



wwPDB EM Validation Summary Report ⓘ

Feb 27, 2025 – 10:10 PM JST

PDB ID : 8Z3P
EMDB ID : EMD-39750
Title : The structure of type III CRISPR-associated deaminase in complex cA6 and ATP, fully activated
Authors : Chen, M.R.; Li, Z.X.; Xiao, Y.B.
Deposited on : 2024-04-15
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 ⓘ 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 : 1.8.5 (274361), 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) : 2.41.2

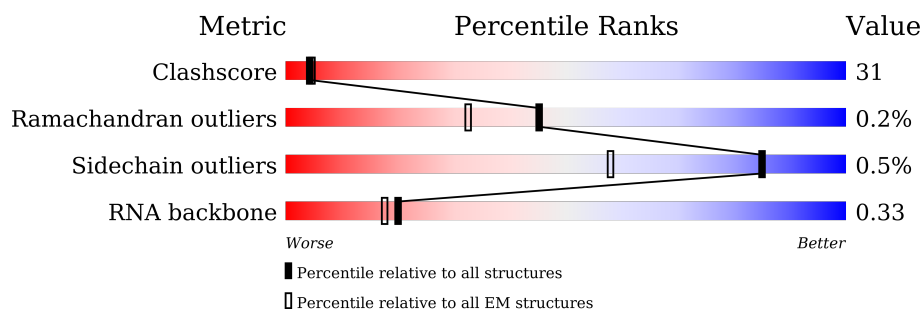
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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 (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	X	6	50% 50%
1	Y	6	17% 50% 33%
1	Z	6	17% 50% 33%
2	A	628	40% 57% ..
2	B	628	48% 49% .
2	C	628	51% 46% .
2	D	628	51% 46% .
2	E	628	52% 46% .

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Mol	Chain	Length	Quality of chain
2	F	628	<div><div></div><div>42%</div><div>55%</div><div>..</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 29566 atoms, of which 72 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.

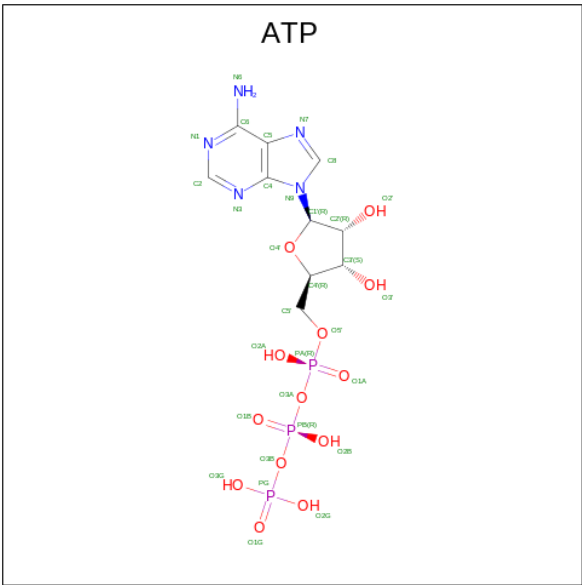
- Molecule 1 is a RNA chain called RNA (5'-R(P*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	6	Total	C	N	O	P	0	0
			132	60	30	36	6		
1	Y	6	Total	C	N	O	P	0	0
			132	60	30	36	6		
1	Z	6	Total	C	N	O	P	0	0
			132	60	30	36	6		

- Molecule 2 is a protein called Adenosine deaminase domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	615	Total	C	N	O	S	0	0
			4820	3044	895	859	22		
2	B	615	Total	C	N	O	S	0	0
			4820	3044	895	859	22		
2	C	615	Total	C	N	O	S	0	0
			4820	3044	895	859	22		
2	D	615	Total	C	N	O	S	0	0
			4820	3044	895	859	22		
2	E	615	Total	C	N	O	S	0	0
			4820	3044	895	859	22		
2	F	612	Total	C	N	O	S	0	0
			4804	3034	892	856	22		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	E	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	F	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	
4	B	1	Total	Zn	0
			1	1	
4	C	1	Total	Zn	0
			1	1	
4	D	1	Total	Zn	0
			1	1	
4	E	1	Total	Zn	0
			1	1	

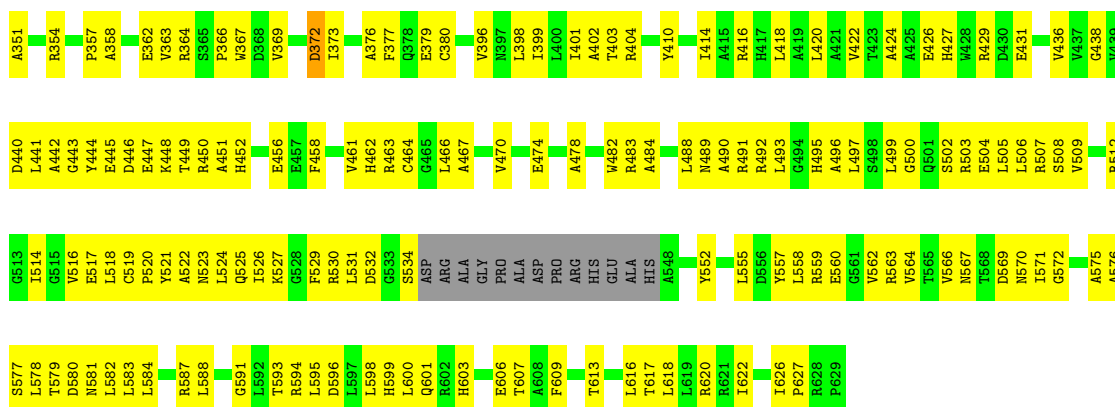
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Mol	Chain	Residues	Atoms		AltConf
4	F	1	Total	Zn	0
			1	1	

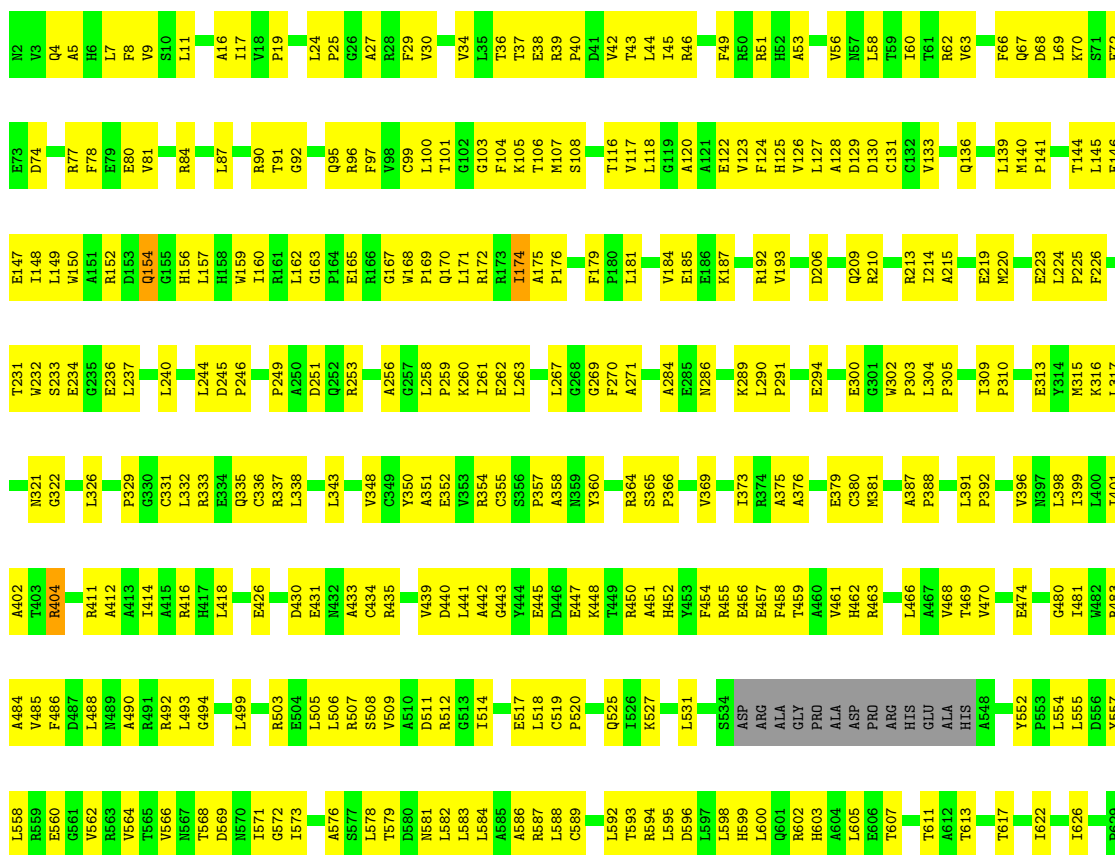
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	C	1	Total	Mg	0
			1	1	
5	D	1	Total	Mg	0
			1	1	



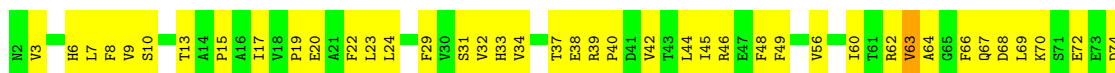
• Molecule 2: Adenosine deaminase domain-containing protein

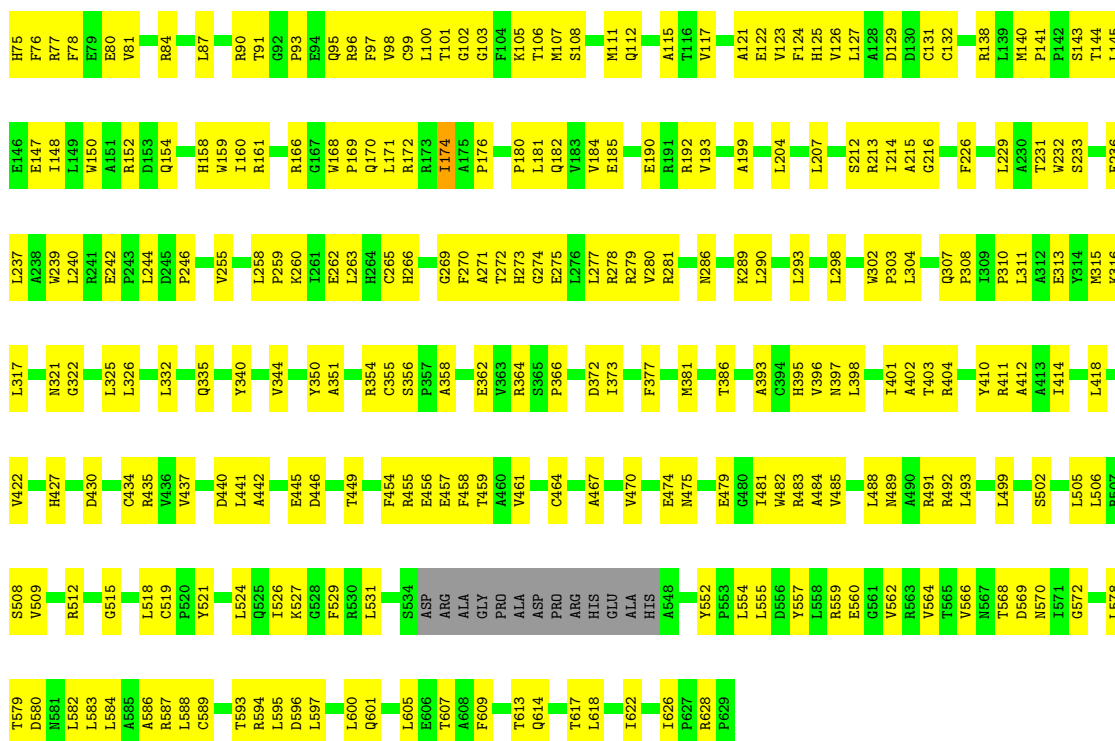
Chain B: 48% 49%



• Molecule 2: Adenosine deaminase domain-containing protein

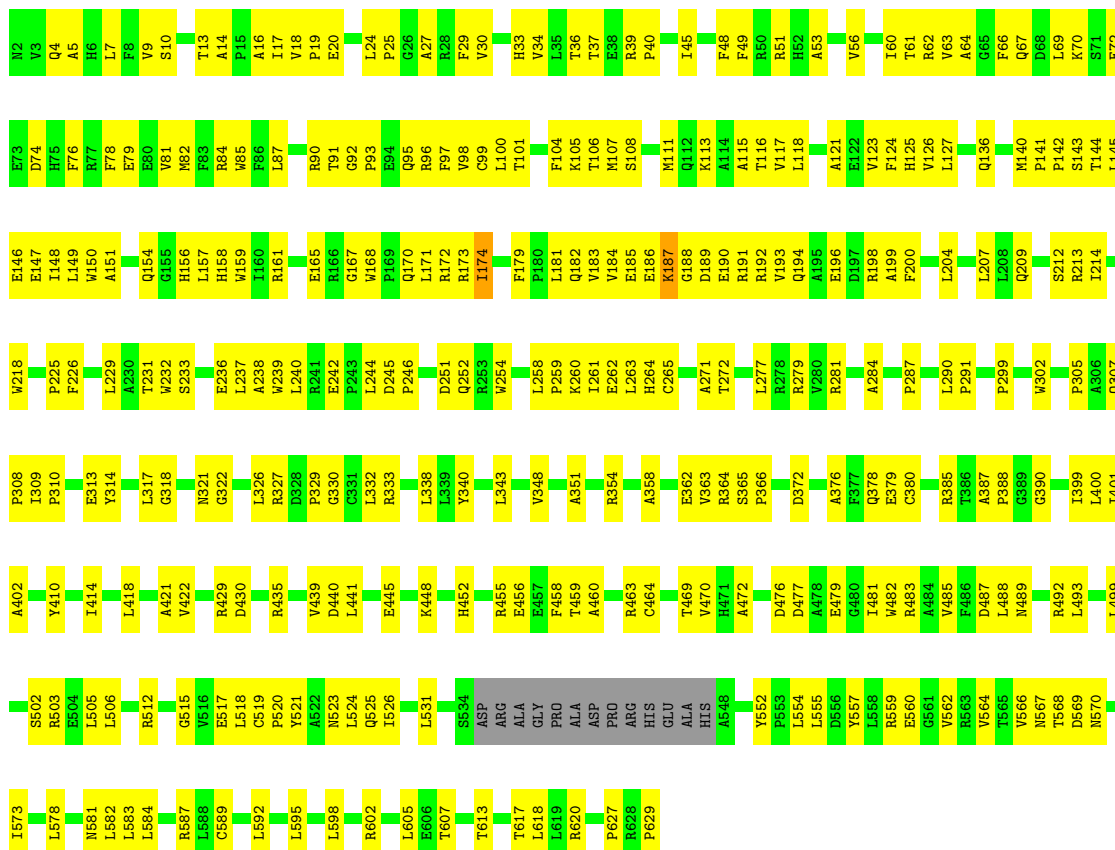
Chain C: 51% 46%



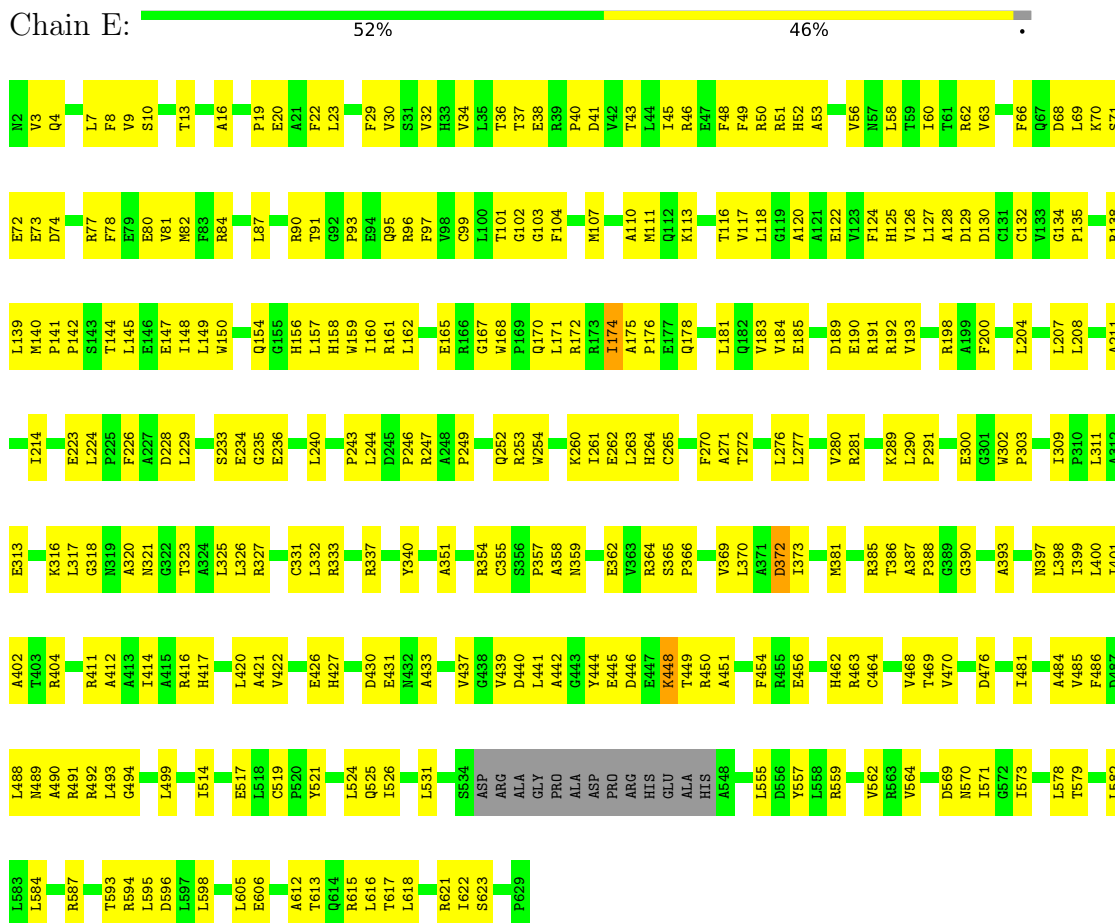


• Molecule 2: Adenosine deaminase domain-containing protein

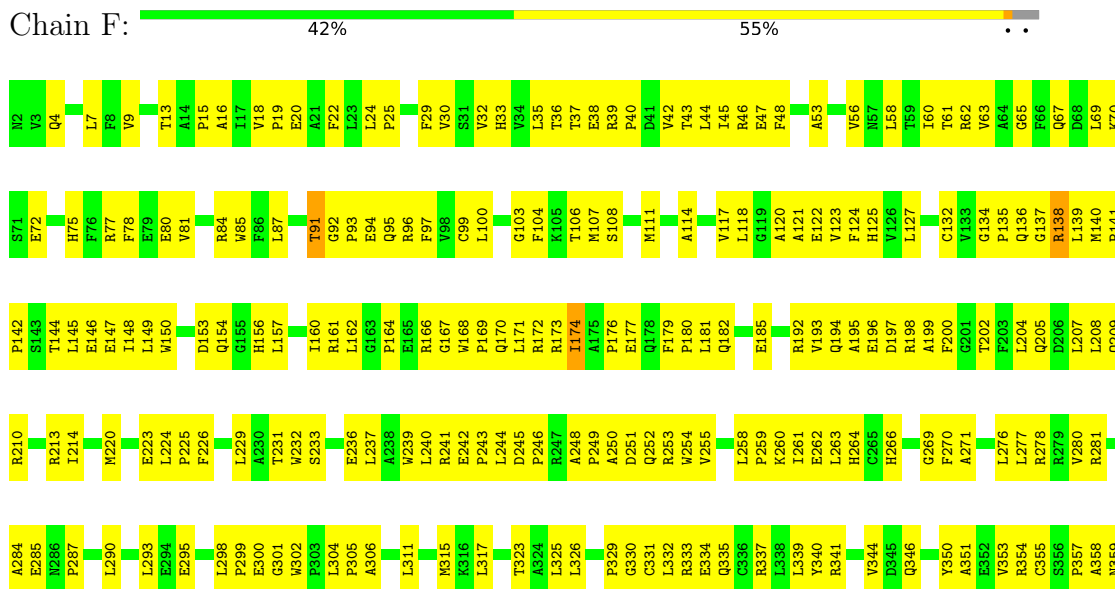
Chain D: 51% 46%



- Molecule 2: Adenosine deaminase domain-containing protein



- Molecule 2: Adenosine deaminase domain-containing protein



D596	L597	L600	Q601	R602	H603	A604	L605	E606	T607	T613	Q614	T617	L618	L619	I622	I626	P627	R628	P629																																		
Q525	R530	L531	S534	ASP	ARG	ALA	GLY	PRO	ALA	ASP	PRO	ARG	HIS	GLU	ALA	HIS	ALA	PRO	GLY	P551	Y552	P553	L554	L555	D556	Y557	L558	R559	E560	R563	V564	T565	V566	N567	T568	D569	N570	I573	L578	T579	D580	N581	L582	L583	L584	A585	A586	R587	L588	L592	T593	R594	L595
E447	R448	T449	R450	A451	H452	Y453	F454	R455	E456	E457	F458	T459	A460	V461	H462	R463	C464	G465	L466	T469	V470	H471	E474	A478	W482	R483	A484	V485	L488	N489	R492	L493	G494	L499	S502	L505	L506	R507	S508	V509	G515	V516	E517	L518	C519	P520	Y521	L524					
V360	A361	E362	V363	R364	S365	P366	V369	Q378	E379	C380	R385	T386	A387	P388	G389	G390	A393	N397	L398	I399	L400	I401	A402	T403	R404	R411	A412	A413	I414	A415	R416	H417	L418	A421	V422	H427	E431	N432	A433	C434	V437	G438	V439	D440	L441	A442	E445	D446					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55742	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k 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, ZN

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	X	0.20	0/149	0.79	0/230
1	Y	0.18	0/149	0.77	0/230
1	Z	0.17	0/149	0.78	0/230
2	A	0.27	0/4936	0.59	2/6712 (0.0%)
2	B	0.26	0/4936	0.56	0/6712
2	C	0.27	0/4936	0.57	0/6712
2	D	0.26	0/4936	0.56	0/6712
2	E	0.27	0/4936	0.57	2/6712 (0.0%)
2	F	0.26	0/4919	0.57	0/6687
All	All	0.26	0/30046	0.57	4/40937 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	372	ASP	CB-CG-OD2	6.56	124.20	118.30
2	A	372	ASP	CB-CG-OD2	6.21	123.89	118.30
2	E	189	ASP	CB-CG-OD1	5.70	123.43	118.30
2	A	345	ASP	CB-CG-OD2	5.12	122.91	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	63	VAL	Peptide

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	X	132	0	67	7	0
1	Y	132	0	67	8	0
1	Z	132	0	67	7	0
2	A	4820	0	4786	361	0
2	B	4820	0	4786	305	0
2	C	4820	0	4786	278	0
2	D	4820	0	4786	308	0
2	E	4820	0	4786	284	0
2	F	4804	0	4772	379	0
3	A	31	12	12	0	0
3	B	31	12	12	1	0
3	C	31	12	12	0	0
3	D	31	12	12	1	0
3	E	31	12	12	1	0
3	F	31	12	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	29494	72	28975	1829	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 31.

The worst 5 of 1829 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:B:171:LEU:HA	2:B:174:ILE:HD11	1.37	1.00
2:F:142:PRO:HD2	2:F:147:GLU:HG2	1.44	0.99
2:D:104:PHE:HB2	2:D:107:MET:HG3	1.43	0.99
2:A:287:PRO:HA	2:A:290:LEU:HD13	1.45	0.98
2:A:171:LEU:HA	2:A:174:ILE:HD11	1.42	0.98

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	
2	A	611/628 (97%)	573 (94%)	37 (6%)	1 (0%)	44	72
2	B	611/628 (97%)	570 (93%)	40 (6%)	1 (0%)	44	72
2	C	611/628 (97%)	567 (93%)	43 (7%)	1 (0%)	44	72
2	D	611/628 (97%)	568 (93%)	42 (7%)	1 (0%)	44	72
2	E	611/628 (97%)	568 (93%)	42 (7%)	1 (0%)	44	72
2	F	608/628 (97%)	561 (92%)	45 (7%)	2 (0%)	37	66
All	All	3663/3768 (97%)	3407 (93%)	249 (7%)	7 (0%)	45	72

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	174	ILE
2	B	174	ILE
2	F	91	THR
2	C	174	ILE
2	E	174	ILE

5.3.2 Protein sidechains ⓘ

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	
2	A	495/504 (98%)	490 (99%)	5 (1%)	73	83
2	B	495/504 (98%)	493 (100%)	2 (0%)	89	93
2	C	495/504 (98%)	495 (100%)	0	100	100
2	D	495/504 (98%)	493 (100%)	2 (0%)	89	93
2	E	495/504 (98%)	493 (100%)	2 (0%)	89	93
2	F	494/504 (98%)	491 (99%)	3 (1%)	84	90
All	All	2969/3024 (98%)	2955 (100%)	14 (0%)	85	91

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	136	GLN
2	D	187	LYS
2	F	530	ARG
2	F	138	ARG
2	F	241	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	397	ASN
2	E	395	HIS
2	F	346	GLN
2	E	154	GLN
2	E	397	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	5/6 (83%)	4 (80%)	0
1	Y	5/6 (83%)	2 (40%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Z	5/6 (83%)	2 (40%)	0
All	All	15/18 (83%)	8 (53%)	0

5 of 8 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	A
1	X	4	A
1	X	5	A
1	X	6	A
1	Y	8	A

There are no RNA pucker outliers to report.

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 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	$\# Z > 2$
3	ATP	C	701	5	26,33,33	0.61	0	31,52,52	1.11	3 (9%)
3	ATP	E	701	-	26,33,33	0.60	0	31,52,52	1.07	3 (9%)
3	ATP	F	701	-	26,33,33	0.58	0	31,52,52	1.10	2 (6%)
3	ATP	D	701	5	26,33,33	0.60	0	31,52,52	1.04	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	B	701	-	26,33,33	0.60	0	31,52,52	1.10	3 (9%)
3	ATP	A	701	-	26,33,33	0.59	0	31,52,52	1.09	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
3	ATP	C	701	5	-	3/18/38/38	0/3/3/3
3	ATP	E	701	-	-	4/18/38/38	0/3/3/3
3	ATP	F	701	-	-	2/18/38/38	0/3/3/3
3	ATP	D	701	5	-	8/18/38/38	0/3/3/3
3	ATP	B	701	-	-	0/18/38/38	0/3/3/3
3	ATP	A	701	-	-	6/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	ATP	C5-C6-N6	2.31	123.86	120.35
3	B	701	ATP	O4'-C1'-C2'	-2.31	103.55	106.93
3	C	701	ATP	O4'-C1'-C2'	-2.29	103.57	106.93
3	C	701	ATP	C5-C6-N6	2.28	123.81	120.35
3	D	701	ATP	C5-C6-N6	2.27	123.80	120.35

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

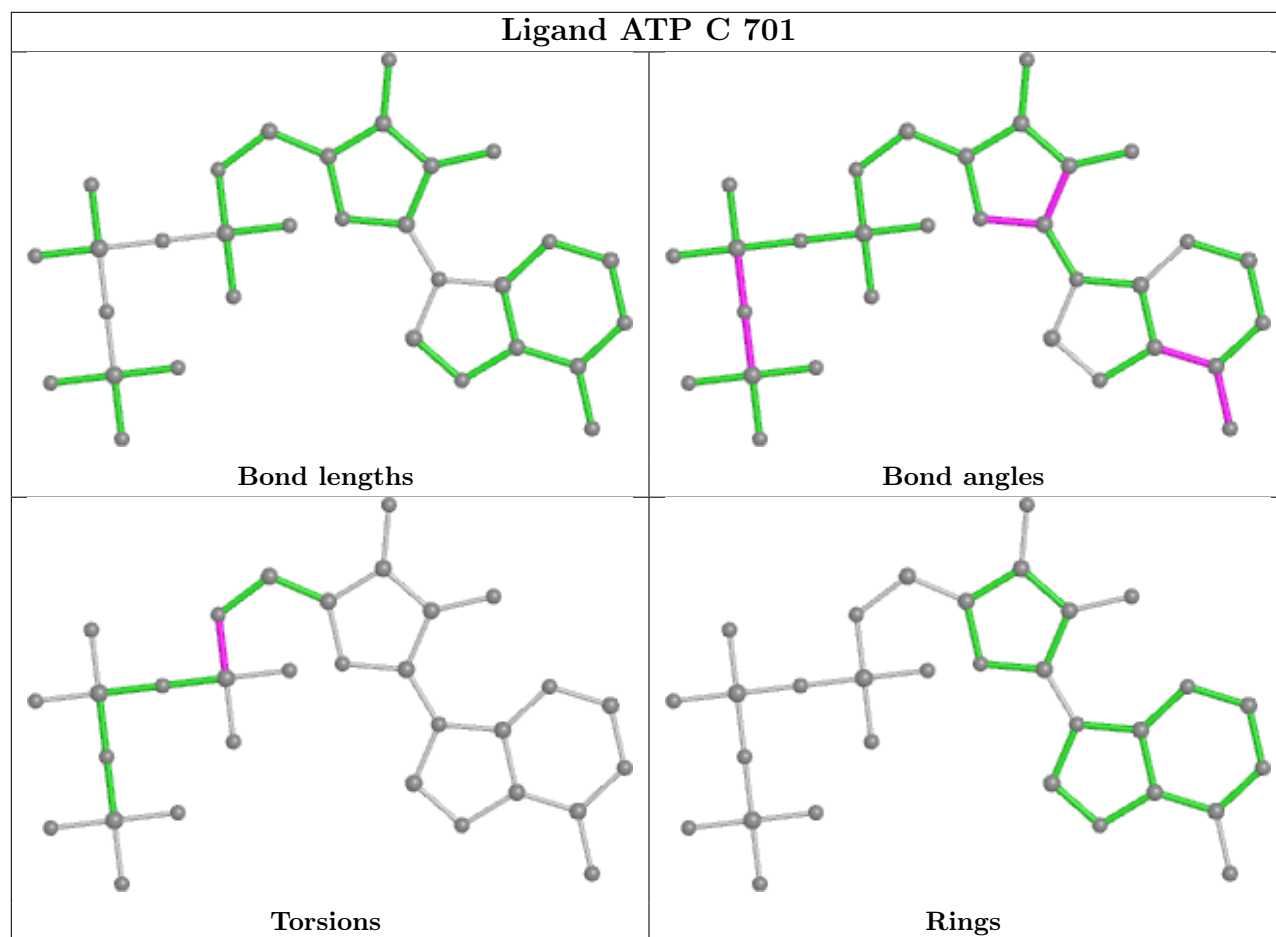
Mol	Chain	Res	Type	Atoms
3	A	701	ATP	O4'-C4'-C5'-O5'
3	C	701	ATP	C5'-O5'-PA-O1A
3	C	701	ATP	C5'-O5'-PA-O2A
3	D	701	ATP	C5'-O5'-PA-O1A
3	E	701	ATP	PB-O3B-PG-O2G

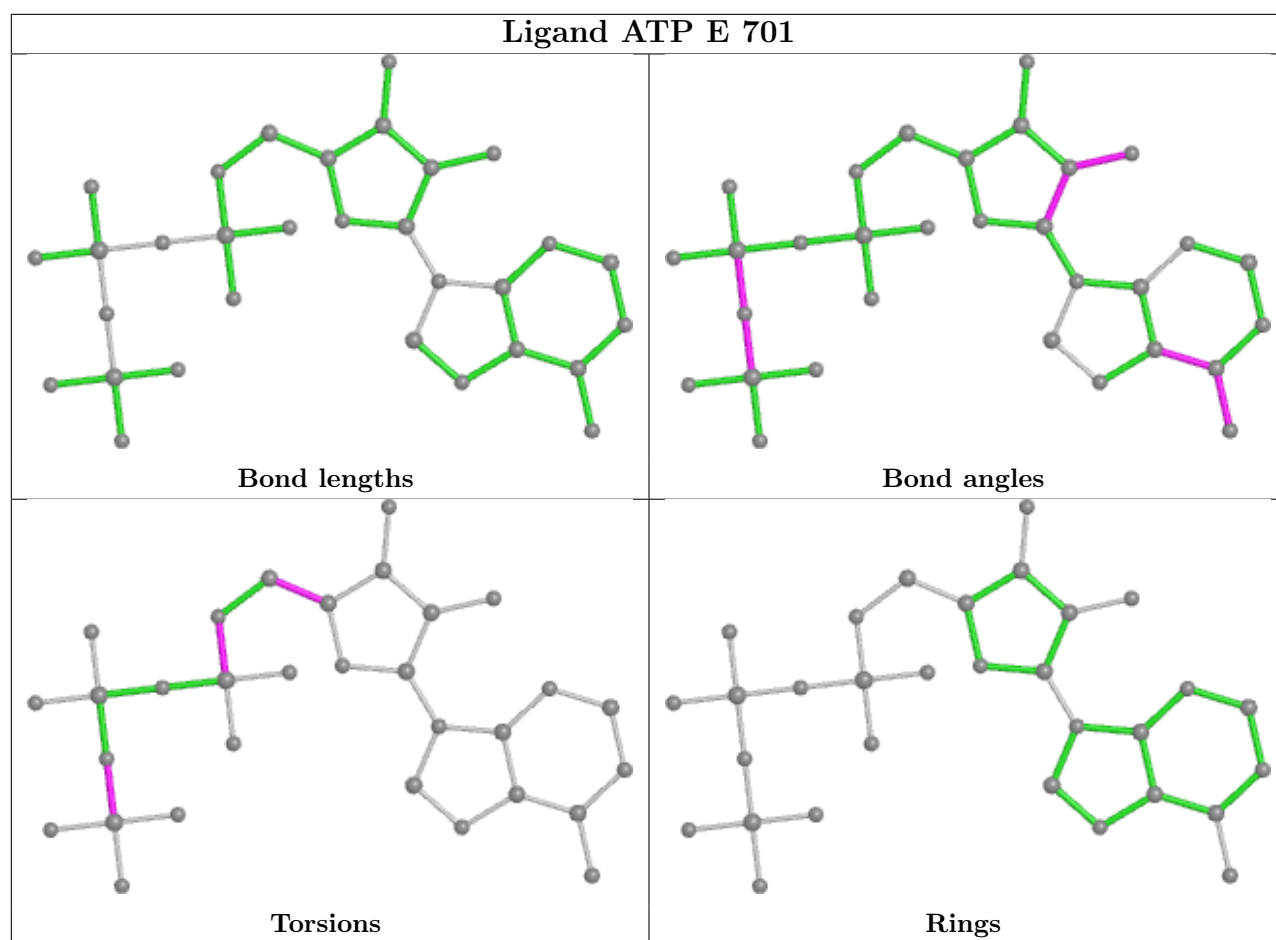
There are no ring outliers.

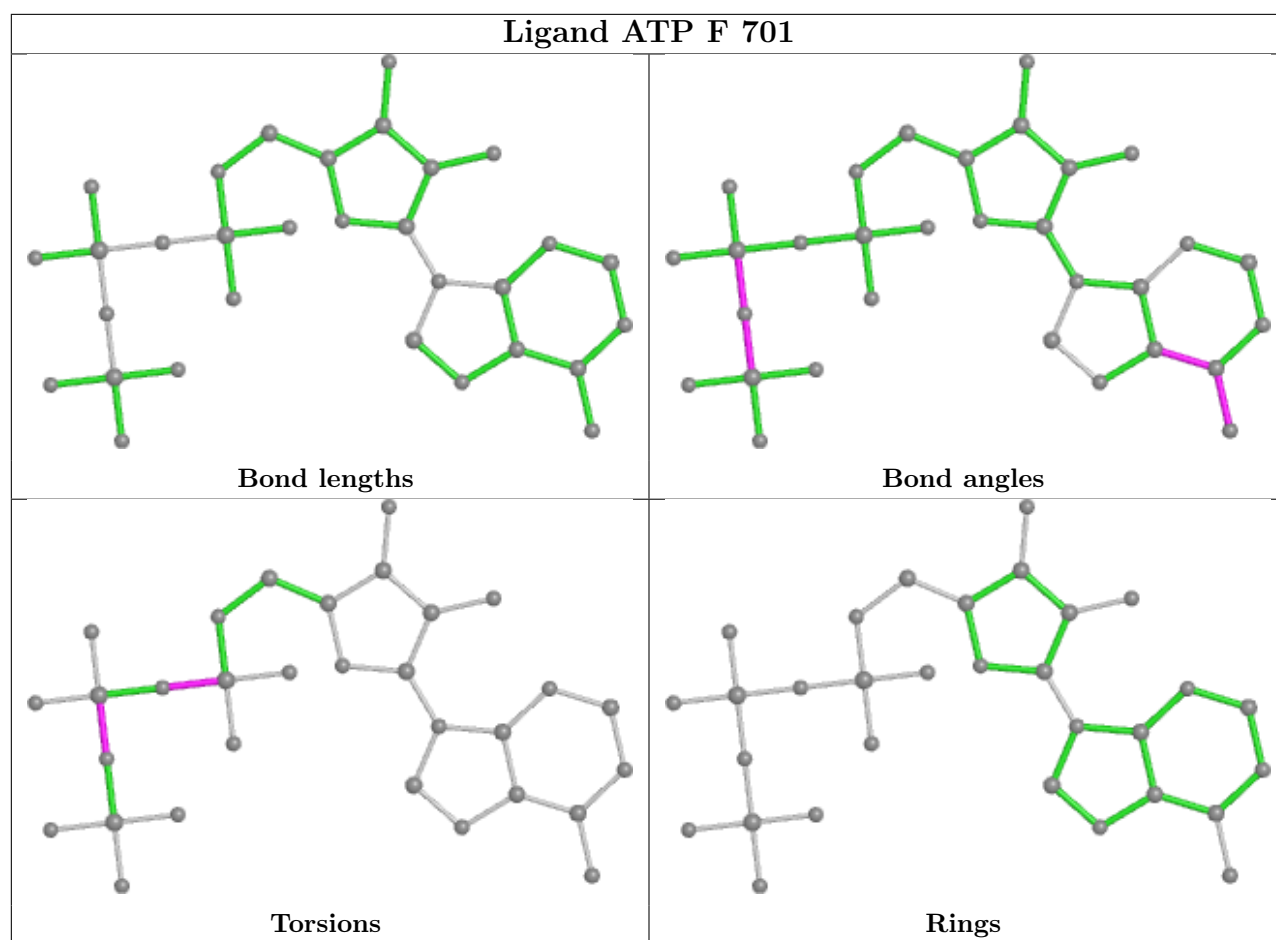
3 monomers are involved in 3 short contacts:

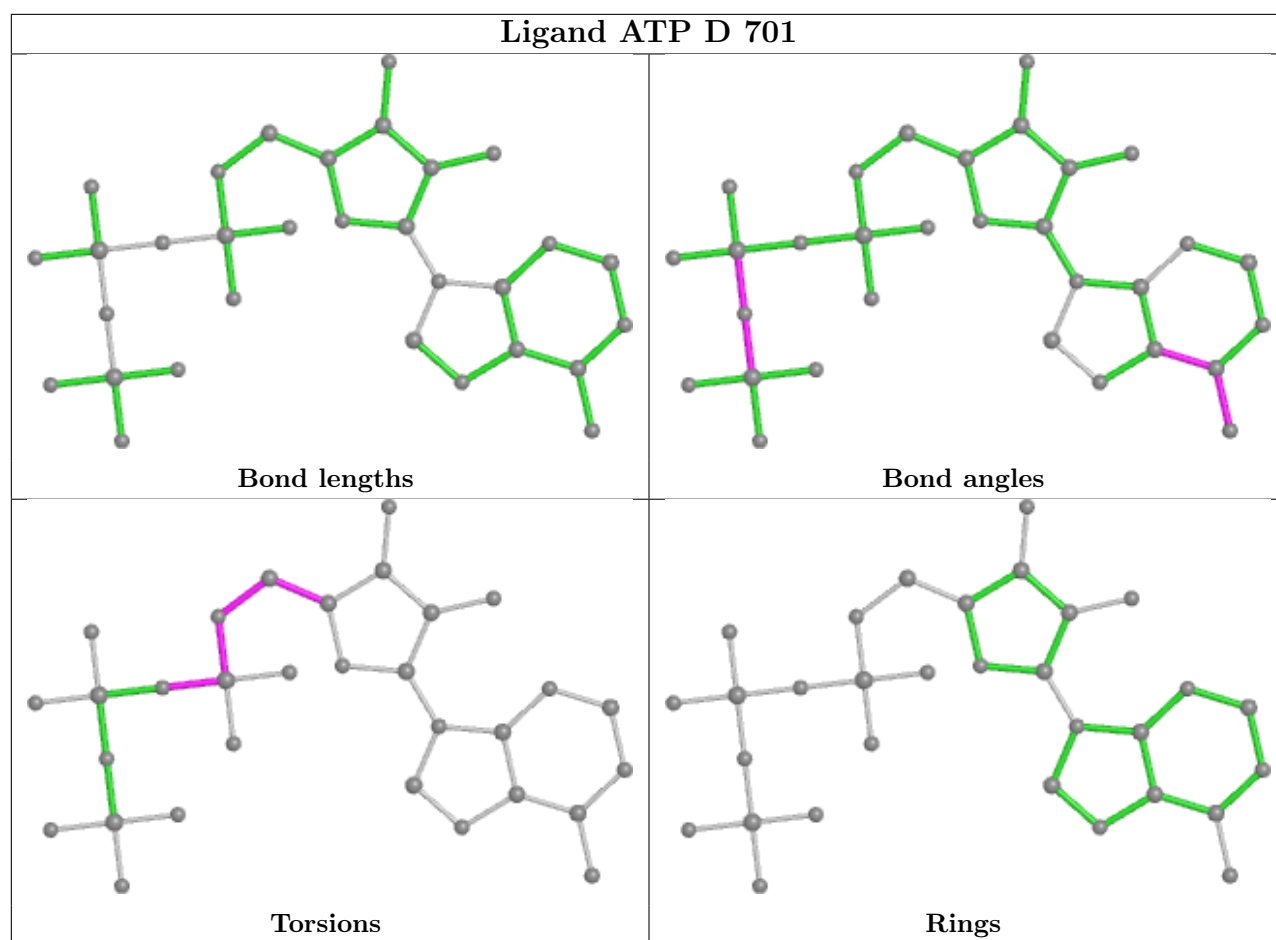
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	701	ATP	1	0
3	D	701	ATP	1	0
3	B	701	ATP	1	0

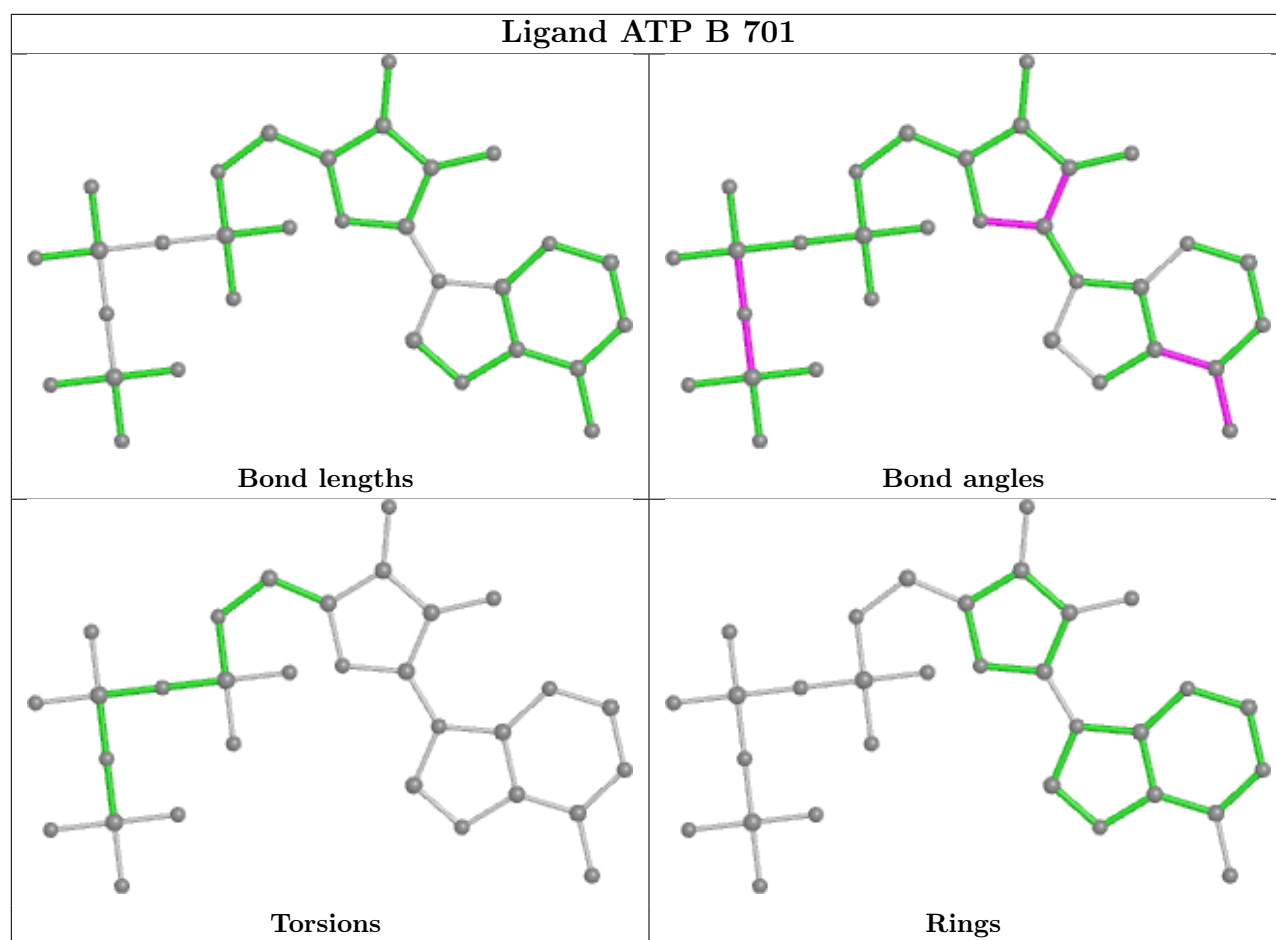
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

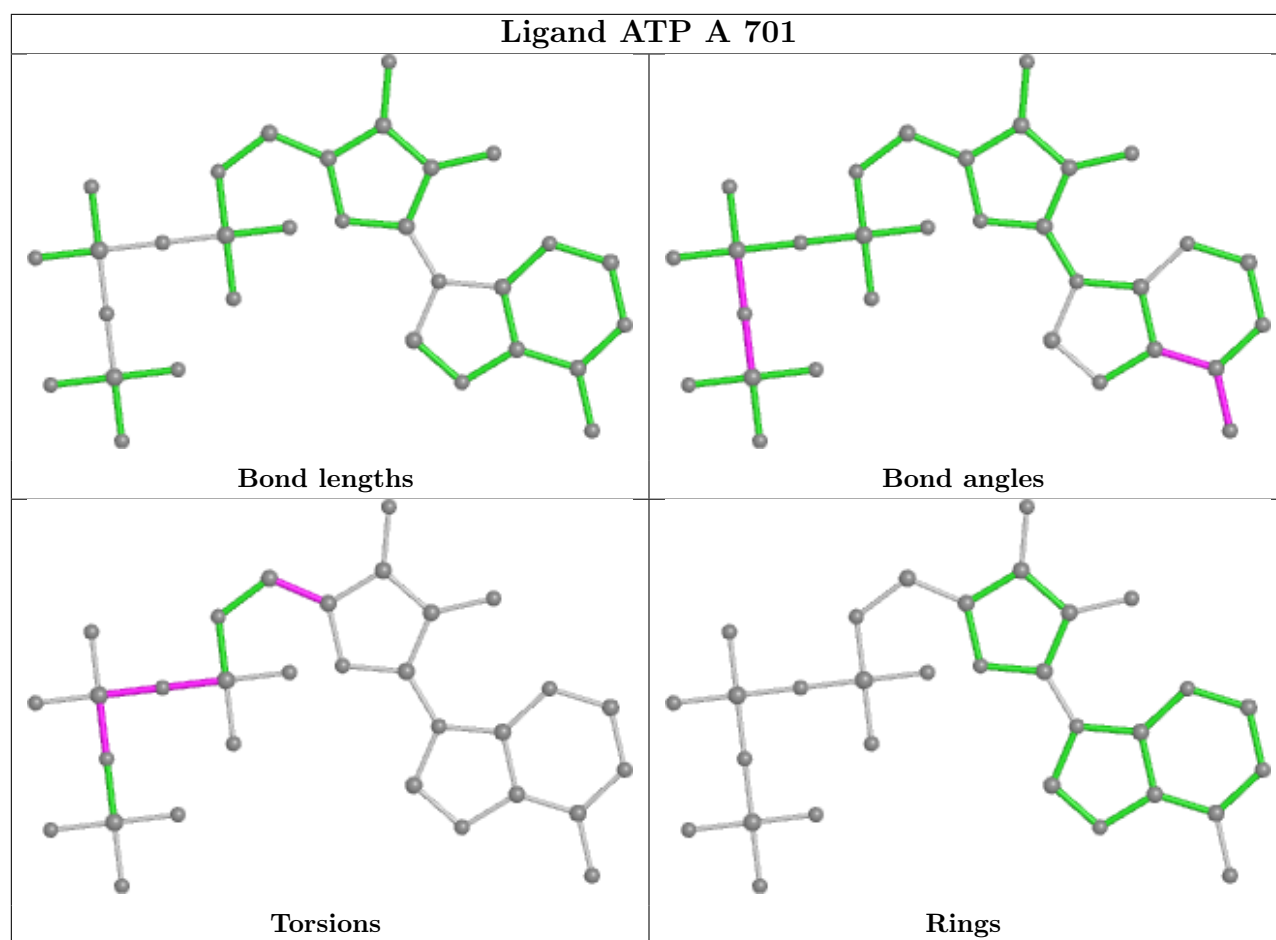












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.