Full wwPDB EM Validation Report (i)

Feb 3, 2024 – 08:37 PM EST

PDB ID	:	1N03
Title	:	Model for Active RecA Filament
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Deposited on	:	2002-10-10
Resolution	:	20.00 Å(reported)
Based on initial model	:	1REA

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB 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 (i)) were used in the production of this report:

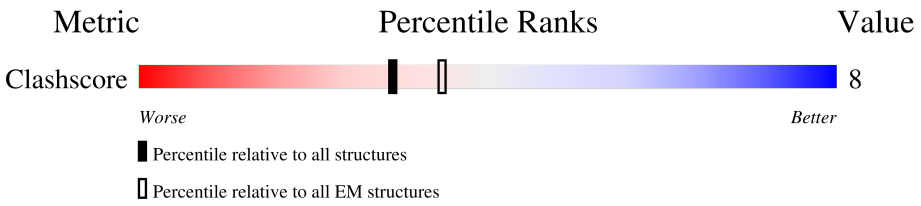
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 20.00 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

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	352	85% · 14%
1	B	352	85% · 14%
1	C	352	85% · 14%
1	D	352	85% · 14%
1	E	352	85% · 14%
1	F	352	85% · 14%
1	G	352	85% · 14%

2 Entry composition (i)

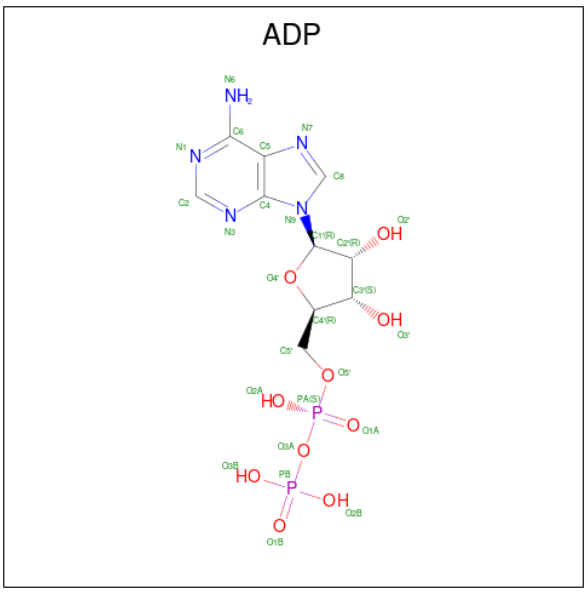
There are 2 unique types of molecules in this entry. The entry contains 2310 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RecA protein.

Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C			
1	A	303	303	303		0	303
1	B	303	303	303		0	303
1	C	303	303	303		0	303
1	D	303	303	303		0	303
1	E	303	303	303		0	303
1	F	303	303	303		0	303
1	G	303	303	303		0	303

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



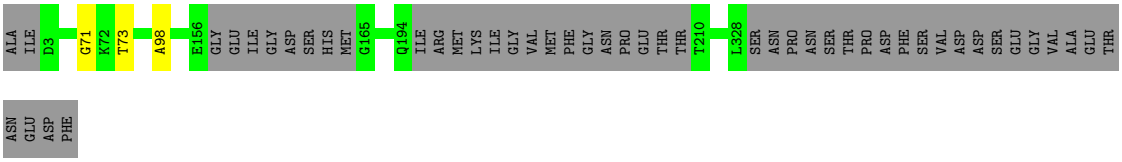
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0
2	B	1	27	10	5	10	2	0
2	C	1	27	10	5	10	2	0
2	D	1	27	10	5	10	2	0
2	E	1	27	10	5	10	2	0
2	F	1	27	10	5	10	2	0
2	G	1	27	10	5	10	2	0

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.

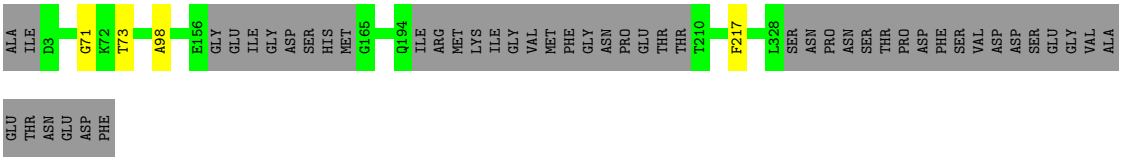
- Molecule 1: RecA protein

Chain A:



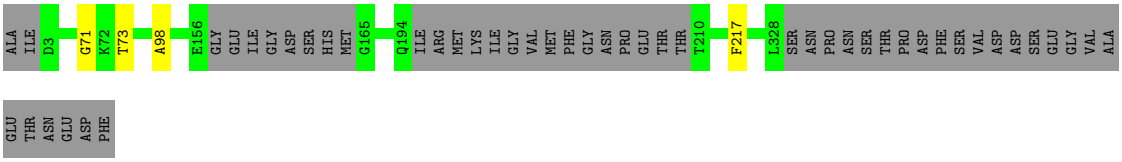
- Molecule 1: RecA protein

Chain B:



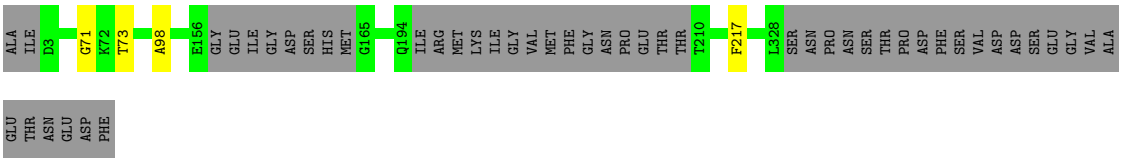
- Molecule 1: RecA protein

Chain C:



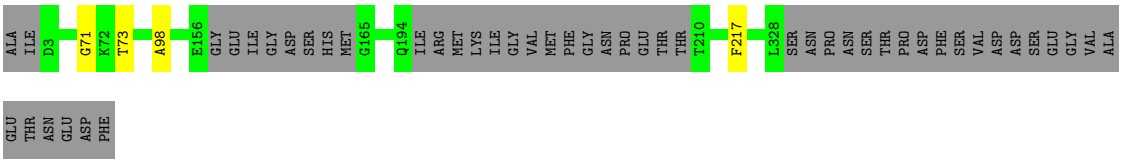
- Molecule 1: RecA protein

Chain D:



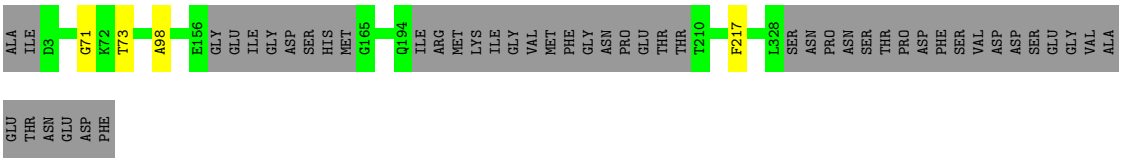
- Molecule 1: RecA protein

Chain E:



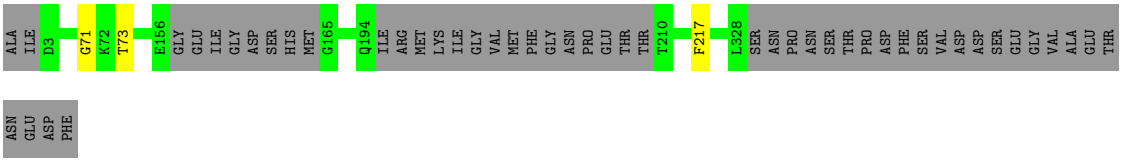
- Molecule 1: RecA protein

Chain F:



- Molecule 1: RecA protein

Chain G:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	1.00Å 1.00Å 1.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 20.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-20.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2310	wwPDB-VP
Average B, all atoms ($Å^2$)	10.0	wwPDB-VP

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: 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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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 (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	303	0	0	3	0
1	B	303	0	0	4	0
1	C	303	0	0	4	0
1	D	303	0	0	4	0
1	E	303	0	0	4	0
1	F	303	0	0	4	0
1	G	303	0	0	3	0
2	A	27	0	12	2	0
2	B	27	0	12	2	0
2	C	27	0	12	2	0
2	D	27	0	12	2	0
2	E	27	0	12	2	0
2	F	27	0	12	2	0
2	G	27	0	12	2	0
All	All	2310	0	84	20	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 8.

All (20) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:THR:CA	2:F:506:ADP:O1A	2.50	0.60
1:G:73:THR:CA	2:G:507:ADP:O1A	2.50	0.60
1:B:73:THR:CA	2:B:502:ADP:O1A	2.50	0.60
1:C:73:THR:CA	2:C:503:ADP:O1A	2.50	0.60
1:E:73:THR:CA	2:E:505:ADP:O1A	2.50	0.60
1:A:73:THR:CA	2:A:501:ADP:O1A	2.50	0.60
1:D:73:THR:CA	2:D:504:ADP:O1A	2.50	0.59
1:C:98:ALA:CA	1:D:217:PHE:CA	2.91	0.49
1:B:98:ALA:CA	1:C:217:PHE:CA	2.91	0.49
1:D:98:ALA:CA	1:E:217:PHE:CA	2.91	0.49
1:A:98:ALA:CA	1:B:217:PHE:CA	2.91	0.49
1:E:98:ALA:CA	1:F:217:PHE:CA	2.91	0.48
1:F:98:ALA:CA	1:G:217:PHE:CA	2.91	0.48
1:D:71:GLY:CA	2:D:504:ADP:H5'1	2.45	0.47
1:F:71:GLY:CA	2:F:506:ADP:H5'1	2.45	0.47
1:C:71:GLY:CA	2:C:503:ADP:H5'1	2.45	0.47
1:G:71:GLY:CA	2:G:507:ADP:H5'1	2.45	0.46
1:A:71:GLY:CA	2:A:501:ADP:H5'1	2.45	0.46
1:B:71:GLY:CA	2:B:502:ADP:H5'1	2.45	0.46
1:E:71:GLY:CA	2:E:505:ADP:H5'1	2.45	0.46

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ADP	B	502	-	24,29,29	1.09	4 (16%)	29,45,45	1.16	2 (6%)
2	ADP	G	507	-	24,29,29	1.09	4 (16%)	29,45,45	1.16	2 (6%)
2	ADP	A	501	-	24,29,29	1.10	4 (16%)	29,45,45	1.15	2 (6%)
2	ADP	C	503	-	24,29,29	1.09	4 (16%)	29,45,45	1.16	2 (6%)
2	ADP	F	506	-	24,29,29	1.09	4 (16%)	29,45,45	1.15	2 (6%)
2	ADP	E	505	-	24,29,29	1.09	4 (16%)	29,45,45	1.16	2 (6%)
2	ADP	D	504	-	24,29,29	1.10	4 (16%)	29,45,45	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
2	ADP	B	502	-	-	3/12/32/32	0/3/3/3
2	ADP	G	507	-	-	3/12/32/32	0/3/3/3
2	ADP	A	501	-	-	3/12/32/32	0/3/3/3
2	ADP	C	503	-	-	3/12/32/32	0/3/3/3
2	ADP	F	506	-	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	E	505	-	-	3/12/32/32	0/3/3/3
2	ADP	D	504	-	-	3/12/32/32	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	ADP	O4'-C1'	2.63	1.44	1.41
2	E	505	ADP	O4'-C1'	2.63	1.44	1.41
2	D	504	ADP	O4'-C1'	2.63	1.44	1.41
2	A	501	ADP	O4'-C1'	2.62	1.44	1.41
2	F	506	ADP	O4'-C1'	2.61	1.44	1.41
2	G	507	ADP	O4'-C1'	2.60	1.44	1.41
2	C	503	ADP	O4'-C1'	2.59	1.44	1.41
2	A	501	ADP	C2'-C1'	-2.14	1.50	1.53
2	D	504	ADP	C2'-C1'	-2.12	1.50	1.53
2	F	506	ADP	C2'-C1'	-2.11	1.50	1.53
2	B	502	ADP	C2'-C1'	-2.09	1.50	1.53
2	E	505	ADP	C2'-C1'	-2.09	1.50	1.53
2	C	503	ADP	C2'-C1'	-2.08	1.50	1.53
2	B	502	ADP	PB-O2B	-2.08	1.46	1.54
2	A	501	ADP	PB-O2B	-2.06	1.46	1.54
2	G	507	ADP	C2'-C1'	-2.06	1.50	1.53
2	G	507	ADP	PB-O2B	-2.06	1.46	1.54
2	G	507	ADP	C8-N7	-2.06	1.31	1.34
2	F	506	ADP	PB-O2B	-2.06	1.46	1.54
2	E	505	ADP	PB-O2B	-2.05	1.46	1.54
2	C	503	ADP	PB-O2B	-2.05	1.46	1.54
2	D	504	ADP	PB-O2B	-2.04	1.47	1.54
2	A	501	ADP	C8-N7	-2.04	1.31	1.34
2	C	503	ADP	C8-N7	-2.04	1.31	1.34
2	F	506	ADP	C8-N7	-2.03	1.31	1.34
2	D	504	ADP	C8-N7	-2.03	1.31	1.34
2	E	505	ADP	C8-N7	-2.02	1.31	1.34
2	B	502	ADP	C8-N7	-2.00	1.31	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	505	ADP	C4-C5-N7	2.17	111.66	109.40
2	C	503	ADP	C4-C5-N7	2.16	111.66	109.40
2	G	507	ADP	O4'-C1'-C2'	-2.16	103.77	106.93
2	C	503	ADP	O4'-C1'-C2'	-2.15	103.78	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	502	ADP	O4'-C1'-C2'	-2.15	103.78	106.93
2	A	501	ADP	O4'-C1'-C2'	-2.15	103.79	106.93
2	E	505	ADP	O4'-C1'-C2'	-2.15	103.79	106.93
2	D	504	ADP	O4'-C1'-C2'	-2.14	103.80	106.93
2	F	506	ADP	O4'-C1'-C2'	-2.14	103.80	106.93
2	B	502	ADP	C4-C5-N7	2.13	111.62	109.40
2	F	506	ADP	C4-C5-N7	2.13	111.61	109.40
2	G	507	ADP	C4-C5-N7	2.12	111.61	109.40
2	D	504	ADP	C4-C5-N7	2.10	111.59	109.40
2	A	501	ADP	C4-C5-N7	2.10	111.58	109.40

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	ADP	PA-O3A-PB-O3B
2	B	502	ADP	PA-O3A-PB-O3B
2	C	503	ADP	PA-O3A-PB-O3B
2	D	504	ADP	PA-O3A-PB-O3B
2	E	505	ADP	PA-O3A-PB-O3B
2	F	506	ADP	PA-O3A-PB-O3B
2	G	507	ADP	PA-O3A-PB-O3B
2	A	501	ADP	PA-O3A-PB-O1B
2	B	502	ADP	PA-O3A-PB-O1B
2	C	503	ADP	PA-O3A-PB-O1B
2	D	504	ADP	PA-O3A-PB-O1B
2	E	505	ADP	PA-O3A-PB-O1B
2	F	506	ADP	PA-O3A-PB-O1B
2	G	507	ADP	PA-O3A-PB-O1B
2	A	501	ADP	PA-O3A-PB-O2B
2	B	502	ADP	PA-O3A-PB-O2B
2	C	503	ADP	PA-O3A-PB-O2B
2	D	504	ADP	PA-O3A-PB-O2B
2	E	505	ADP	PA-O3A-PB-O2B
2	F	506	ADP	PA-O3A-PB-O2B
2	G	507	ADP	PA-O3A-PB-O2B

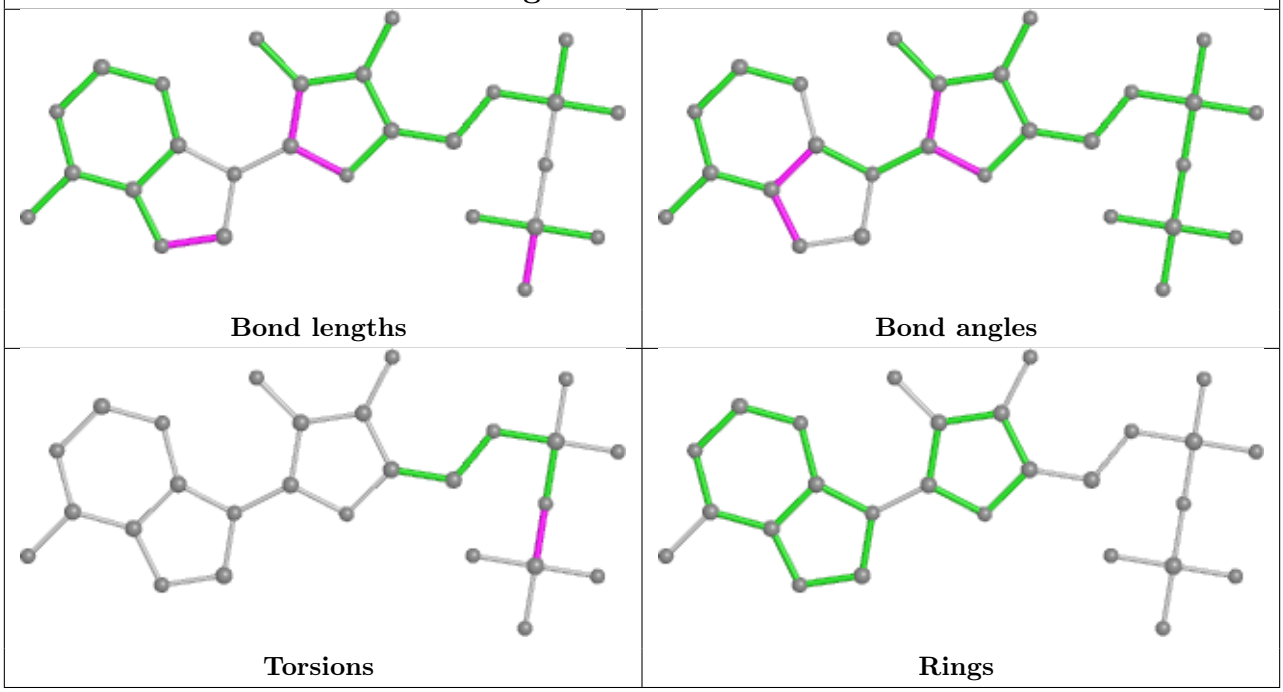
There are no ring outliers.

7 monomers are involved in 14 short contacts:

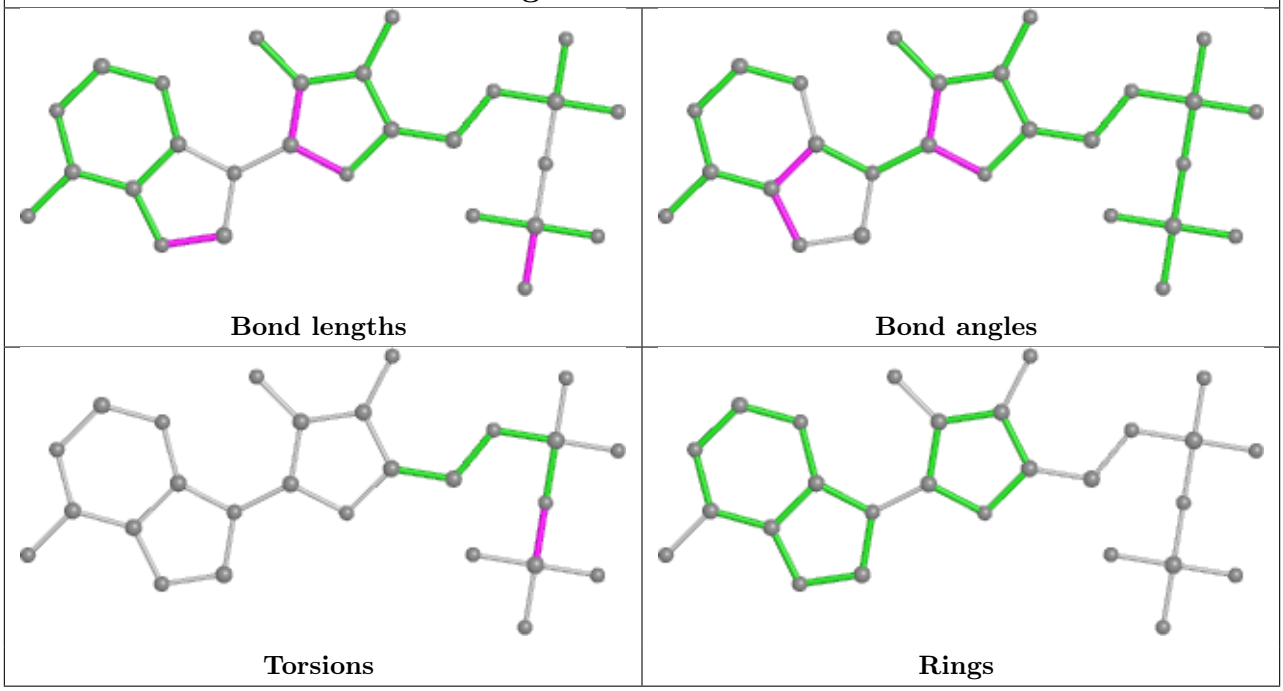
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	ADP	2	0
2	G	507	ADP	2	0
2	A	501	ADP	2	0
2	C	503	ADP	2	0
2	F	506	ADP	2	0
2	E	505	ADP	2	0
2	D	504	ADP	2	0

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.

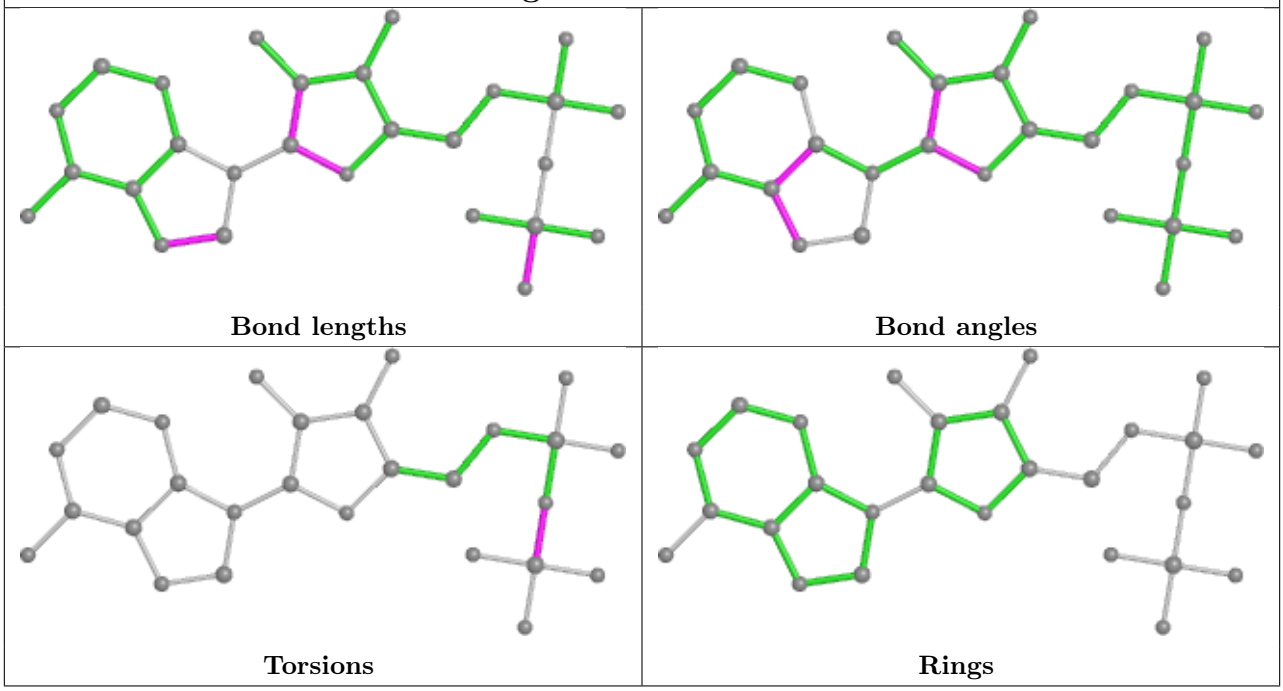
Ligand ADP B 502



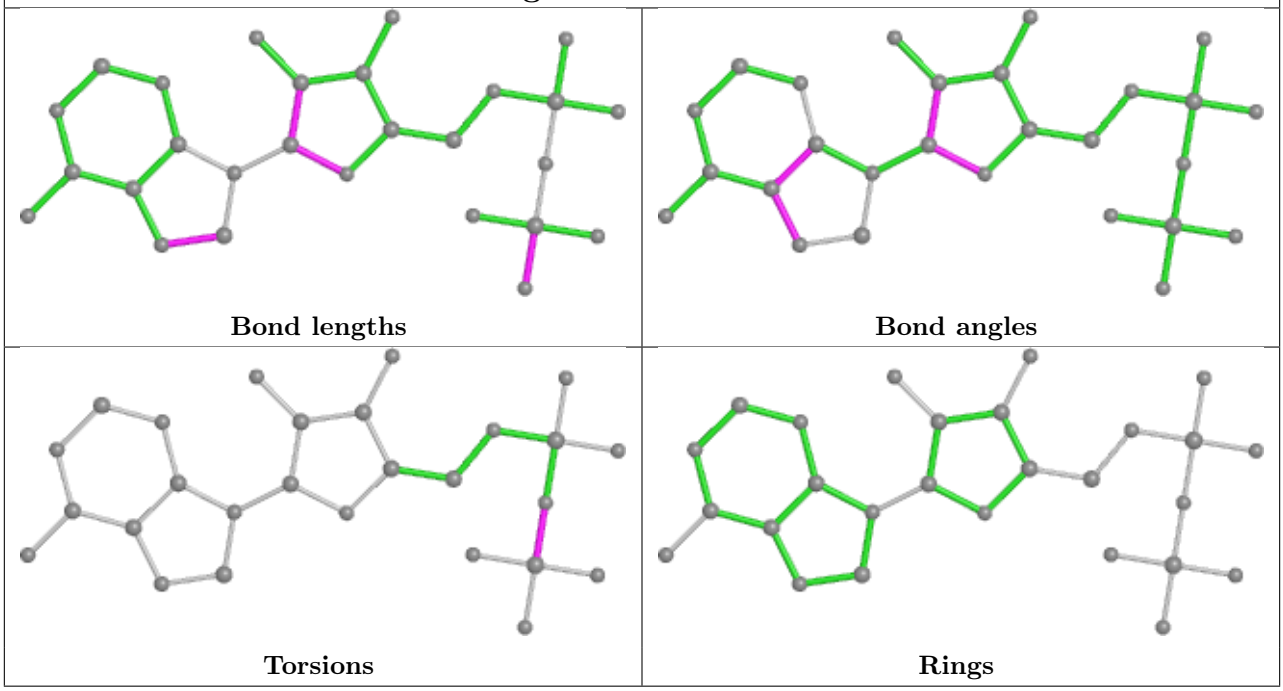
Ligand ADP G 507



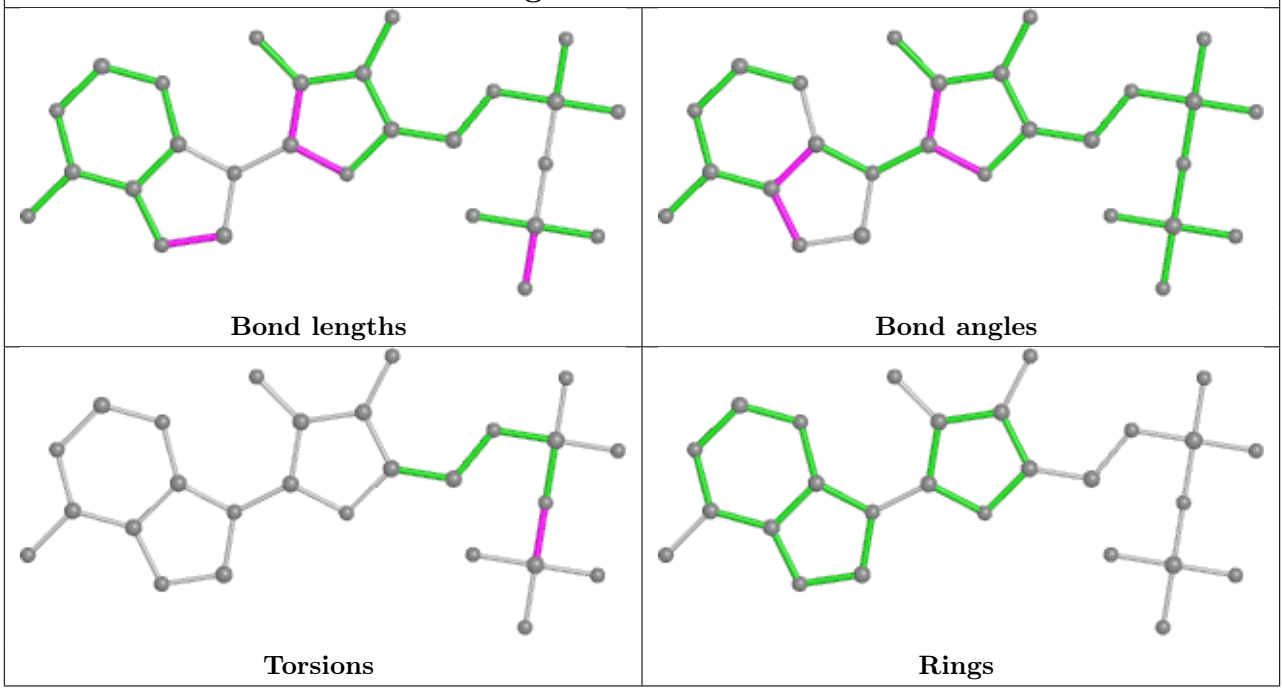
Ligand ADP A 501



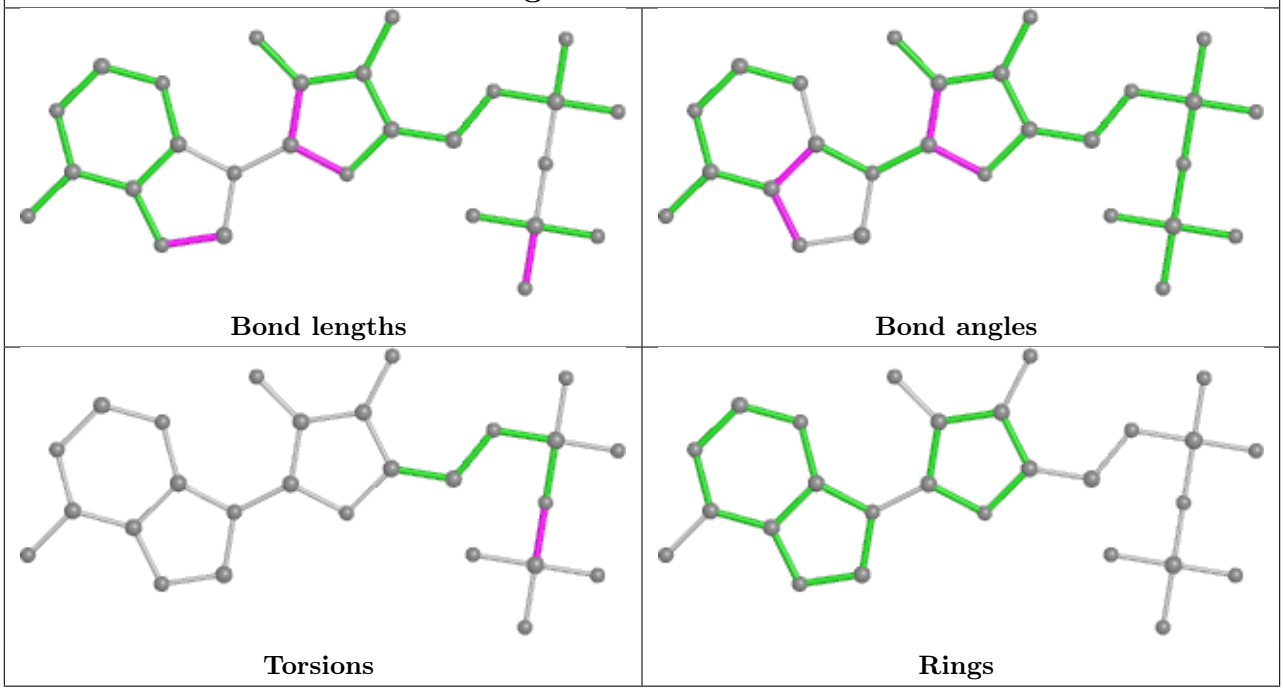
Ligand ADP C 503



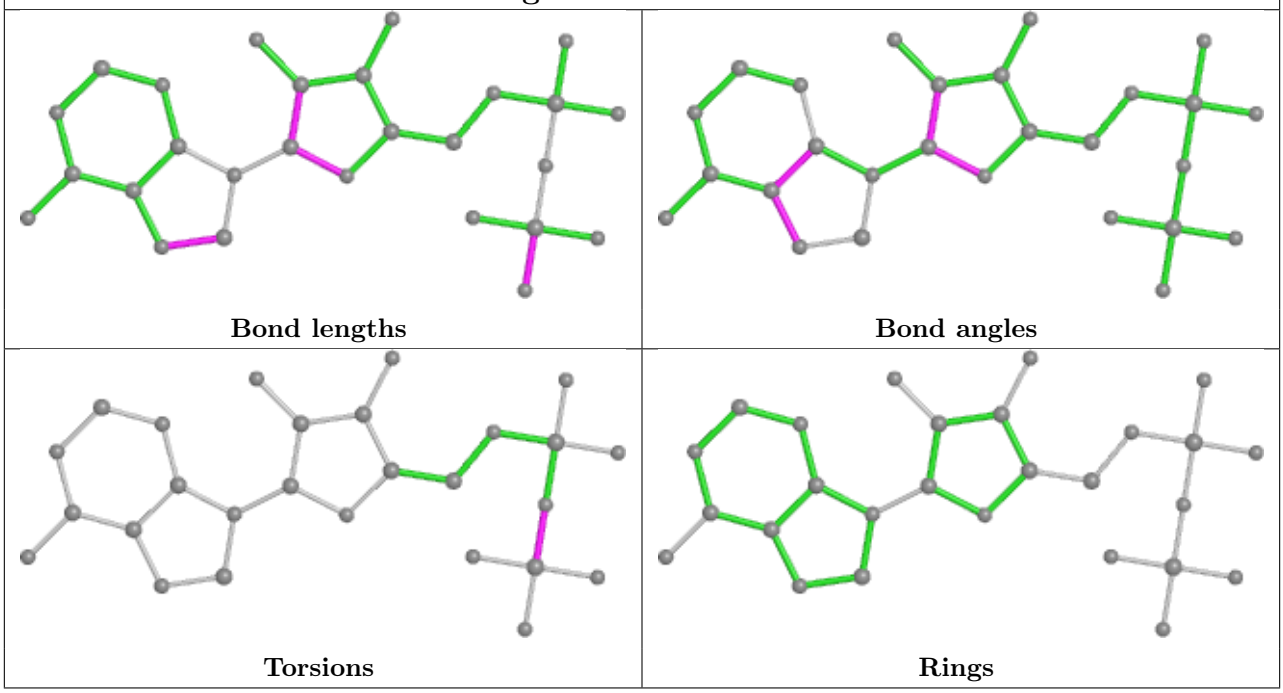
Ligand ADP F 506



Ligand ADP E 505



Ligand ADP D 504



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.