

wwPDB EM Validation Summary Report (i)

Nov 29, 2022 – 01:12 AM EST

PDB ID : 7UFI

EMDB ID : EMD-26476

Title: VchTnsC AAA+ ATPase with DNA, single heptamer

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Deposited on : 2022-03-22

Resolution : 3.40 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 : 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)

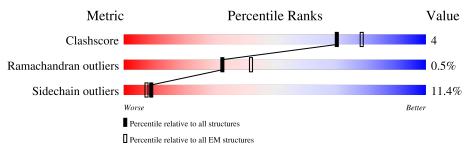
 $\begin{tabular}{lll} Validation Pipeline (wwPDB-VP) & : & 2.31.2 \end{tabular}$

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 3.40 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 $(\# \mathrm{Entries})$	${ m EM\ structures} \ (\#{ m Entries})$		
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	21	100%		
2	В	21	95%	_	5%
3	1	311	83%	.5%	.
3	2	311	84%	14%	•
3	3	311	84%	15%	-
3	4	311	84%	14%	•
3	5	311	84%	15%	_
3	6	311	85%	14%	•
3	7	311	84%	15%	- :



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18319 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 DNA chain called DNA (5'-D(P*CP*TP*CP*CP*AP*GP*TP*AP*CP*AP *GP*CP*GP*CP*GP*CP*TP*GP*AP*A)-3').

Mol	Chain	Residues	\mathbf{Atoms}				AltConf	Trace	
1	A	21	Total 430	C 203	N 82	O 124	P 21	0	0

• Molecule 2 is a DNA chain called DNA (5'-D(P*TP*TP*CP*AP*GP*CP*GP*CP*GP*CP*GP*CP*GP*TP*AP*CP*TP*GP*TP*AP*CP*TP*GP*AP*G)-3').

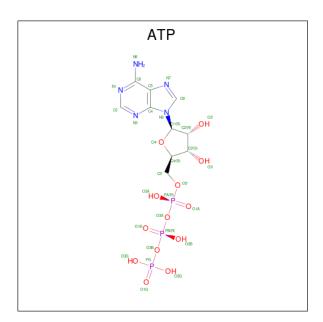
Mol	Chain	Residues	Atoms				AltConf	Trace	
2	В	21	Total 431	C 204	N 78	O 128	P 21	0	0

• Molecule 3 is a protein called VchTnsC.

Mol	Chain	Residues		At	oms			AltConf	Trace
3	1	311	Total	С	N	О	S	0	0
9	1	511	2463	1567	426	459	11	0	0
3	2	311	Total	С	N	О	S	0	0
J	۷	311	2463	1567	426	459	11	U	U
3	3	311	Total	\mathbf{C}	N	О	S	0	0
0	5	511	2463	1567	426	459	11	U	
3	4	4 311	Total	$^{\mathrm{C}}$	N	Ο	S	0	0
3	4	311	2463	1567	426	459	11	U	
3	5	311	Total	$^{\mathrm{C}}$	N	O	\mathbf{S}	0	0
0	5	311	2463	1567	426	459	11	U	U
3	6	311	Total	С	N	Ο	\mathbf{S}	0	0
	3 0	911	2463	1567	426	459	11	U	
3	3 7	311	Total	$^{\mathrm{C}}$	N	О	S	0	0
			2463	1567	426	459	11		U

• Molecule 4 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		Ato	oms			AltConf	
4	1	1	Total	С	N	О	Р	0	
4	1	1	31	10	5	13	3	0	
4	2	1	Total	С	N	О	Р	0	
4	<u> </u>	1	31	10	5	13	3	U	
4	3	1	Total	С	N	О	Р	0	
4	4 3	1	31	10	5	13	3	U	
4	4	4	1	Total	С	N	О	Р	0
4	4	1	31	10	5	13	3	U	
4	5	1	Total	С	N	О	Р	0	
4	9	1	31	10	5	13	3	U	
4	6	1	Total	С	N	О	Р	0	
4	4 0	1	31	10	5	13	3	U	
4	7	1	Total	С	N	О	Р	0	
4		7 1	31	10	5	13	3	U	



3 Residue-property plots (i)

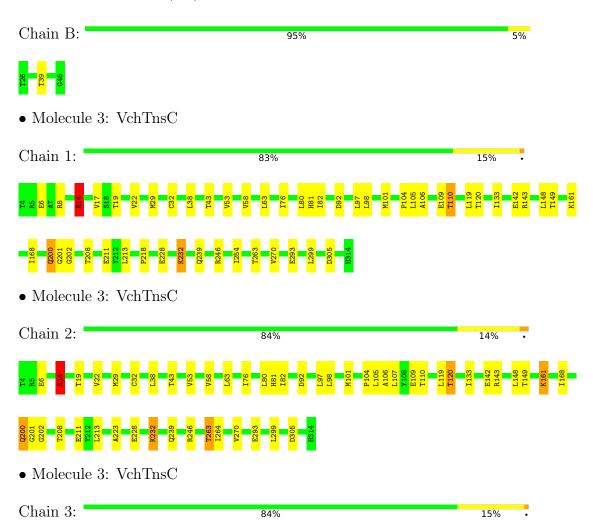
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

 \bullet Molecule 1: DNA (5'-D(P*CP*TP*CP*CP*AP*GP*TP*AP*CP*AP*GP*CP*GP*GP*GP*CP*TP*GP*AP*A)-3')

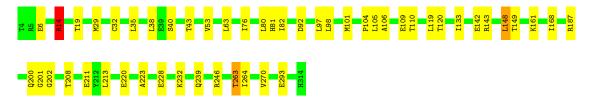
Chain A:

There are no outlier residues recorded for this chain.

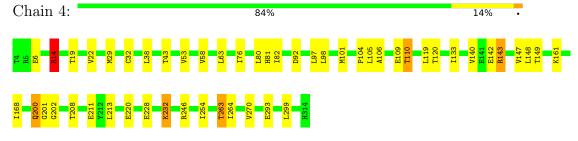
 \bullet Molecule 2: DNA (5'-D(P*TP*TP*CP*AP*GP*CP*CP*GP*CP*GP*CP*TP*GP*TP*AP*C P*TP*GP*AP*G)-3')



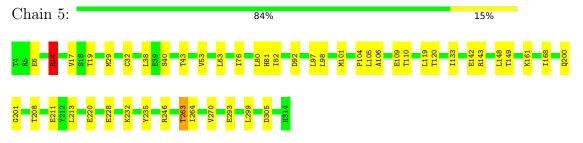




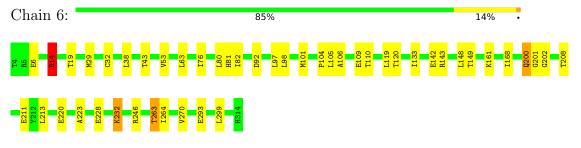
• Molecule 3: VchTnsC



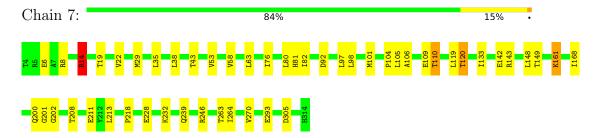
• Molecule 3: VchTnsC



• Molecule 3: VchTnsC



• Molecule 3: VchTnsC





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	65	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
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: ATP

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	0.19	0/482	0.70	0/741	
2	В	0.21	0/482	0.73	0/742	
3	1	0.67	0/2511	0.82	2/3395 (0.1%)	
3	2	0.67	0/2511	0.81	$2/3395 \ (0.1\%)$	
3	3	0.67	0/2511	0.81	2/3395 (0.1%)	
3	4	0.68	0/2511	0.82	2/3395~(0.1%)	
3	5	0.70	0/2511	0.83	2/3395 (0.1%)	
3	6	0.67	0/2511	0.81	2/3395 (0.1%)	
3	7	0.67	0/2511	0.82	2/3395 (0.1%)	
All	All	0.66	0/18541	0.81	14/25248 (0.1%)	

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	7	14	ARG	NE-CZ-NH1	7.01	123.80	120.30
3	5	14	ARG	NE-CZ-NH1	6.89	123.75	120.30
3	1	14	ARG	NE-CZ-NH1	6.85	123.73	120.30
3	3	14	ARG	NE-CZ-NH1	6.85	123.72	120.30
3	2	14	ARG	NE-CZ-NH1	6.78	123.69	120.30

There are no chirality outliers.

There are no planarity outliers.

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	430	0	235	0	0
2	В	431	0	237	1	0
3	1	2463	0	2497	20	0
3	2	2463	0	2497	18	0
3	3	2463	0	2497	14	0
3	4	2463	0	2497	18	0
3	5	2463	0	2497	34	0
3	6	2463	0	2497	15	0
3	7	2463	0	2497	15	0
4	1	31	0	12	2	0
4	2	31	0	12	1	0
4	3	31	0	12	1	0
4	4	31	0	12	2	0
4	5	31	0	12	2	0
4	6	31	0	11	1	0
4	7	31	0	12	1	0
All	All	18319	0	18034	129	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 4.

The worst 5 of 129 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1 Atom-2		$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$	
3:5:200:GLN:CD	3:5:299:LEU:HD22	1.34	1.48	
3:5:200:GLN:HE22	3:5:299:LEU:CD2	1.31	1.44	
3:5:200:GLN:NE2	3:5:299:LEU:HD22	1.12	1.42	
3:5:200:GLN:OE1	3:5:299:LEU:CG	1.65	1.42	
3:5:200:GLN:OE1	3:5:299:LEU:CB	1.71	1.38	

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	Perce	entiles
3	1	309/311 (99%)	277 (90%)	30 (10%)	2 (1%)	25	57
3	2	309/311 (99%)	278 (90%)	29 (9%)	2 (1%)	25	57
3	3	309/311 (99%)	280 (91%)	27 (9%)	2 (1%)	25	57
3	4	309/311 (99%)	280 (91%)	28 (9%)	1 (0%)	41	72
3	5	309/311 (99%)	280 (91%)	28 (9%)	1 (0%)	41	72
3	6	309/311 (99%)	280 (91%)	28 (9%)	1 (0%)	41	72
3	7	309/311 (99%)	280 (91%)	27 (9%)	2 (1%)	25	57
All	All	2163/2177 (99%)	1955 (90%)	197 (9%)	11 (0%)	32	61

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	1	201	GLY
3	3	201	GLY
3	6	201	GLY
3	7	201	GLY
3	2	201	GLY

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	Perc	entiles
3	1	$268/268 \; (100\%)$	237 (88%)	31 (12%)	5	20
3	2	$268/268 \; (100\%)$	236 (88%)	32 (12%)	5	19
3	3	$268/268 \; (100\%)$	238 (89%)	30 (11%)	6	22
3	4	$268/268 \; (100\%)$	237 (88%)	31 (12%)	5	20
3	5	$268/268 \; (100\%)$	237 (88%)	31 (12%)	5	20
3	6	$268/268\ (100\%)$	237 (88%)	31 (12%)	5	20
3	7	268/268 (100%)	240 (90%)	28 (10%)	7	25

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Mol	Chain	Analysed	Analysed Rotameric		Percentiles	
All	All	1876/1876 (100%)	1662 (89%)	214 (11%)	9 21	

5 of 214 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	4	208	THR
3	5	149	THR
3	7	119	LEU
3	4	228	GLU
3	5	43	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	1	200	GLN
3	4	200	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)

7 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	Во	ond leng	ths	В	ond ang	les
WIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	5	401	-	26,33,33	0.69	0	31,52,52	0.83	0
4	ATP	1	401	-	26,33,33	0.73	0	31,52,52	1.17	2 (6%)
4	ATP	6	401	-	26,33,33	0.66	0	31,52,52	1.18	3 (9%)
4	ATP	4	401	-	26,33,33	0.71	0	31,52,52	1.04	2 (6%)
4	ATP	3	401	-	26,33,33	0.72	0	31,52,52	1.23	2 (6%)
4	ATP	7	401	-	26,33,33	0.71	0	31,52,52	1.12	2 (6%)
4	ATP	2	401	-	26,33,33	0.73	0	31,52,52	1.15	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
4	ATP	5	401	-	-	5/18/38/38	0/3/3/3
4	ATP	1	401	-	-	5/18/38/38	0/3/3/3
4	ATP	6	401	-	-	5/18/38/38	0/3/3/3
4	ATP	4	401	-	-	5/18/38/38	0/3/3/3
4	ATP	3	401	-	-	5/18/38/38	0/3/3/3
4	ATP	7	401	-	-	5/18/38/38	0/3/3/3
4	ATP	2	401	-	-	5/18/38/38	0/3/3/3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
4	3	401	ATP	PA-O3A-PB	-3.91	119.42	132.83
4	1	401	ATP	PA-O3A-PB	-3.61	120.42	132.83
4	2	401	ATP	PB-O3B-PG	-3.60	120.47	132.83
4	1	401	ATP	PB-O3B-PG	-3.57	120.58	132.83
4	7	401	ATP	PB-O3B-PG	-3.51	120.77	132.83

There are no chirality outliers.

5 of 35 torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
4	1	401	ATP	C5'-O5'-PA-O1A
4	1	401	ATP	C5'-O5'-PA-O2A
4	1	401	ATP	C5'-O5'-PA-O3A
4	2	401	ATP	C5'-O5'-PA-O1A
4	2	401	ATP	C5'-O5'-PA-O3A

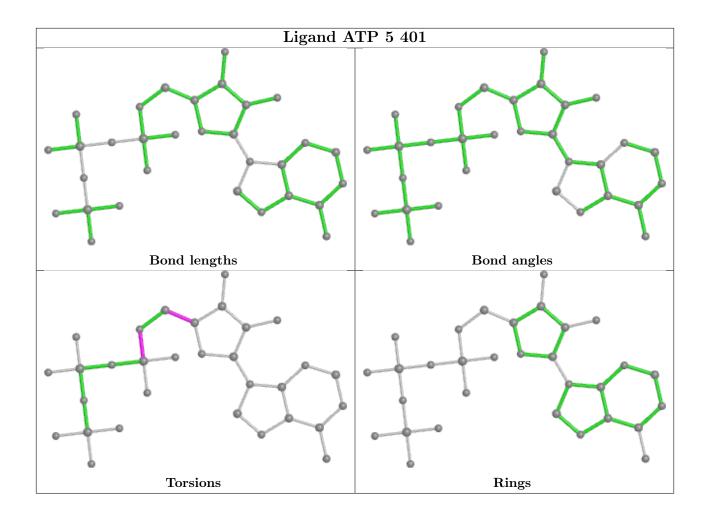
There are no ring outliers.

7 monomers are involved in 10 short contacts:

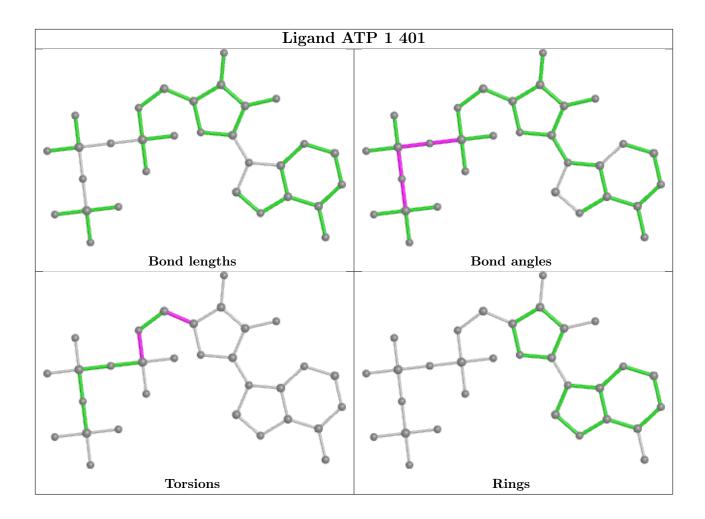
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	5	401	ATP	2	0
4	1	401	ATP	2	0
4	6	401	ATP	1	0
4	4	401	ATP	2	0
4	3	401	ATP	1	0
4	7	401	ATP	1	0
4	2	401	ATP	1	0

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.

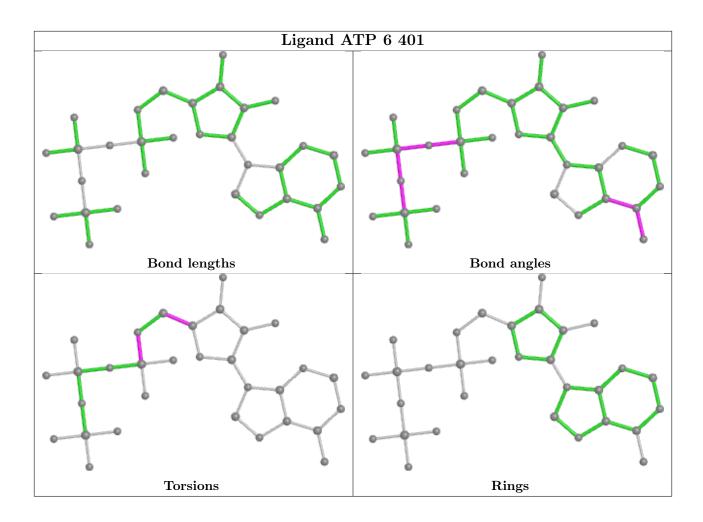




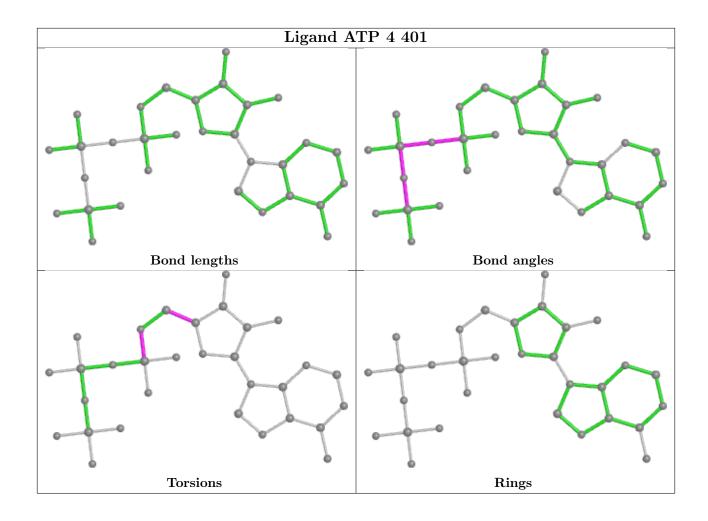




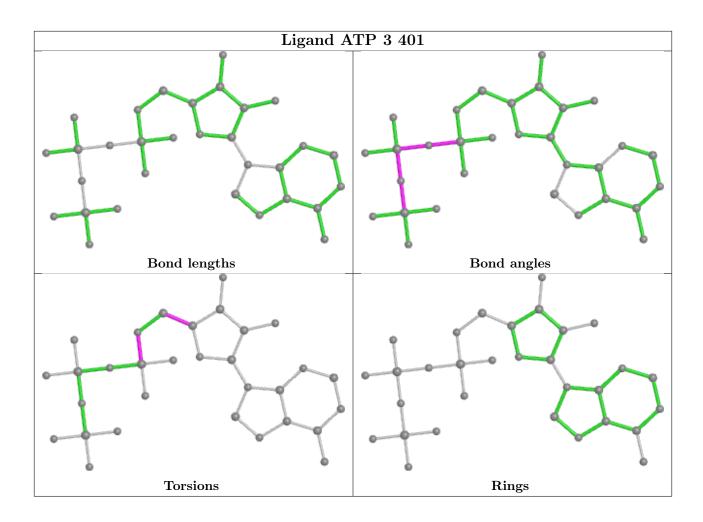




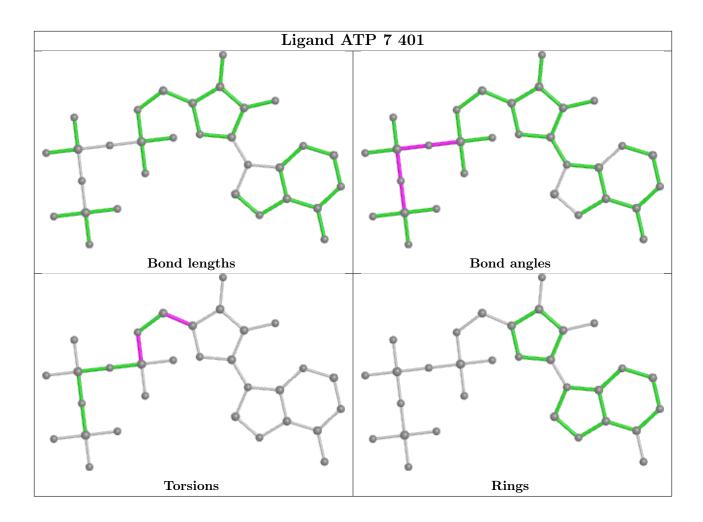




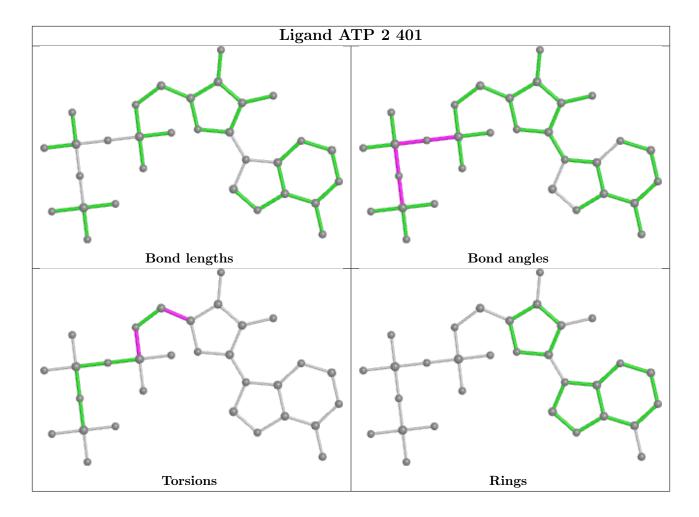












5.7 Other polymers (i)

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 (i)

This section contains visualisations of the EMDB entry EMD-26476. 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 (i)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

6.4 Orthogonal surface views (i)

This section was not generated.

6.5 Mask visualisation (i)

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



7 Map analysis (i)

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

7.1 Map-value distribution (i)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

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 (i)

This section was not generated.

