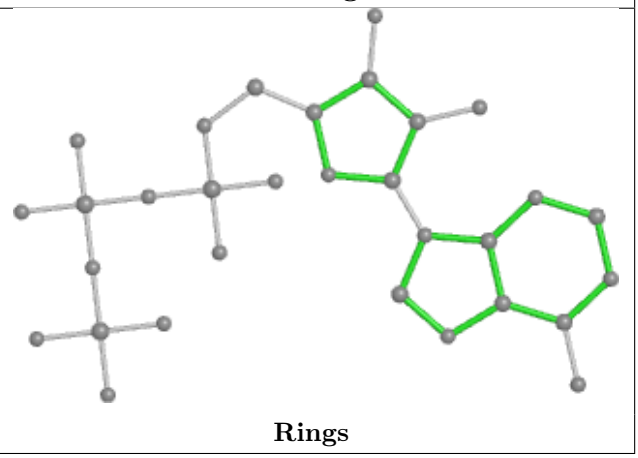
Bond lengths



Bond angles

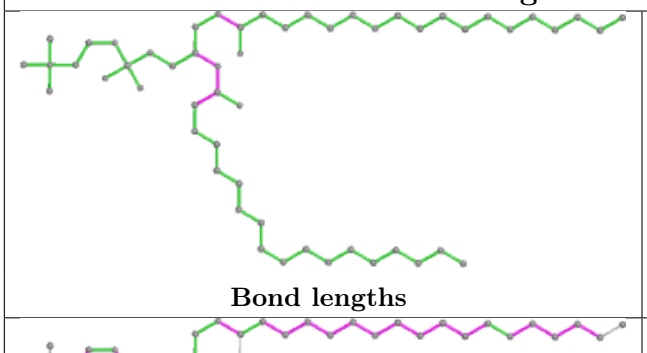


Torsions

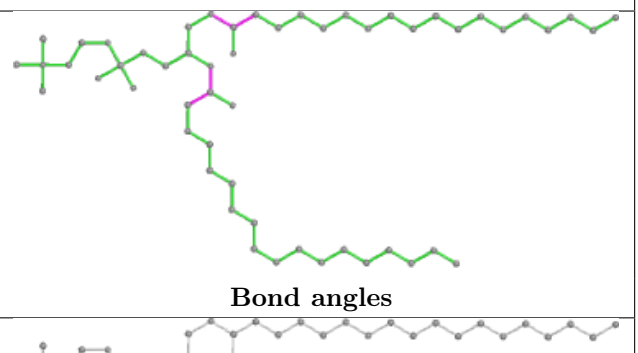


Rings

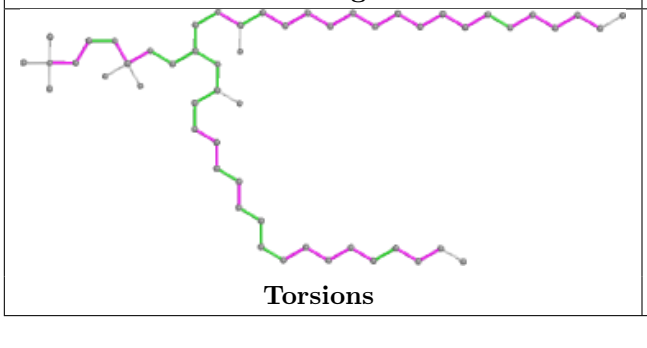
Ligand L9R A 5308



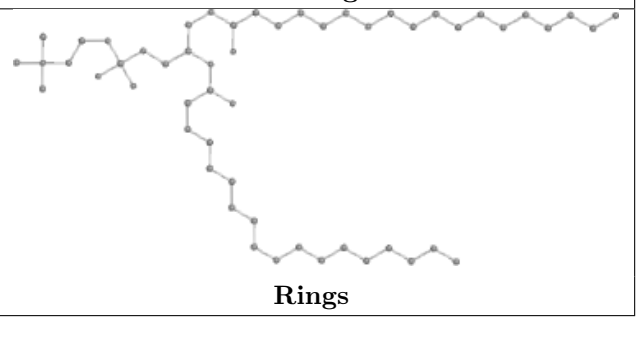
Bond lengths



Bond angles

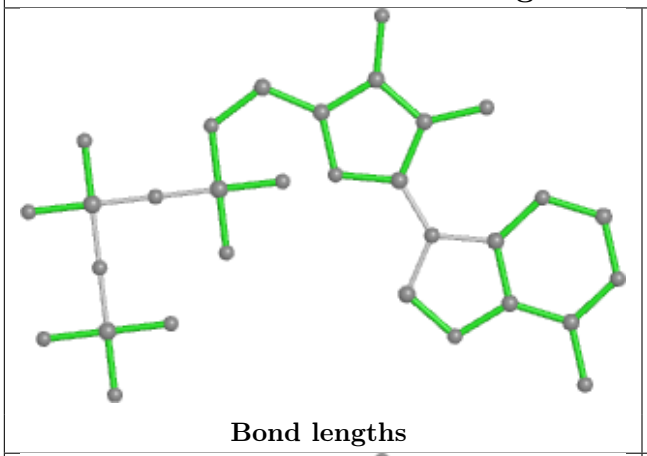


Torsions

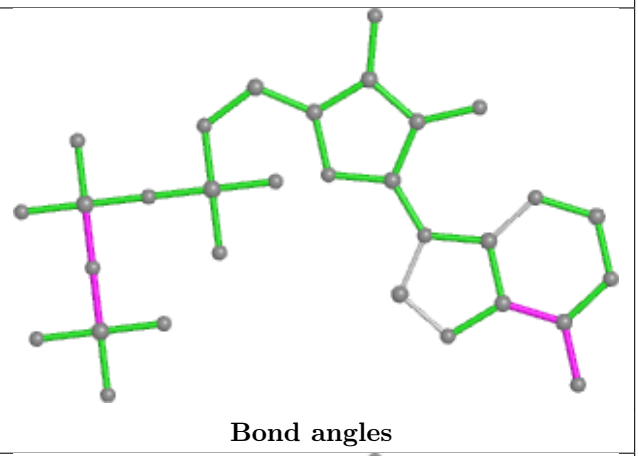


Rings

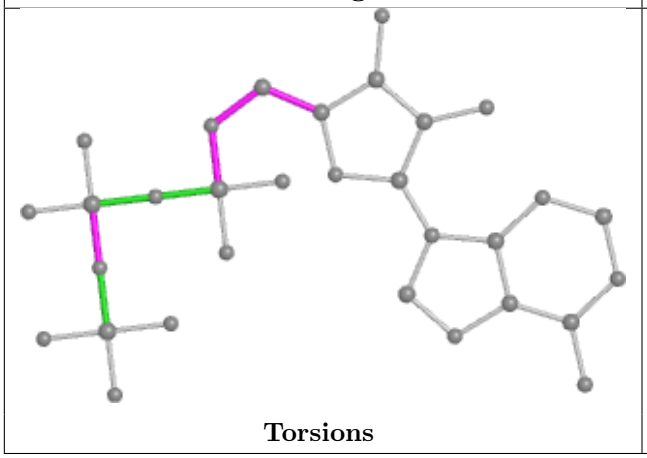
Ligand ATP A 5301



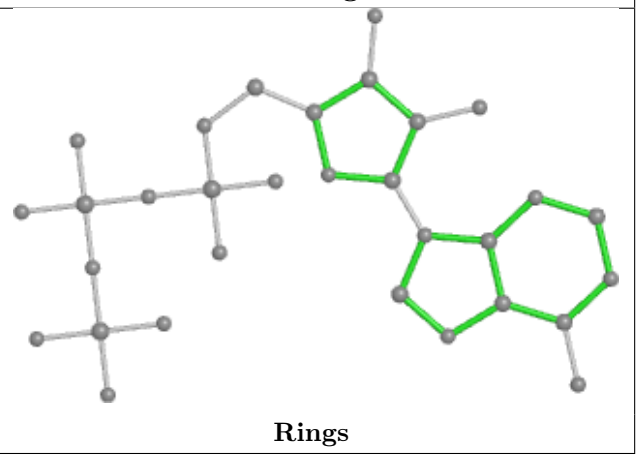
Bond lengths



Bond angles

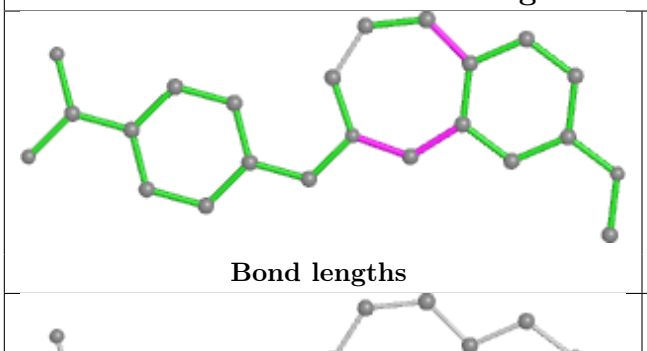


Torsions

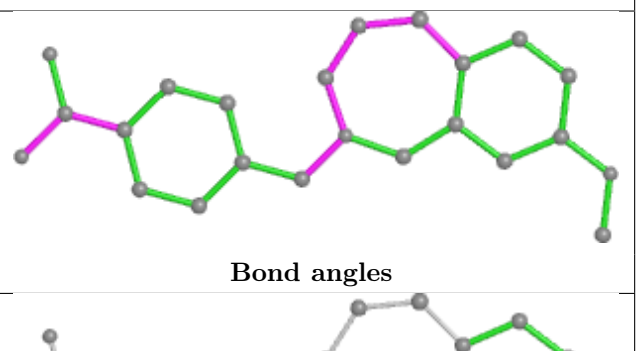


Rings

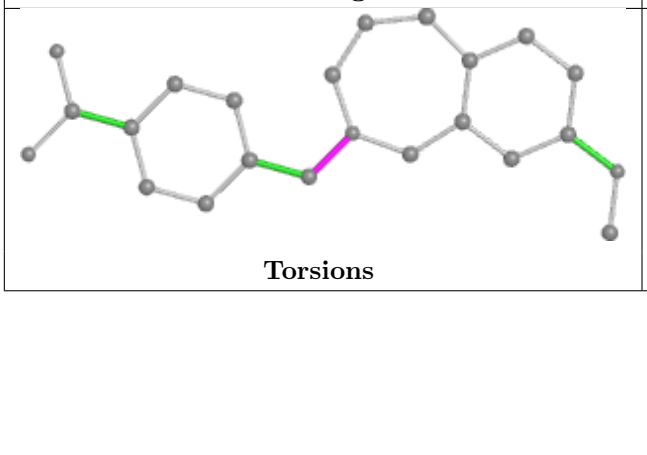
Ligand KVR I 5107



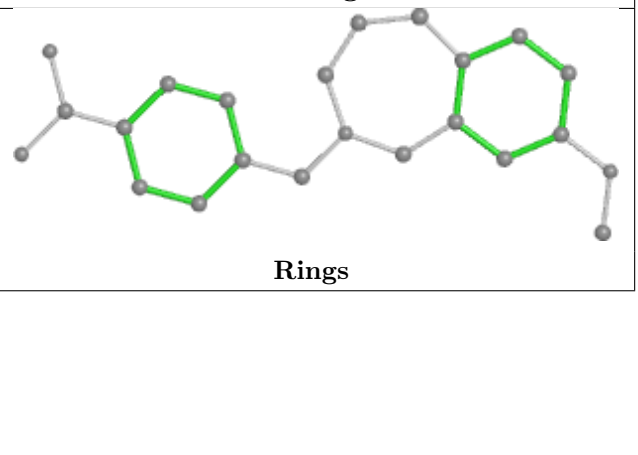
Bond lengths



Bond angles

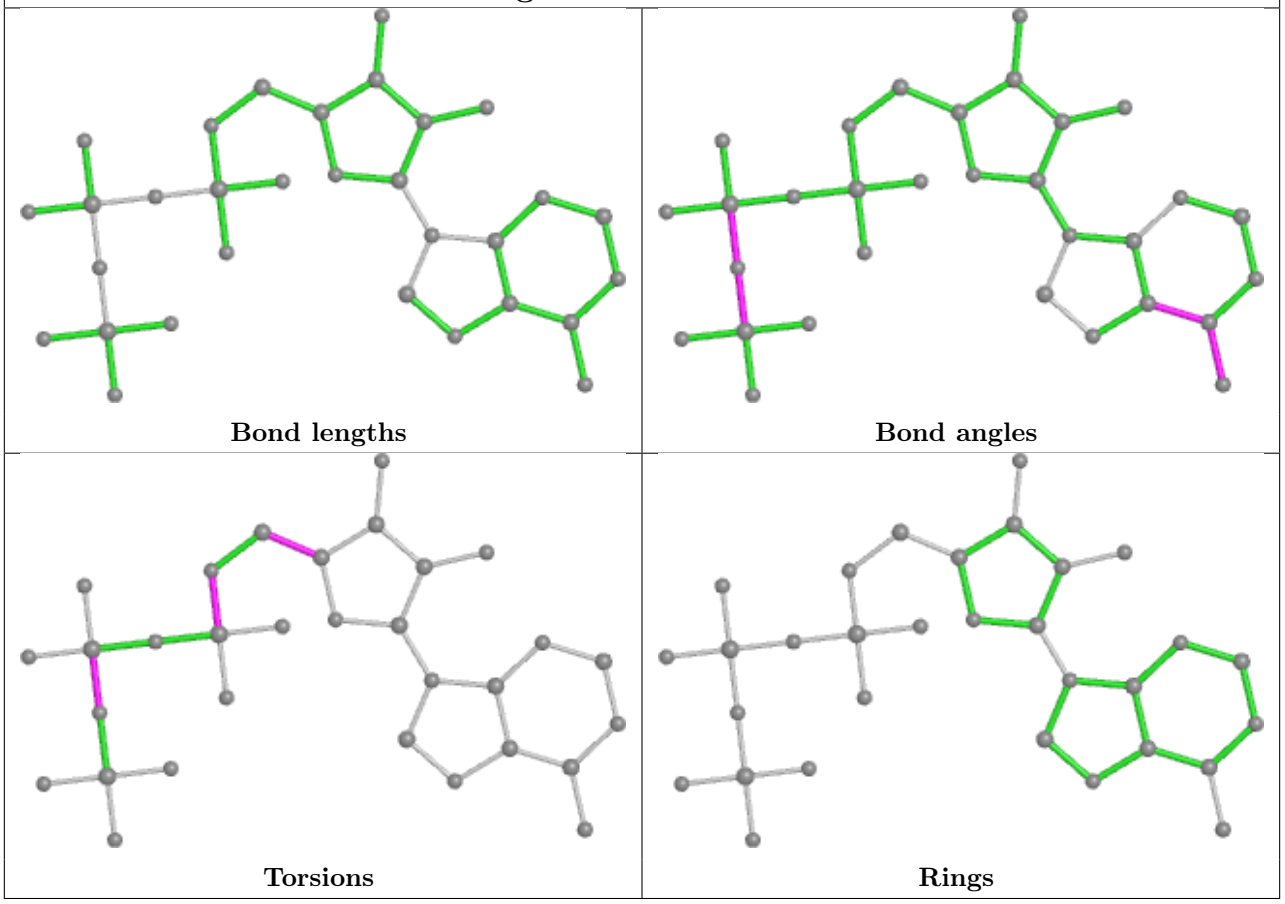


Torsions



Rings

Ligand ATP A 5305



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 Map visualisation

This section contains visualisations of the EMDB entry EMD-26205. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.