



wwPDB EM Validation Summary Report ⓘ

Apr 23, 2024 – 06:54 am BST

PDB ID : 6ZYW
EMDB ID : EMD-11576
Title : Outer Dynein Arm-Shulin complex - overall structure (Tetrahymena thermophila)
Authors : Mali, G.R.; Abid Ali, F.; Lau, C.K.; Carter, A.P.
Deposited on : 2020-08-03
Resolution : 8.78 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	: 1.8.4, 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)	: 2.36.2

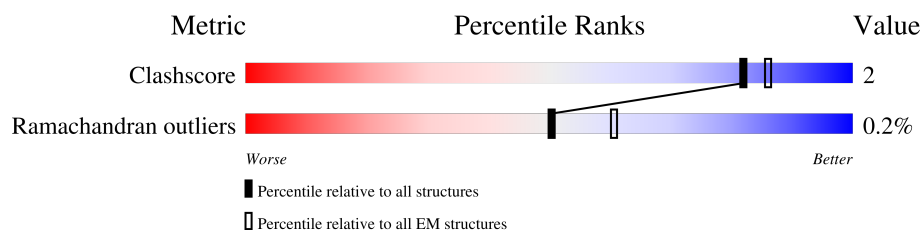
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



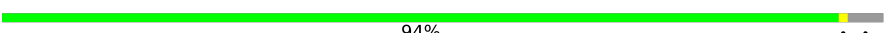







The reported resolution of this entry is 8.78 Å.

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.







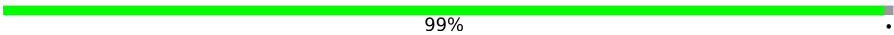

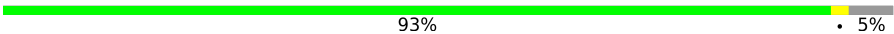

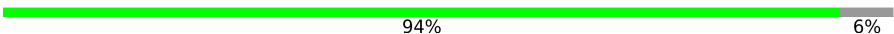
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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	A	4168	 85% 6% 9%
2	B	4595	 91% 5% 5%
3	C	4620	 94% 2% 4%
4	D	667	 47% 52%
4	d	667	 19% 81%
5	E	670	 51% 49%
5	e	670	 15% 85%
6	F	133	 74% 26%
7	G	103	 90% 8%
8	H	92	 90% 8%

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Mol	Chain	Length	Quality of chain
9	I	110	 81%19%
10	J	93	 90%10%
11	K	111	 86%14%
12	L	111	 87%13%
13	M	87	 99%.
14	N	132	 83%17%
15	O	117	 93%. 5%
16	P	110	 90%. 6%
17	Y	1200	 94%6%

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 73897 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 Dynein-1-alpha heavy chain, flagellar inner arm I1 complex protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	3795	Total	C	N	O	0	0
			18787	11198	3795	3794		

- Molecule 2 is a protein called Outer arm dynein beta heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	4370	Total	C	N	O	0	417
			20008	12102	3953	3953		

- Molecule 3 is a protein called Dynein heavy chain, outer arm protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	4433	Total	C	N	O	0	563
			19737	11997	3870	3870		

- Molecule 4 is a protein called Dynein intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	321	Total	C	N	O	0	0
			1588	946	321	321		
4	d	128	Total	C	N	O	0	0
			637	381	128	128		

- Molecule 5 is a protein called Flagellar outer dynein arm intermediate protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	341	Total	C	N	O	0	0
			1678	996	341	341		
5	e	102	Total	C	N	O	0	0
			501	297	102	102		

- Molecule 6 is a protein called Dynein light chain roadblock-type 2 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	98	Total	C	N	O	0	0
			486	290	98	98		

- Molecule 7 is a protein called Dynein light chain roadblock-type 2 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	95	Total	C	N	O	0	0
			470	280	95	95		

- Molecule 8 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	85	Total	C	N	O	0	0
			420	250	85	85		

- Molecule 9 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	89	Total	C	N	O	0	0
			439	261	89	89		

- Molecule 10 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	84	Total	C	N	O	0	0
			416	248	84	84		

- Molecule 11 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	95	Total	C	N	O	0	0
			470	280	95	95		

- Molecule 12 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	97	Total	C	N	O	0	0
			479	285	97	97		

- Molecule 13 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	86	Total	C	N	O	0	0
			426	254	86	86		

- Molecule 14 is a protein called Dynein light chain 2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	109	Total	C	N	O	0	0
			537	319	109	109		

- Molecule 15 is a protein called Dynein light chain tctex-type 1 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	111	Total	C	N	O	0	0
			550	328	111	111		

- Molecule 16 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	103	Total	C	N	O	0	0
			513	307	103	103		

- Molecule 17 is a protein called Shulin.

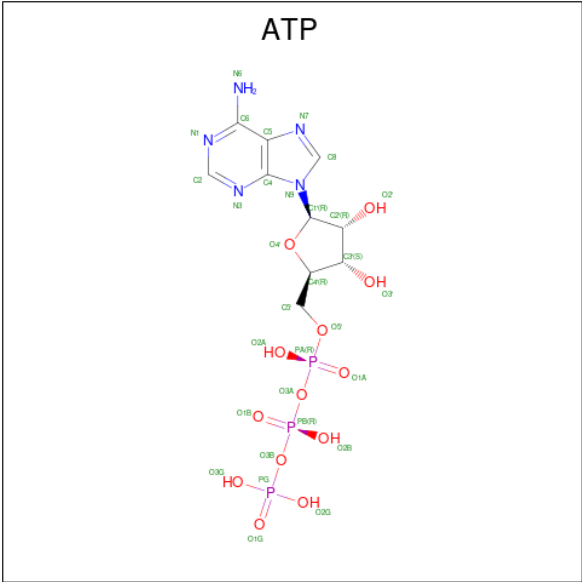
Mol	Chain	Residues	Atoms				AltConf	Trace
17	Y	1133	Total	C	N	O	0	0
			5611	3345	1133	1133		

- Molecule 18 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



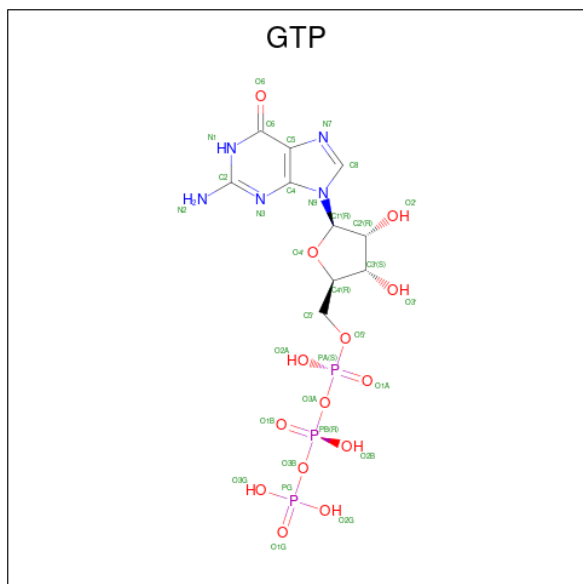
Mol	Chain	Residues	Atoms					AltConf
18	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
18	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
18	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 19 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

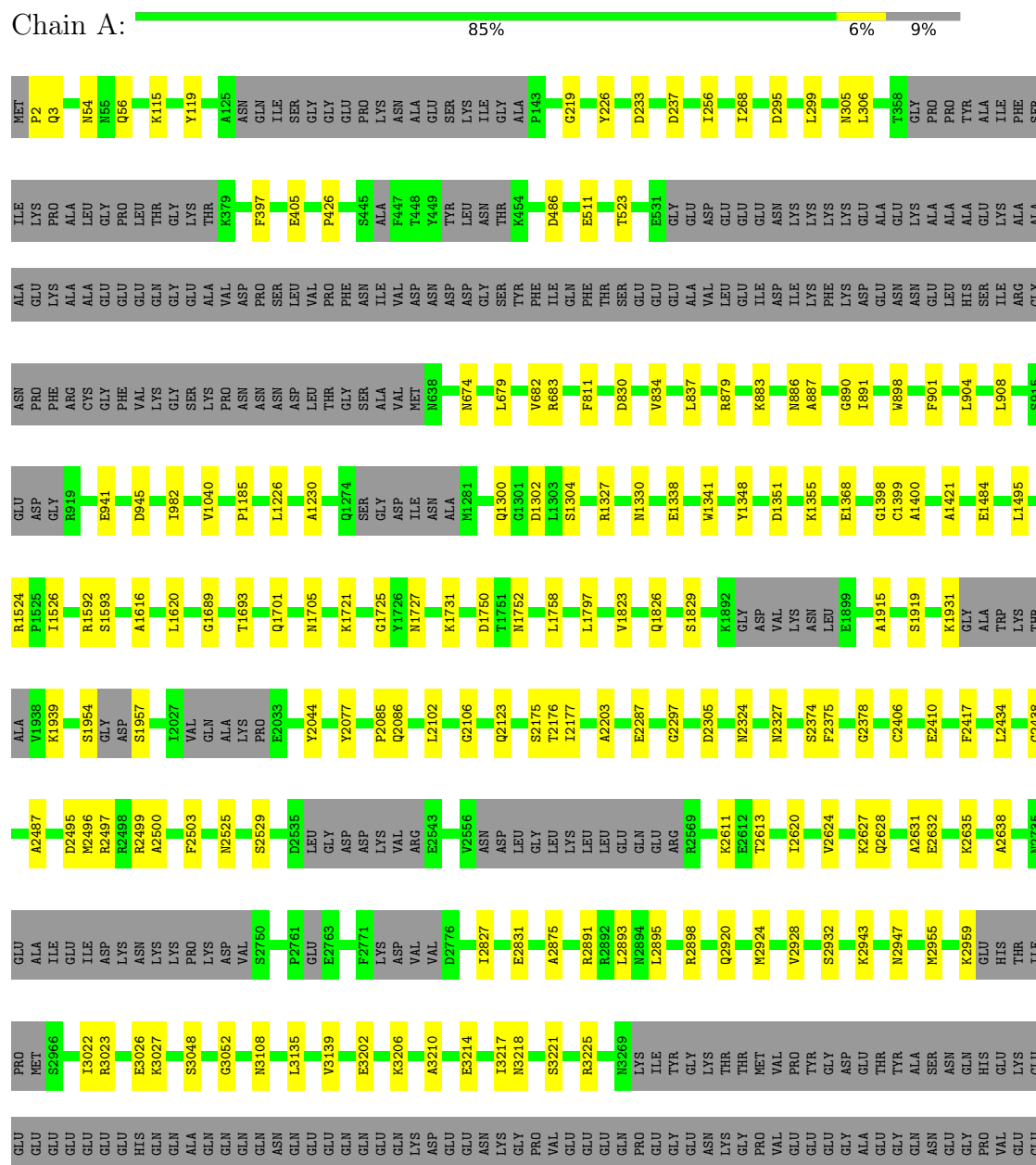
- Molecule 20 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



3 Residue-property plots

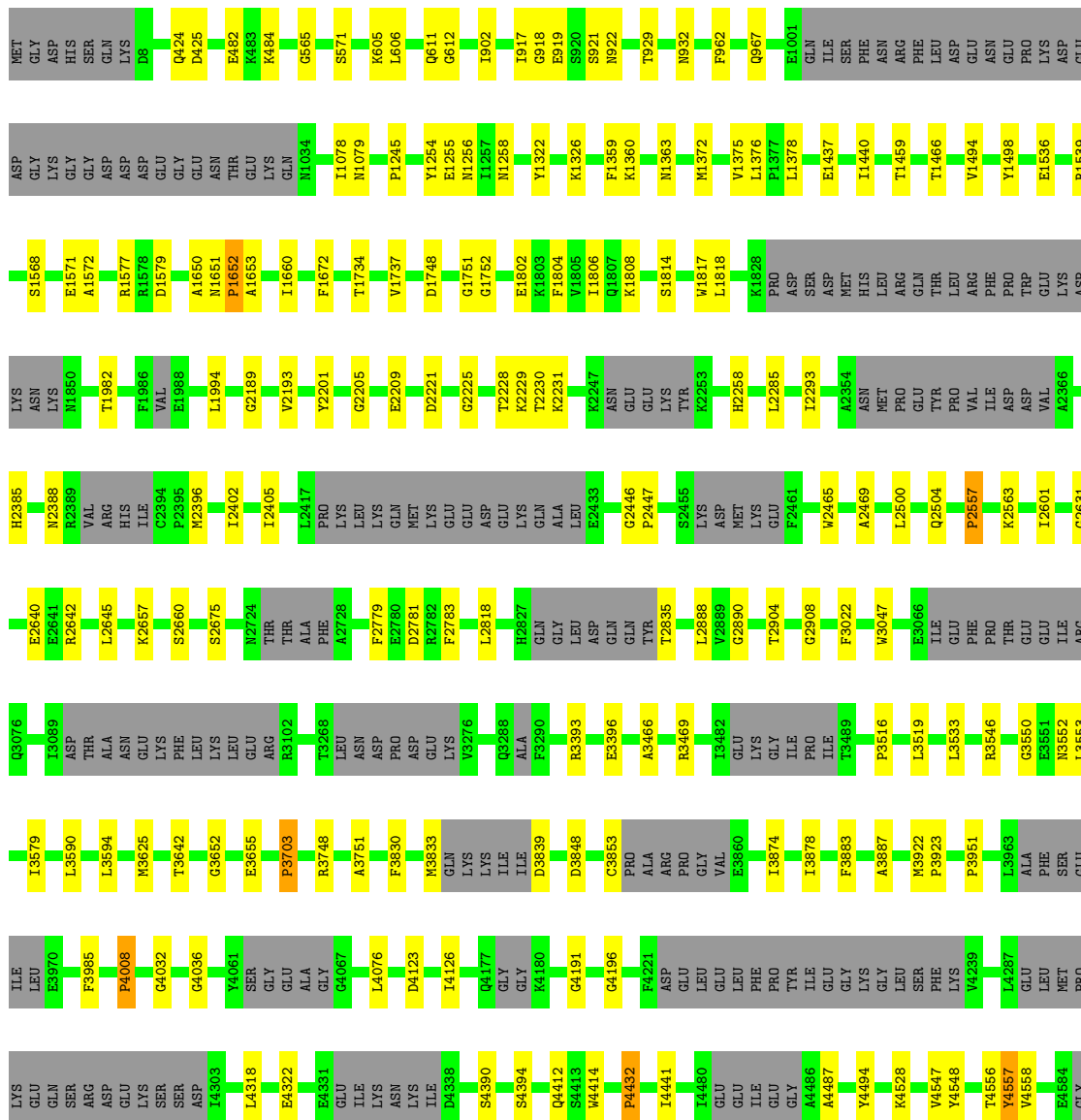
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Dynein-1-alpha heavy chain, flagellar inner arm I1 complex protein, putative



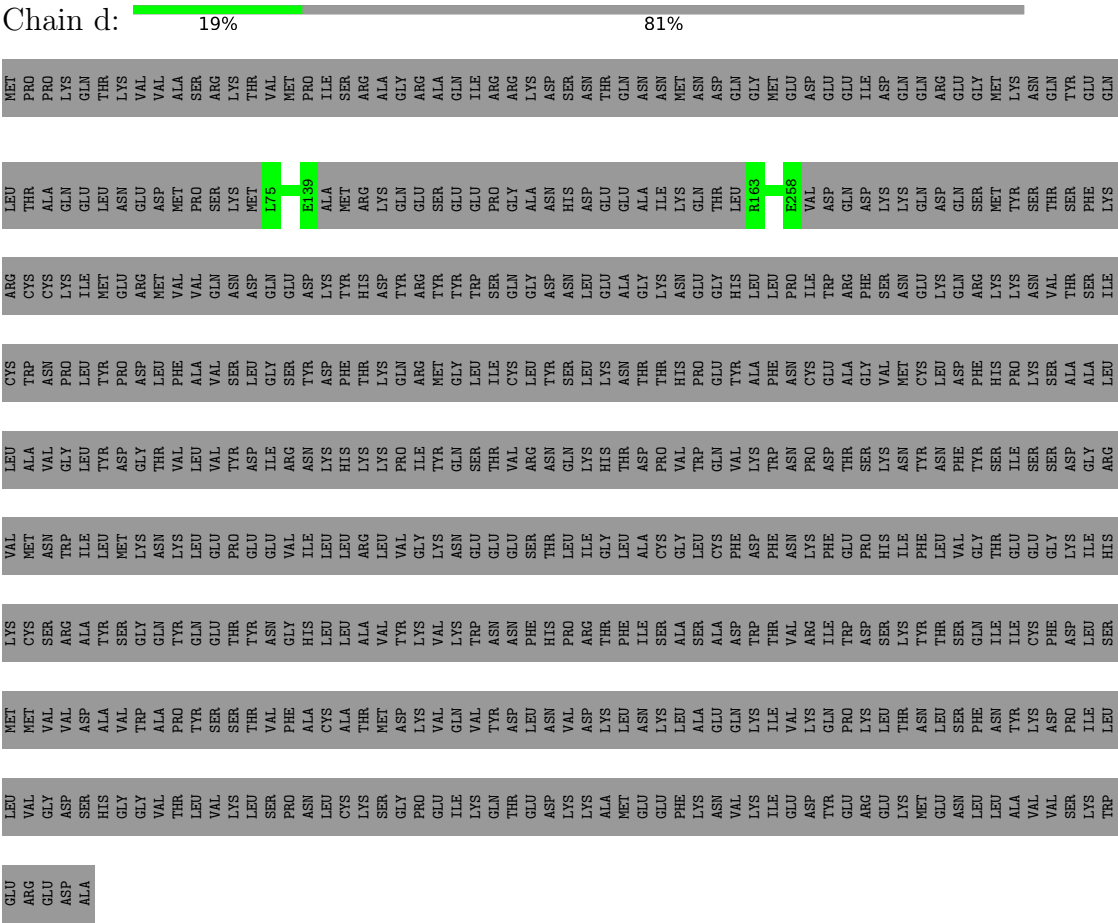
- Molecule 2: Outer arm dynein beta heavy chain

Chain B: 91% • 5%

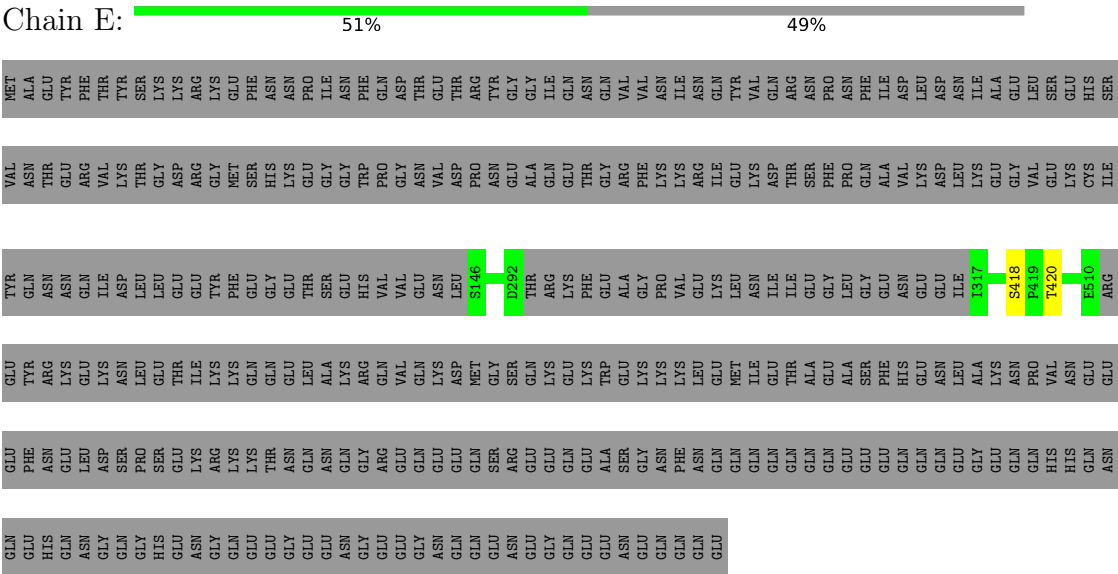


VAL VAL
SER SER
LYS LYS
TRP TRP
GLU GLU
ARG ARG
ASP ASP
ALA ALA

● Molecule 4: Dynein intermediate chain 2



● Molecule 5: Flagellar outer dynein arm intermediate protein, putative



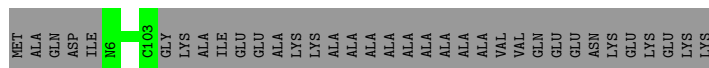
- Molecule 5: Flagellar outer dynein arm intermediate protein, putative

Chain e: 15% 85%



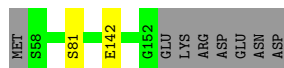
- Molecule 6: Dynein light chain roadblock-type 2 protein

Chain F:  74% 26%



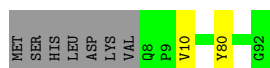
- Molecule 7: Dynein light chain roadblock-type 2 protein

Chain G:  90% . 8%




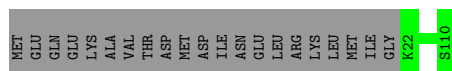
- Molecule 8: Dynein light chain

Chain H: 90% • 8%



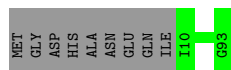
- Molecule 9: Dynein light chain

Chain I:  81% 19%



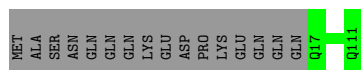
- Molecule 10: Dynein light chain

Chain J:  90% 10%



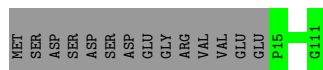
- Molecule 11: Dynein light chain

Chain K:  86% 14%



- Molecule 12: Dynein light chain

Chain L:  87% 13%




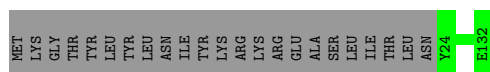
- Molecule 13: Dynein light chain

Chain M:  99% 1%



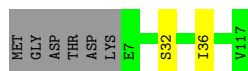
- Molecule 14: Dynein light chain 2A

Chain N:  83% 17%

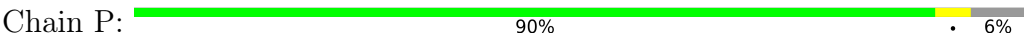


- Molecule 15: Dynein light chain tctex-type 1 protein

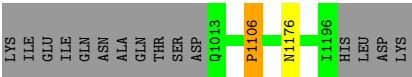
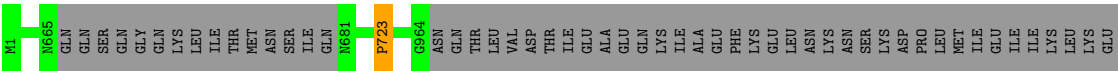
Chain O:  93% 5%



- Molecule 16: Thioredoxin



● Molecule 17: Shulin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	131142	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (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, ADP, GTP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.34	0/18743	0.69	1/26057 (0.0%)
2	B	0.39	0/19561	0.65	6/27233 (0.0%)
3	C	0.31	0/19162	0.56	8/26702 (0.0%)
4	D	0.36	0/1584	0.84	0/2201
4	d	0.31	0/634	0.61	0/881
5	E	0.36	0/1676	0.78	0/2327
5	e	0.44	0/498	0.76	3/687 (0.4%)
6	F	0.46	0/485	0.86	0/675
7	G	0.37	0/469	0.73	0/652
8	H	0.42	0/419	0.84	0/582
9	I	0.40	0/438	0.86	0/608
10	J	0.31	0/415	0.57	0/577
11	K	0.28	0/469	0.56	0/652
12	L	0.28	0/478	0.57	0/664
13	M	0.29	0/425	0.55	0/591
14	N	0.28	0/536	0.57	0/744
15	O	0.24	0/549	0.50	0/764
16	P	0.78	0/512	0.92	0/714
17	Y	0.29	1/5608 (0.0%)	0.55	2/7814 (0.0%)
All	All	0.35	1/72661 (0.0%)	0.64	20/101125 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	1176	ASN	C-N	6.01	1.47	1.34

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4432	PRO	N-CA-CB	8.75	113.80	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4182	PRO	N-CA-CB	6.65	111.28	103.30
3	C	4188	PRO	N-CA-CB	6.65	111.28	103.30
17	Y	1106	PRO	N-CA-CB	6.55	111.16	103.30
3	C	2978	PRO	N-CA-CB	6.33	110.89	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	18787	0	8282	131	0
2	B	20008	0	8566	89	0
3	C	19737	0	8300	29	0
4	D	1588	0	693	3	0
4	d	637	0	261	0	0
5	E	1678	0	724	1	0
5	e	501	0	215	0	0
6	F	486	0	218	0	0
7	G	470	0	203	1	0
8	H	420	0	185	1	0
9	I	439	0	202	0	0
10	J	416	0	184	0	0
11	K	470	0	215	0	0
12	L	479	0	209	0	0
13	M	426	0	189	0	0
14	N	537	0	231	0	0
15	O	550	0	247	1	0
16	P	513	0	213	2	0
17	Y	5611	0	2410	0	0
18	C	81	0	36	0	0
19	C	31	0	12	0	0
20	Y	32	0	12	0	0
All	All	73897	0	31807	258	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 2.

The worst 5 of 258 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:917:ILE:O	2:B:921:SER:CB	2.17	0.92
3:C:617:ILE:C	3:C:618:THR:CA	2.46	0.84
2:B:4318:LEU:O	2:B:4322:GLU:N	2.12	0.83
3:C:642:ASN:CA	3:C:643:THR:N	2.43	0.81
2:B:2229:LYS:O	2:B:2230:THR:N	2.13	0.81

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3707/4168 (89%)	3206 (86%)	493 (13%)	8 (0%)	47	81
2	B	3893/4595 (85%)	3484 (90%)	398 (10%)	11 (0%)	41	77
3	C	3846/4620 (83%)	3509 (91%)	330 (9%)	7 (0%)	47	81
4	D	313/667 (47%)	268 (86%)	45 (14%)	0	100	100
4	d	122/667 (18%)	112 (92%)	10 (8%)	0	100	100
5	E	337/670 (50%)	287 (85%)	50 (15%)	0	100	100
5	e	96/670 (14%)	86 (90%)	10 (10%)	0	100	100
6	F	96/133 (72%)	79 (82%)	17 (18%)	0	100	100
7	G	93/103 (90%)	81 (87%)	12 (13%)	0	100	100
8	H	83/92 (90%)	76 (92%)	7 (8%)	0	100	100
9	I	87/110 (79%)	79 (91%)	8 (9%)	0	100	100
10	J	82/93 (88%)	77 (94%)	5 (6%)	0	100	100
11	K	93/111 (84%)	83 (89%)	10 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	95/111 (86%)	90 (95%)	5 (5%)	0	100	100
13	M	84/87 (97%)	77 (92%)	7 (8%)	0	100	100
14	N	107/132 (81%)	100 (94%)	7 (6%)	0	100	100
15	O	109/117 (93%)	99 (91%)	10 (9%)	0	100	100
16	P	101/110 (92%)	97 (96%)	4 (4%)	0	100	100
17	Y	1127/1200 (94%)	1071 (95%)	54 (5%)	2 (0%)	47	81
All	All	14471/18456 (78%)	12961 (90%)	1482 (10%)	28 (0%)	50	81

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1823	VAL
2	B	1651	ASN
2	B	1652	PRO
2	B	2557	PRO
2	B	3703	PRO

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](#)

5 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	$\# Z > 2$
20	GTP	Y	1301	-	26,34,34	1.21	2 (7%)	32,54,54	1.65	6 (18%)
18	ADP	C	4704	-	24,29,29	0.92	1 (4%)	29,45,45	1.49	4 (13%)
18	ADP	C	4701	-	24,29,29	0.96	1 (4%)	29,45,45	1.49	3 (10%)
19	ATP	C	4702	-	26,33,33	0.87	1 (3%)	31,52,52	1.68	5 (16%)
18	ADP	C	4703	-	24,29,29	0.93	1 (4%)	29,45,45	1.54	4 (13%)

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
20	GTP	Y	1301	-	-	6/18/38/38	0/3/3/3
18	ADP	C	4704	-	-	3/12/32/32	0/3/3/3
18	ADP	C	4701	-	-	1/12/32/32	0/3/3/3
19	ATP	C	4702	-	-	4/18/38/38	0/3/3/3
18	ADP	C	4703	-	-	4/12/32/32	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Y	1301	GTP	C5-C6	-4.38	1.38	1.47
18	C	4704	ADP	C5-C4	2.25	1.46	1.40
18	C	4701	ADP	C5-C4	2.18	1.46	1.40
20	Y	1301	GTP	C2-N3	2.17	1.38	1.33
18	C	4703	ADP	C5-C4	2.13	1.46	1.40

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	C	4702	ATP	PA-O3A-PB	-5.12	115.25	132.83
18	C	4701	ADP	PA-O3A-PB	-4.56	117.17	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	4704	ADP	PA-O3A-PB	-4.21	118.36	132.83
19	C	4702	ATP	PB-O3B-PG	-4.13	118.64	132.83
18	C	4703	ADP	PA-O3A-PB	-4.13	118.66	132.83

There are no chirality outliers.

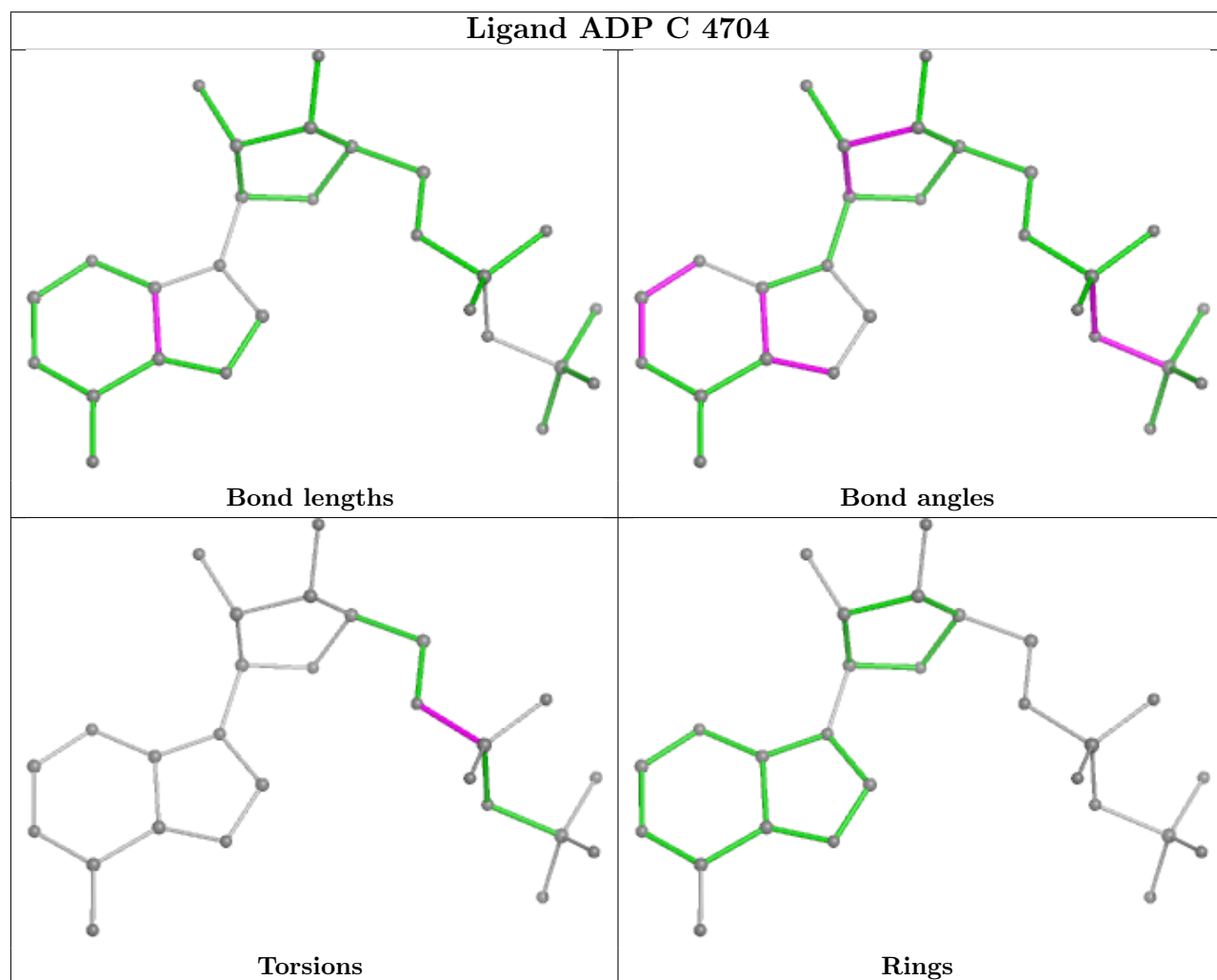
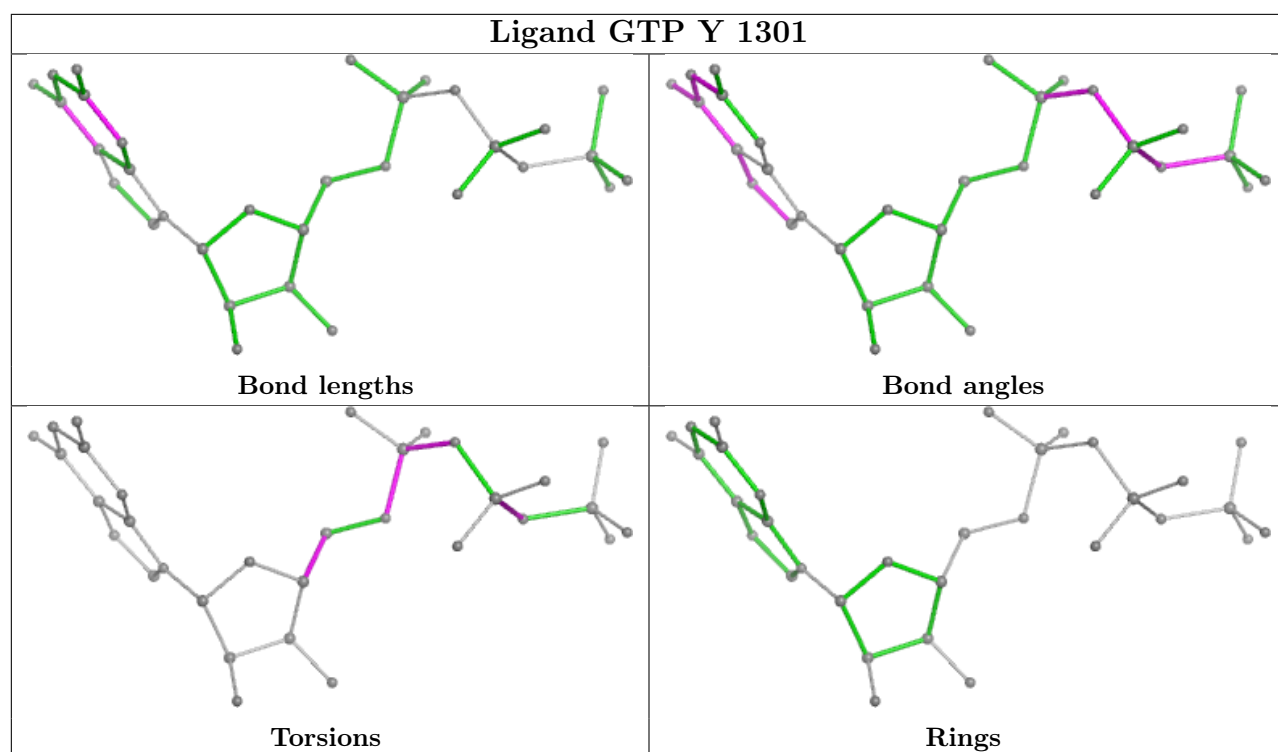
5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	C	4703	ADP	C5'-O5'-PA-O1A
18	C	4703	ADP	C5'-O5'-PA-O2A
18	C	4704	ADP	C5'-O5'-PA-O2A
19	C	4702	ATP	C5'-O5'-PA-O1A
19	C	4702	ATP	C5'-O5'-PA-O3A

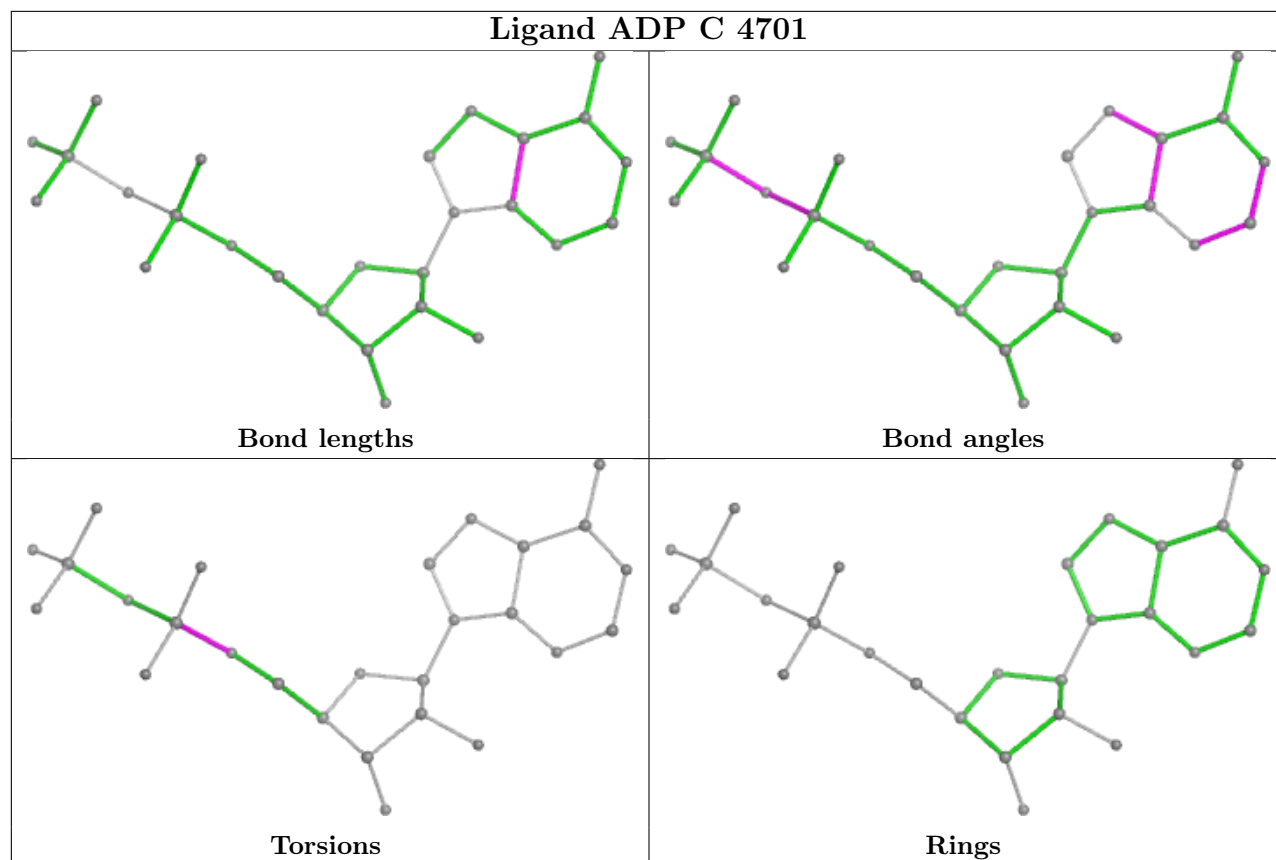
There are no ring outliers.

No monomer is involved in short contacts.

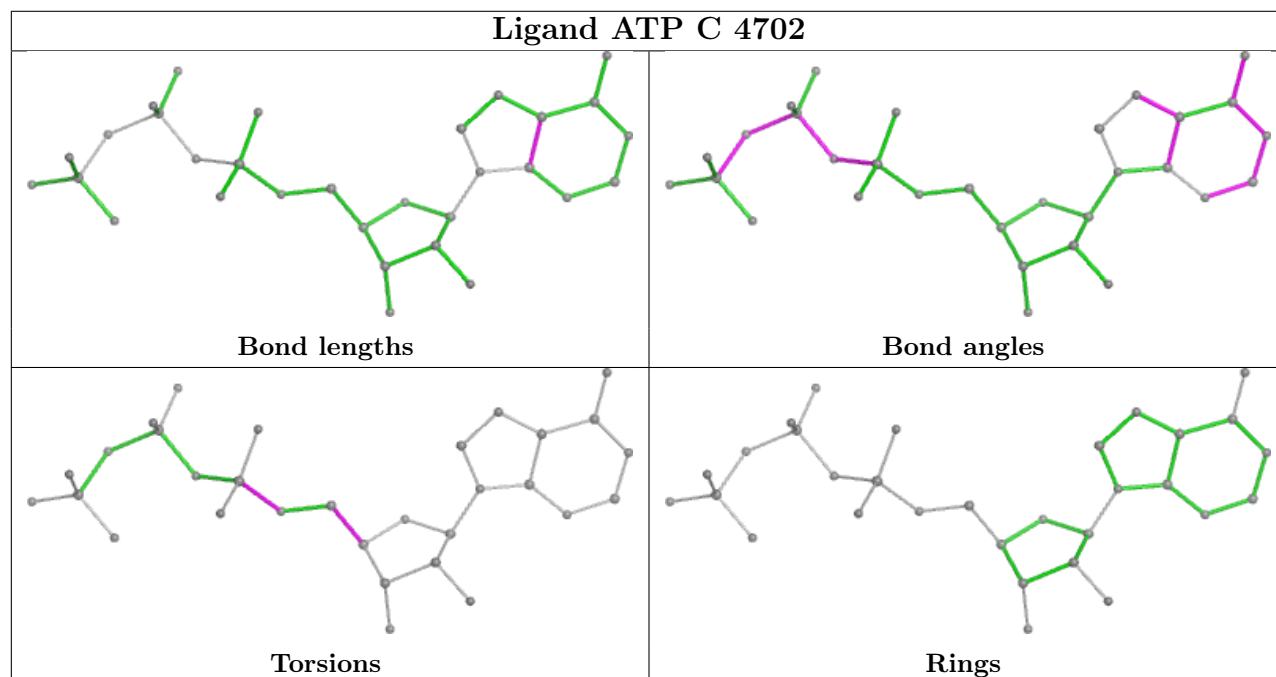
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

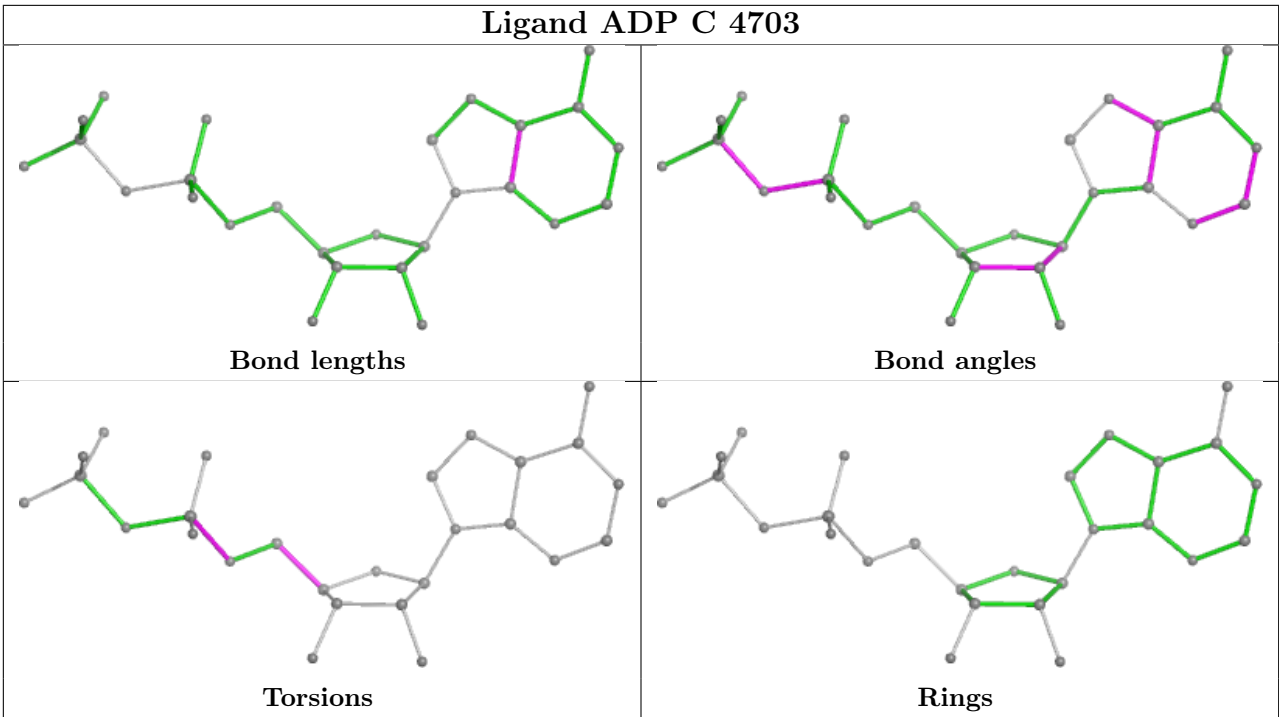


Ligand ADP C 4701



Ligand ATP C 4702





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	23
2	B	12
5	e	2
4	d	1

The worst 5 of 38 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	d	201:GLN	C	235:TRP	N	31.73
1	A	389:ASP	C	390:THR	N	29.62
1	A	486:ASP	C	487:GLN	N	21.39
1	A	1299:VAL	C	1300:GLN	N	17.01
1	A	2300:SER	C	2301:ASP	N	13.90