



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 3, 2019 – 04:02 PM EST

PDB ID : 6F3A
EMDB ID: : EMD-2860
Title : Cryo-EM structure of a single dynein tail domain bound to dynactin and BICD2N
Authors : Urnavicius, L.; Lau, C.K.; Elshenawy, M.M.; Morales-Rios, E.; Motz, C.; Yildiz, A.; Carter, A.P.
Deposited on : 2017-11-28
Resolution : 8.20 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary 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 ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

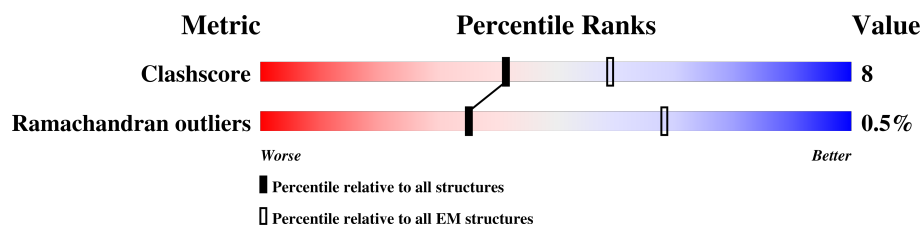
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.20 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.




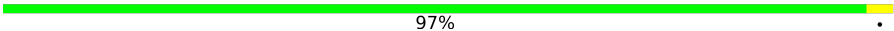
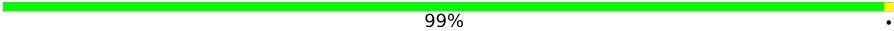


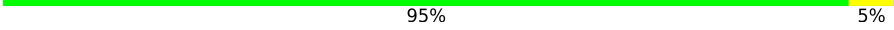
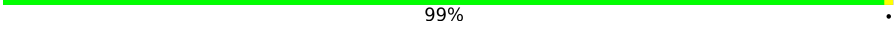



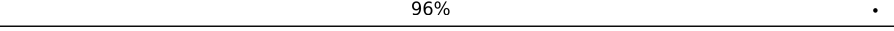
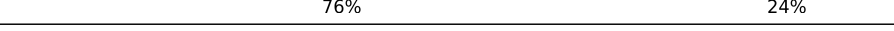







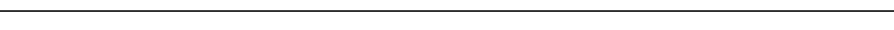

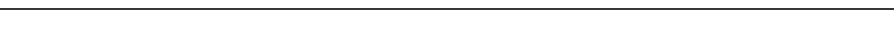
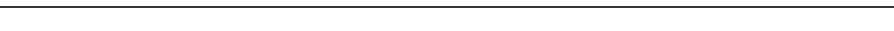


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	376	 87% 12% .
1	B	376	 81% 17% .
1	C	376	 85% 14% .
1	D	376	 83% 16% .
1	E	376	 81% 18% .
1	F	376	 83% 15% .
1	G	376	 88% 10% .
1	I	376	 84% 14% .
2	H	375	 87% 12% .
3	J	390	 83% 12% 5%
4	K	286	 82% 15% .

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Mol	Chain	Length	Quality of chain
5	L	272	 89% 10%
6	M	587	 97%
7	N	616	 99%
8	O	65	 89% 11%
8	P	65	 94% 6%
9	Q	87	 95% 5%
9	R	87	 99%
10	U	190	 85% 6% 9%
11	V	182	 77% 14% 9%
12	Y	264	 91% 9%
13	Z	52	 96%
14	a	68	 76% 24%
15	b	89	 84% 16%
15	c	89	 39% 61%
15	d	89	 27% 73%
16	e	1455	 54% 46%
16	f	1455	 57% 43%
17	g	612	 65% 35%
17	h	612	 65% 34%
18	j	492	 97%
19	k	96	 97%
19	l	96	 97%
20	z	53	 100%
21	5	275	 81% 19%
21	6	275	 81% 19%

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 48864 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 ARP1 actin related protein 1 homolog A.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	B	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	C	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	D	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	E	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	F	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	G	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	I	370	Total	C	N	O	0	0
			1822	1082	370	370		

- Molecule 2 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	H	370	Total	C	N	O	0	0
			1822	1082	370	370		

- Molecule 3 is a protein called Actin related protein 10 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	J	369	Total	C	N	O	0	0
			1819	1081	369	369		

- Molecule 4 is a protein called Capping protein (Actin filament) muscle Z-line, alpha 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	278	Total	C	N	O	0	0
			1378	822	278	278		

- Molecule 5 is a protein called F-actin capping protein beta subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	L	269	Total	C	N	O	0	0
			1327	789	269	269		

- Molecule 6 is a protein called Dynactin Subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	M	587	Total	C	N	O	0	0
			2935	1761	587	587		

- Molecule 7 is a protein called Dynactin Subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	N	616	Total	C	N	O	0	0
			3080	1848	616	616		

- Molecule 8 is a protein called Dynactin Subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	O	65	Total	C	N	O	0	0
			323	193	65	65		
8	P	65	Total	C	N	O	0	0
			323	193	65	65		

- Molecule 9 is a protein called Dynactin Subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	Q	87	Total	C	N	O	0	0
			435	261	87	87		
9	R	87	Total	C	N	O	0	0
			435	261	87	87		

- Molecule 10 is a protein called Dynactin 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	U	172	Total	C	N	O	0	1
			843	500	171	172		

- Molecule 11 is a protein called Dynactin subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	V	165	Total	C	N	O	0	0
			812	482	165	165		

- Molecule 12 is a protein called Dynactin Subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	Y	264	Total	C	N	O	0	0
			1320	792	264	264		

- Molecule 13 is a protein called Dynactin Subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	Z	52	Total	C	N	O	0	0
			260	156	52	52		

- Molecule 14 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	a	52	Total	C	N	O	0	0
			259	155	52	52		

- Molecule 15 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	b	75	Total	C	N	O	0	0
			369	219	75	75		
15	c	35	Total	C	N	O	0	0
			174	104	35	35		
15	d	24	Total	C	N	O	0	0
			119	71	24	24		

- Molecule 16 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	e	785	Total	C	N	O	0	0
			3898	2328	785	785		
16	f	832	Total	C	N	O	0	0
			4128	2470	832	826		

- Molecule 17 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	g	397	Total	C	N	O	0	0
			1961	1167	397	397		
17	h	401	Total	C	N	O	0	0
			1980	1178	401	401		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	484	SER	THR	conflict	UNP Q13409
g	499	GLY	ASP	conflict	UNP Q13409
h	484	SER	THR	conflict	UNP Q13409
h	499	GLY	ASP	conflict	UNP Q13409

- Molecule 18 is a protein called Cytoplasmic dynein 1 light intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	j	15	Total	C	N	O	0	0
			75	45	15	15		

- Molecule 19 is a protein called Dynein light chain roadblock-type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	k	93	Total	C	N	O	0	0
			462	276	93	93		
19	l	93	Total	C	N	O	0	0
			462	276	93	93		

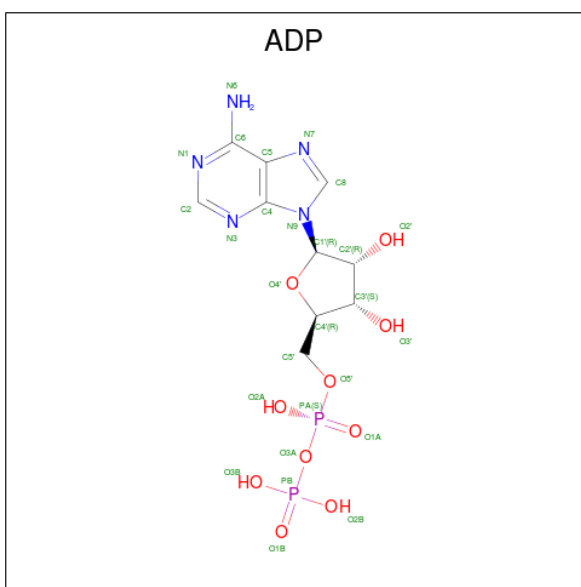
- Molecule 20 is a protein called Dynactin Subunit 1.

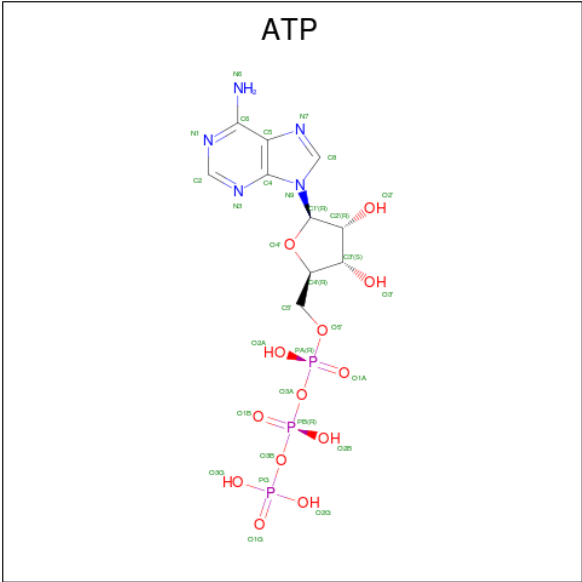
Mol	Chain	Residues	Atoms				AltConf	Trace
20	z	53	Total	C	N	O	0	0
			265	159	53	53		

- Molecule 21 is a protein called BICD2N.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	5	275	Total	C	N	O	0	0
			1375	825	275	275		
21	6	275	Total	C	N	O	0	0
			1375	825	275	275		

- Molecule 22 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



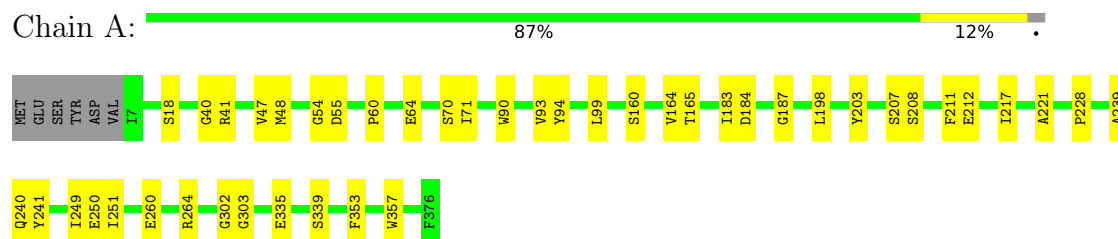


Mol	Chain	Residues	Atoms					AltConf
23	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

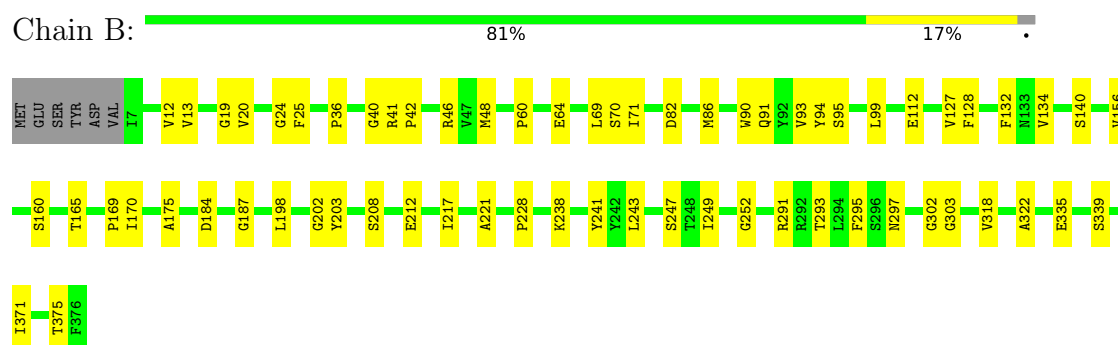
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

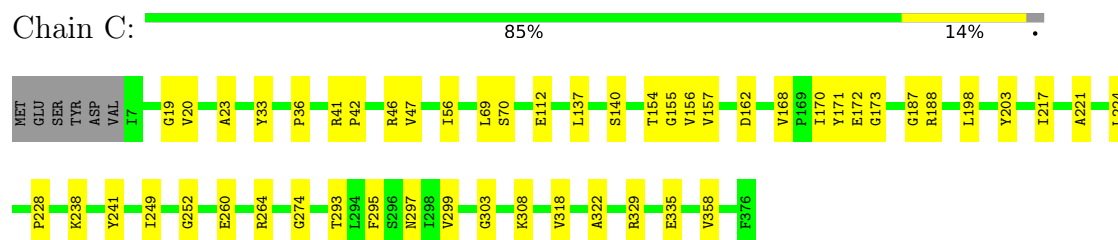
- Molecule 1: ARP1 actin related protein 1 homolog A



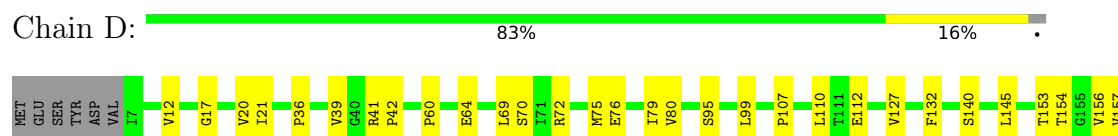
- Molecule 1: ARP1 actin related protein 1 homolog A



- Molecule 1: ARP1 actin related protein 1 homolog A



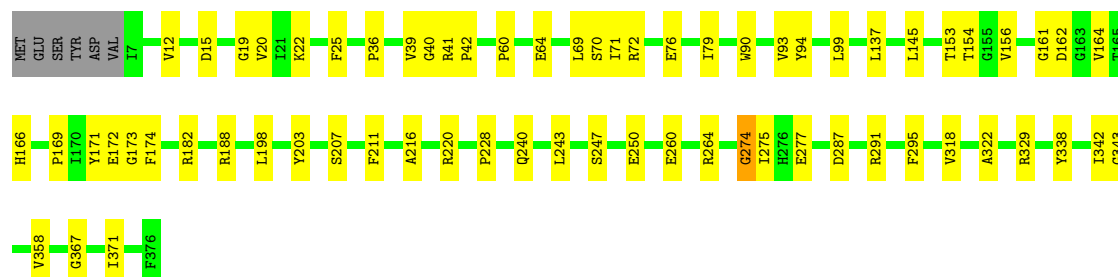
- Molecule 1: ARP1 actin related protein 1 homolog A





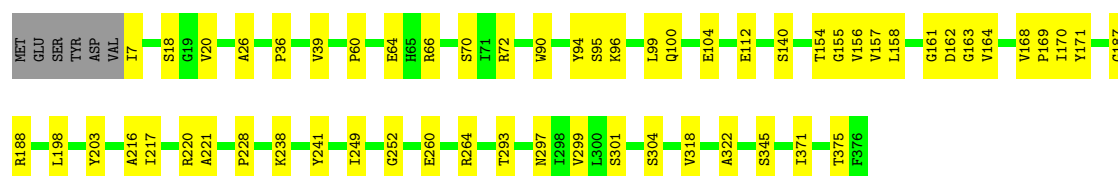
- Molecule 1: ARP1 actin related protein 1 homolog A

Chain E: 81% 18% .



- Molecule 1: ARP1 actin related protein 1 homolog A

Chain F: 83% 15% .



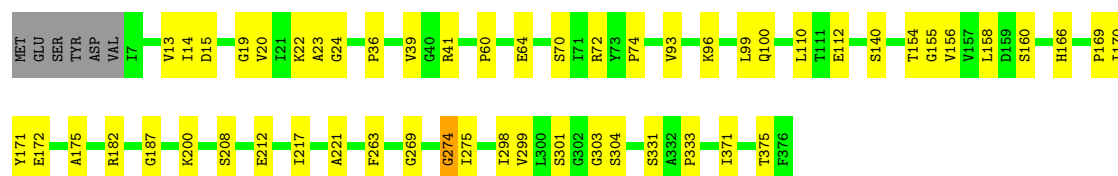
- Molecule 1: ARP1 actin related protein 1 homolog A

Chain G: 88% 10% .



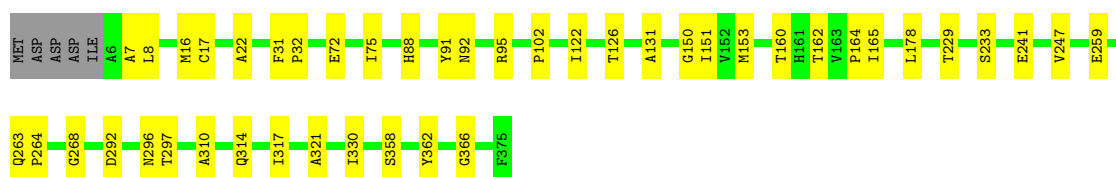
- Molecule 1: ARP1 actin related protein 1 homolog A

Chain I: 84% 14% .



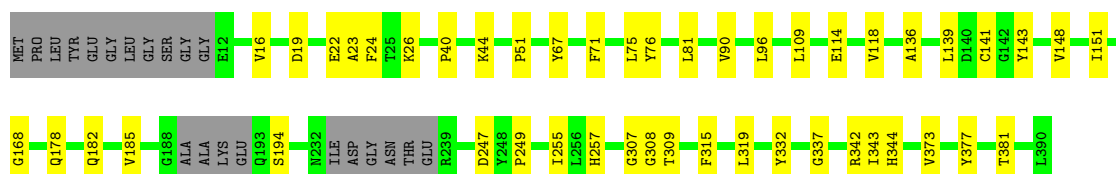
- Molecule 2: Actin, cytoplasmic 1

Chain H: 87% 12% .



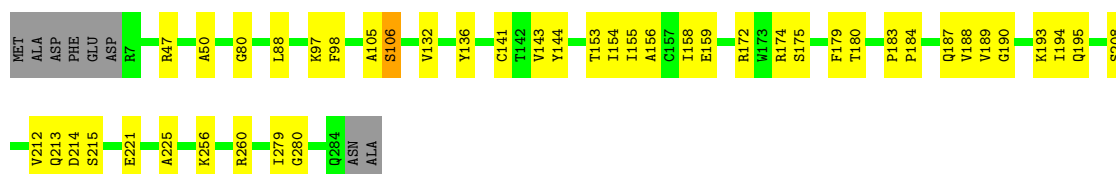
- Molecule 3: Actin related protein 10 homolog

Chain J: 83% 12% 5%



- Molecule 4: Capping protein (Actin filament) muscle Z-line, alpha 1

Chain K: 82% 15% .



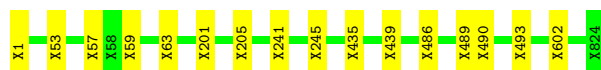
- Molecule 5: F-actin capping protein beta subunit

Chain L: 89% 10% .



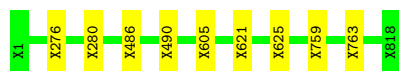
- Molecule 6: Dynactin Subunit 2

Chain M: 97% .



- Molecule 7: Dynactin Subunit 2

Chain N: 99% .



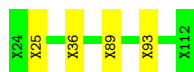
- Molecule 8: Dynactin Subunit 3

Chain O: 89% 11%



• Molecule 8: Dynactin Subunit 3

Chain P: 94% 6%



• Molecule 9: Dynactin Subunit 2

Chain Q: 95% 5%



• Molecule 9: Dynactin Subunit 2

Chain R: 99% .



• Molecule 10: Dynactin 6

Chain U: 85% 6% 9%



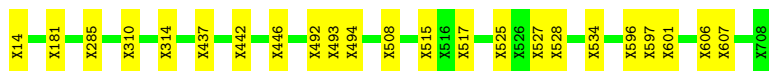
• Molecule 11: Dynactin subunit 5

Chain V: 77% 14% 9%



• Molecule 12: Dynactin Subunit 4

Chain Y: 91% 9%

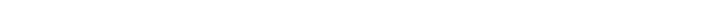


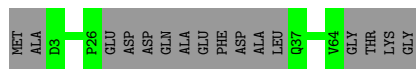
• Molecule 13: Dynactin Subunit 1

Chain Z: 96% .



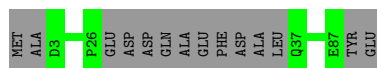
- Molecule 14: Dynactin subunit 2

Chain a:  76% 24%



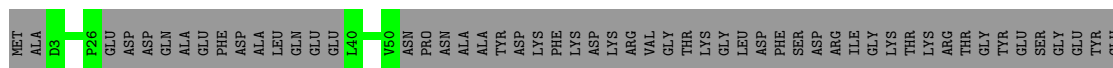
- Molecule 15: Dynactin subunit 2

Chain b: 84% 16%



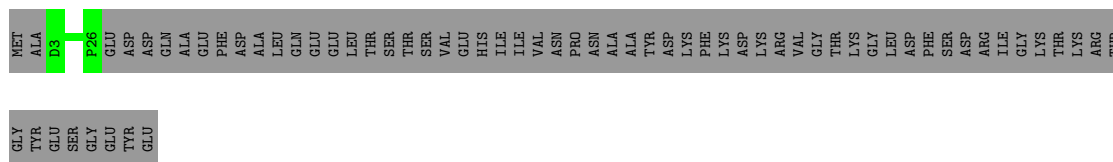
- Molecule 15: Dynactin subunit 2

Chain c: 39% 61%



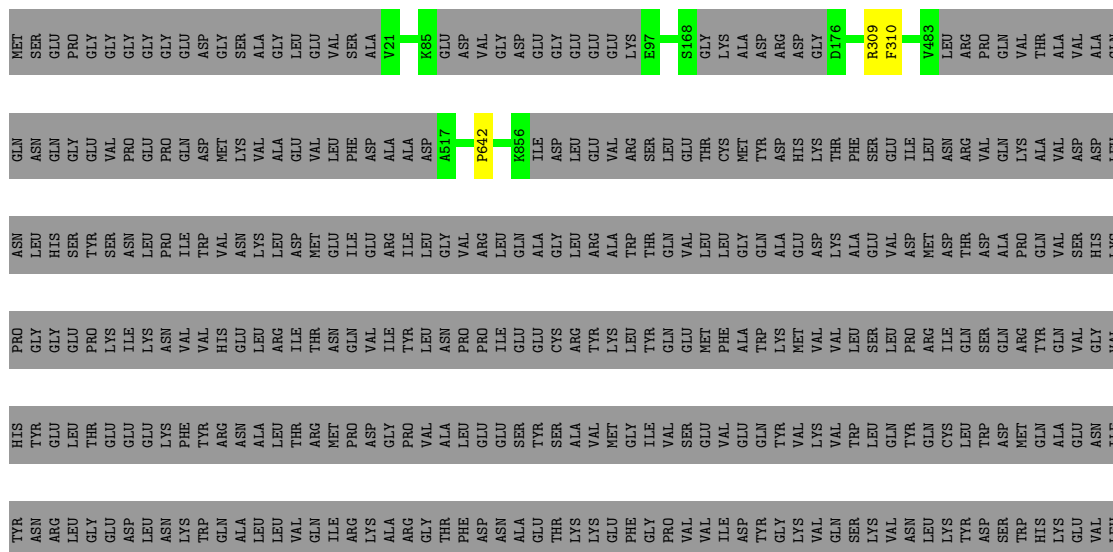
- Molecule 15: Dynactin subunit 2

Chain d: 27% 73%



- Molecule 16: Cytoplasmic dynein 1 heavy chain 1

Chain e:  54% 46%



LEU	THR	GLN	THR	ALA	LEU	SER
LEU	THR	LEU	GLY	VAL	TYR	LYS
GLY	GLY	LEU	LEU	GLU	ARG	PHE
GLN	SER	SER	LEU	SER	ASN	GLY
ILE	PHE	GLY	GLY	THR	GLN	THR
TRP	ALA	PRO	SER	THR	ARG	LEU
ASP	ARG	ALA	GLU	ASP	LEU	GLY
VAL	LEU	LEU	GLU	LEU	LEU	SER
ASP	ASP	ARG	ARG	LEU	GLU	ASN
LEU	GLN	GLN	VAL	THR	LEU	MET
GLN	TYR	TYR	GLN	ASP	GLN	THR
LYS	ALA	ALA	VAL	TRP	ARG	GLU
ASN	SER	SER	ALA	GLU	PHE	PHE
GLU	TYR	TYR	LEU	LYS	GLN	HIS
ALA	GLU	GLU	GLU	THR	GLN	SER
ALA	ALA	PHE	GLU	THR	PHE	SER
ILE	ILE	ILE	GLU	LYS	PRO	GLN
VAL	VAL	VAL	LEU	PRO	PRO	ILE
LYS	ASP	GLN	GLN	VAL	SER	SER
ASP	ARG	ARG	ASP	THR	TRP	LYS
GLU	TYR	LEU	LEU	GLY	LEU	SER
VAL	GLU	LEU	LEU	ASN	TYR	ARG
LEU	LEU	LYS	GLY	LEU	ILE	GLN
VAL	VAL	GLY	VAL	ARG	GLU	GLU
ALA	ALA	TYR	TRP	PRO	ASN	LEU
GLN	GLN	MET	SER	GLU	ASN	GLU
GLY	GLY	ILE	LEU	ALA	GLY	HIS
		ILE	LEU	ALA	GLU	SER
		MET	LYS	GLN	TRP	VAL
		LEU	VAL	ALA	GLY	ASP
		VAL	TRP	LEU	ALA	THR
		ILE	GLU	THR	ALA	ALA
		GLU	GLN	ILE	ASN	SER
		GLU	ILE	TYR	ASP	THR
		LYS	ASP	GLU	ILE	SER
		SER	GLN	GLY	MET	ASP
		GLU	MET	LYS	ARG	ALA
		ALA	LYS	PHE	ARG	VAL
		LEU	GLU	GLY	LYS	THR
		LYS	GLN	ARG	ASP	PHE
		ASP	PRO	LEU	SER	ILE
		ARG	TRP	LYS	ALA	THR
		HIS	VAL	ASP	ILE	TYR
		TRP	SER	ASP	GLN	VAL
		LYS	VAL	ARG	GLN	GLN
		GLN	GLN	GLU	GLN	SER
		LEU	PRO	LYS	VAL	LEU
		MET	ARG	CYS	ALA	LYS
		LYS	LYS	ALA	ASN	ARG
		ARG	LEU	LYS	LEU	LYS
		LEU	ARG	ALA	GLN	ILE
		HIS	GLN	LYS	MET	LYS
		VAL	ASN	GLU	LYS	GLN
		ASN	LEU	ALA	ILE	PHE
		TRP	ASP	LEU	VAL	GLU
		VAL	ALA	GLU	GLU	GLN
		VAL	LEU	LEU	GLU	GLN
		SER	LEU	THR	ASP	GLU
		GLN	ASN	ASP	ARG	THR

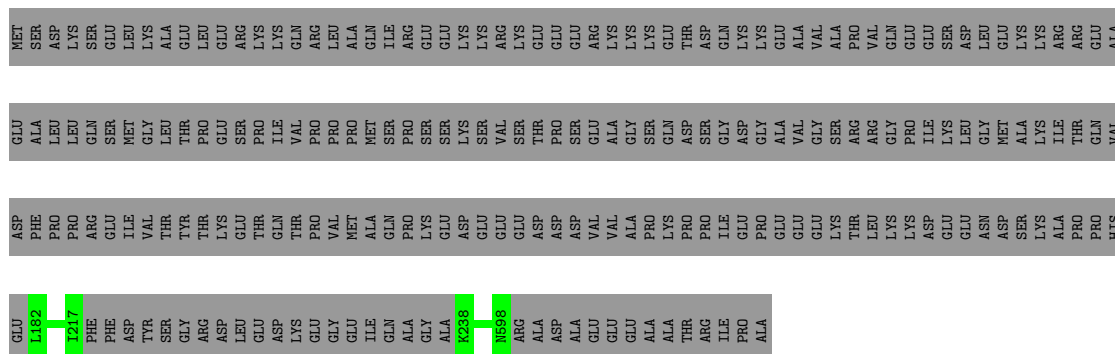
- Molecule 16: Cytoplasmic dynein 1 heavy chain 1

Chain f:  57% 43%

[illegible]

- Molecule 17: Cytoplasmic dynein 1 intermediate chain 2

Chain g: 65% 35%



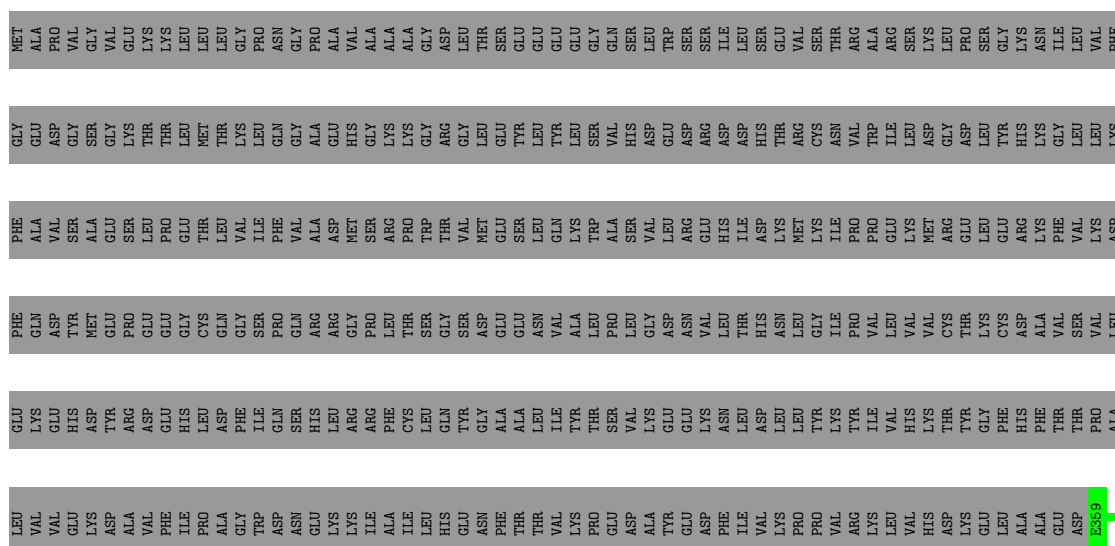
- Molecule 17: Cytoplasmic dynein 1 intermediate chain 2

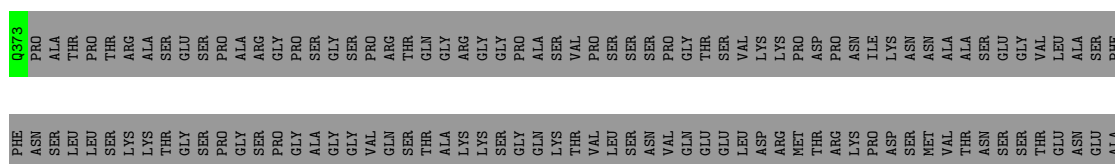
Chain h: 65% 34%



- Molecule 18: Cytoplasmic dynein 1 light intermediate chain 2

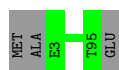
Chain j: 97%





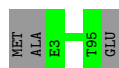
- Molecule 19: Dynein light chain roadblock-type 1

Chain k: 97%



- Molecule 19: Dynein light chain roadblock-type 1

Chain l: 97%



- Molecule 20: Dynactin Subunit 1

Chain z: 100%

There are no outlier residues recorded for this chain.

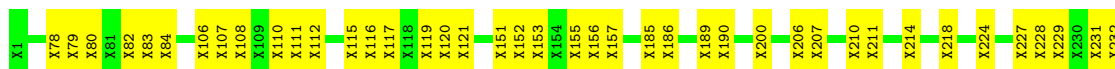
- Molecule 21: BICD2N

Chain 5: 81%



- Molecule 21: BICD2N

Chain 6: 81%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	85744	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 ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (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, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	A	0.41	0/1821	0.76	1/2531 (0.0%)
1	B	0.43	0/1821	0.74	0/2531
1	C	0.47	1/1821 (0.1%)	0.82	2/2531 (0.1%)
1	D	0.47	0/1821	0.78	1/2531 (0.0%)
1	E	0.46	0/1821	0.80	1/2531 (0.0%)
1	F	0.48	0/1821	0.78	1/2531 (0.0%)
1	G	0.46	0/1821	0.84	1/2531 (0.0%)
1	I	0.43	0/1821	0.76	2/2531 (0.1%)
10	U	0.38	0/841	0.65	0/1168
11	V	0.29	0/811	0.63	0/1126
14	a	0.39	0/257	0.82	0/356
15	b	0.42	0/367	0.88	0/507
15	c	0.39	0/172	0.82	0/237
15	d	0.36	0/118	0.76	0/163
16	e	0.29	0/3894	0.52	1/5429 (0.0%)
16	f	0.33	0/4123	0.62	1/5745 (0.0%)
17	g	0.33	0/1959	0.73	0/2725
17	h	0.35	0/1978	0.81	0/2751
18	j	0.26	0/74	0.55	0/102
19	k	0.31	0/461	0.61	0/642
19	l	0.28	0/461	0.57	0/642
2	H	0.42	0/1821	0.76	0/2531
3	J	0.41	0/1816	0.73	0/2522
4	K	0.35	0/1377	0.74	1/1919 (0.1%)
5	L	0.40	0/1326	0.71	1/1844 (0.1%)
All	All	0.39	1/36424 (0.0%)	0.72	13/50657 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	335	GLU	CA-CB	-6.00	1.40	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	274	GLY	N-CA-C	-10.65	86.47	113.10
1	I	274	GLY	N-CA-C	-9.15	90.23	113.10
1	C	274	GLY	N-CA-C	-8.38	92.16	113.10
1	G	274	GLY	N-CA-C	-7.54	94.24	113.10
1	E	274	GLY	N-CA-C	-7.18	95.16	113.10

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	1822	0	820	22	0
1	B	1822	0	820	35	0
1	C	1822	0	820	27	0
1	D	1822	0	820	29	0
1	E	1822	0	820	34	0
1	F	1822	0	820	31	0
1	G	1822	0	820	22	0
1	I	1822	0	820	28	0
2	H	1822	0	835	22	0
3	J	1819	0	794	28	0
4	K	1378	0	611	22	0
5	L	1327	0	585	13	0
6	M	2935	0	601	9	0
7	N	3080	0	632	5	0
8	O	323	0	73	4	0
8	P	323	0	74	2	0
9	Q	435	0	93	3	0
9	R	435	0	93	1	0
10	U	843	0	376	5	0
11	V	812	0	344	14	0
12	Y	1320	0	339	14	0
13	Z	260	0	57	1	0
14	a	259	0	110	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	b	369	0	161	0	0
15	c	174	0	71	0	0
15	d	119	0	50	0	0
16	e	3898	0	1725	0	0
16	f	4128	0	1822	0	0
17	g	1961	0	883	0	0
17	h	1980	0	889	0	0
18	j	75	0	32	0	0
19	k	462	0	192	0	0
19	l	462	0	192	0	0
20	z	265	0	57	0	0
21	5	1375	0	277	53	0
21	6	1375	0	277	43	0
22	A	27	0	12	1	0
22	B	27	0	12	1	0
22	C	27	0	12	2	0
22	D	27	0	12	0	0
22	E	27	0	12	1	0
22	F	27	0	12	2	0
22	G	27	0	12	2	0
22	I	27	0	12	1	0
22	J	27	0	12	4	0
23	H	31	0	12	0	0
All	All	48864	0	18925	442	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.

The worst 5 of 442 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)
21:5:268:UNK:CB	21:6:269:UNK:CB	1.95	1.44
21:5:137:UNK:O	21:5:141:UNK:N	1.68	1.25
21:6:238:UNK:O	21:6:242:UNK:N	1.70	1.24
21:5:138:UNK:O	21:5:142:UNK:N	1.90	1.05
21:6:117:UNK:O	21:6:121:UNK:N	1.92	1.02

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	368/376 (98%)	319 (87%)	46 (12%)	3 (1%)	21	65
1	B	368/376 (98%)	321 (87%)	45 (12%)	2 (0%)	31	74
1	C	368/376 (98%)	325 (88%)	40 (11%)	3 (1%)	21	65
1	D	368/376 (98%)	316 (86%)	49 (13%)	3 (1%)	21	65
1	E	368/376 (98%)	321 (87%)	45 (12%)	2 (0%)	31	74
1	F	368/376 (98%)	316 (86%)	50 (14%)	2 (0%)	31	74
1	G	368/376 (98%)	325 (88%)	40 (11%)	3 (1%)	21	65
1	I	368/376 (98%)	333 (90%)	30 (8%)	5 (1%)	12	52
2	H	368/375 (98%)	326 (89%)	42 (11%)	0	100	100
3	J	363/390 (93%)	310 (85%)	53 (15%)	0	100	100
4	K	276/286 (96%)	236 (86%)	38 (14%)	2 (1%)	24	67
5	L	267/272 (98%)	237 (89%)	30 (11%)	0	100	100
10	U	169/190 (89%)	126 (75%)	41 (24%)	2 (1%)	14	56
11	V	163/182 (90%)	126 (77%)	36 (22%)	1 (1%)	27	70
14	a	48/68 (71%)	39 (81%)	9 (19%)	0	100	100
15	b	71/89 (80%)	55 (78%)	16 (22%)	0	100	100
15	c	31/89 (35%)	22 (71%)	9 (29%)	0	100	100
15	d	22/89 (25%)	18 (82%)	4 (18%)	0	100	100
16	e	777/1455 (53%)	694 (89%)	81 (10%)	2 (0%)	43	81
16	f	822/1455 (56%)	750 (91%)	71 (9%)	1 (0%)	53	88
17	g	393/612 (64%)	341 (87%)	52 (13%)	0	100	100
17	h	397/612 (65%)	328 (83%)	67 (17%)	2 (0%)	31	74
18	j	13/492 (3%)	11 (85%)	2 (15%)	0	100	100
19	k	91/96 (95%)	75 (82%)	16 (18%)	0	100	100
19	l	91/96 (95%)	85 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	7306/9856 (74%)	6355 (87%)	918 (13%)	33 (0%)	35	74

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	K	279	ILE
10	U	79	PRO
17	h	491	LEU
1	A	187	GLY
1	B	187	GLY

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 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
22	ADP	A	800	-	24,29,29	0.96	1 (4%)	25,45,45	1.55	4 (16%)
22	ADP	B	800	-	24,29,29	0.94	1 (4%)	25,45,45	1.71	7 (28%)
22	ADP	C	800	-	24,29,29	0.94	1 (4%)	25,45,45	2.68	8 (32%)
22	ADP	D	800	-	24,29,29	0.91	1 (4%)	25,45,45	2.00	6 (24%)
22	ADP	E	800	-	24,29,29	1.13	2 (8%)	25,45,45	1.69	8 (32%)
22	ADP	F	800	-	24,29,29	1.00	1 (4%)	25,45,45	1.48	4 (16%)
22	ADP	G	800	-	24,29,29	0.95	1 (4%)	25,45,45	1.71	3 (12%)
23	ATP	H	401	-	26,33,33	0.94	1 (3%)	27,52,52	1.59	4 (14%)
22	ADP	I	800	-	24,29,29	1.00	1 (4%)	25,45,45	1.56	4 (16%)
22	ADP	J	800	-	24,29,29	1.02	1 (4%)	25,45,45	1.78	7 (28%)

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
22	ADP	A	800	-	-	3/12/32/32	0/3/3/3
22	ADP	B	800	-	-	4/12/32/32	0/3/3/3
22	ADP	C	800	-	-	5/12/32/32	0/3/3/3
22	ADP	D	800	-	-	3/12/32/32	0/3/3/3
22	ADP	E	800	-	-	3/12/32/32	0/3/3/3
22	ADP	F	800	-	-	2/12/32/32	0/3/3/3
22	ADP	G	800	-	-	1/12/32/32	0/3/3/3
23	ATP	H	401	-	-	3/18/38/38	0/3/3/3
22	ADP	I	800	-	-	1/12/32/32	0/3/3/3
22	ADP	J	800	-	-	5/12/32/32	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	800	ADP	C5-C4	2.95	1.47	1.40
22	F	800	ADP	C5-C4	2.83	1.46	1.40
23	H	401	ATP	C5-C4	2.82	1.46	1.40
22	E	800	ADP	C5-C4	2.77	1.46	1.40
22	G	800	ADP	C5-C4	2.75	1.46	1.40

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	800	ADP	C4'-O4'-C1'	-10.44	98.94	109.83
22	G	800	ADP	PA-O3A-PB	-5.29	115.75	132.57
22	A	800	ADP	PA-O3A-PB	-5.09	116.40	132.57
22	D	800	ADP	C4'-O4'-C1'	-4.86	104.77	109.83
22	D	800	ADP	PA-O3A-PB	-4.55	118.11	132.57

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

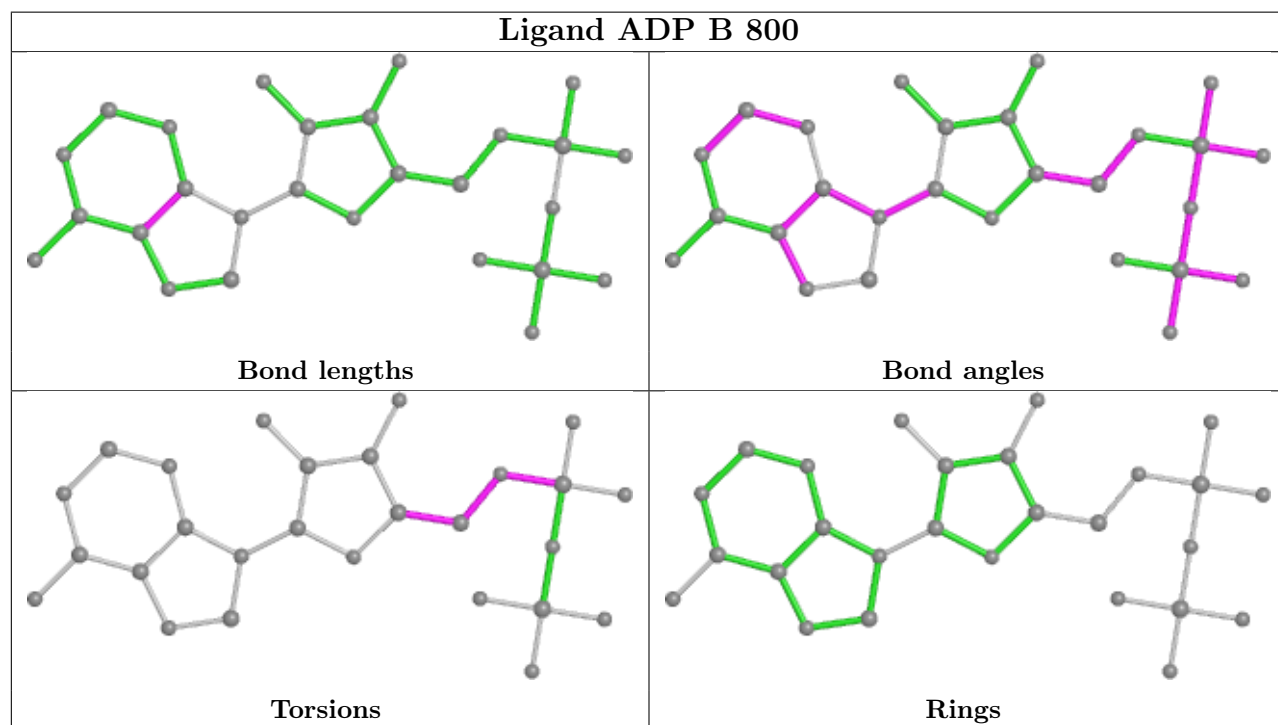
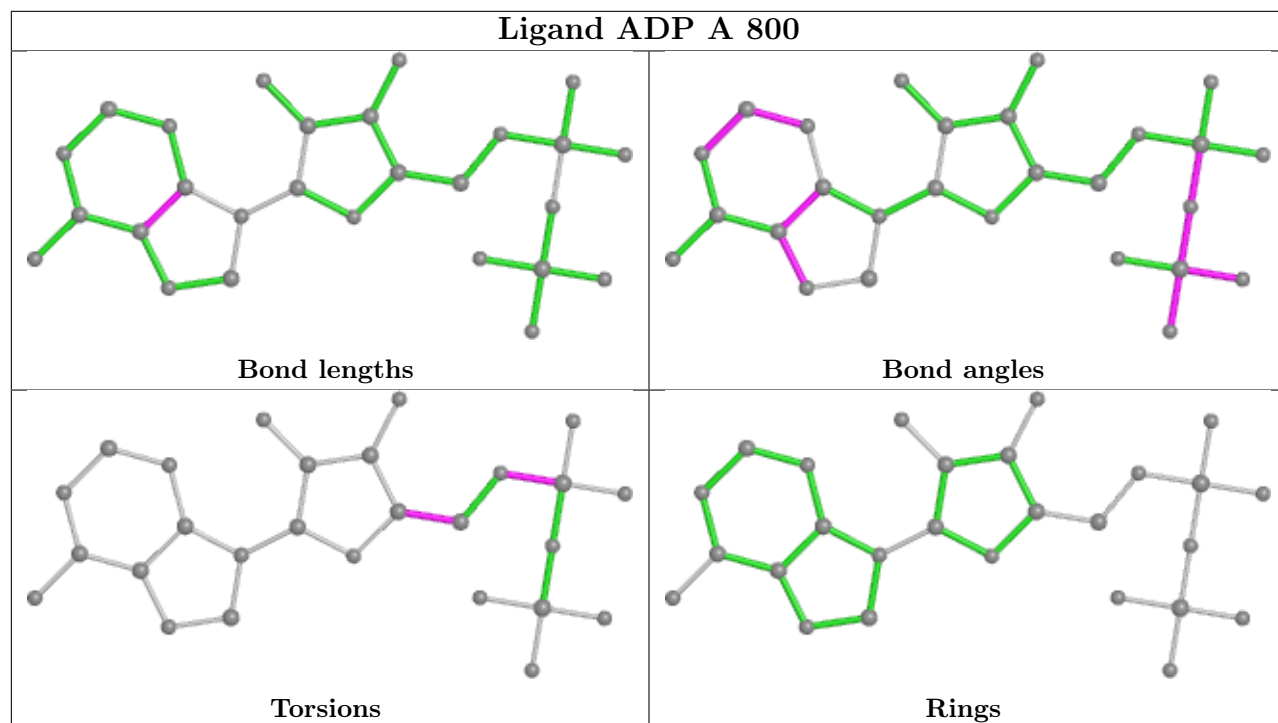
Mol	Chain	Res	Type	Atoms
22	A	800	ADP	O4'-C4'-C5'-O5'
22	A	800	ADP	C3'-C4'-C5'-O5'
22	C	800	ADP	C5'-O5'-PA-O3A
22	C	800	ADP	C3'-C4'-C5'-O5'
22	J	800	ADP	C5'-O5'-PA-O3A

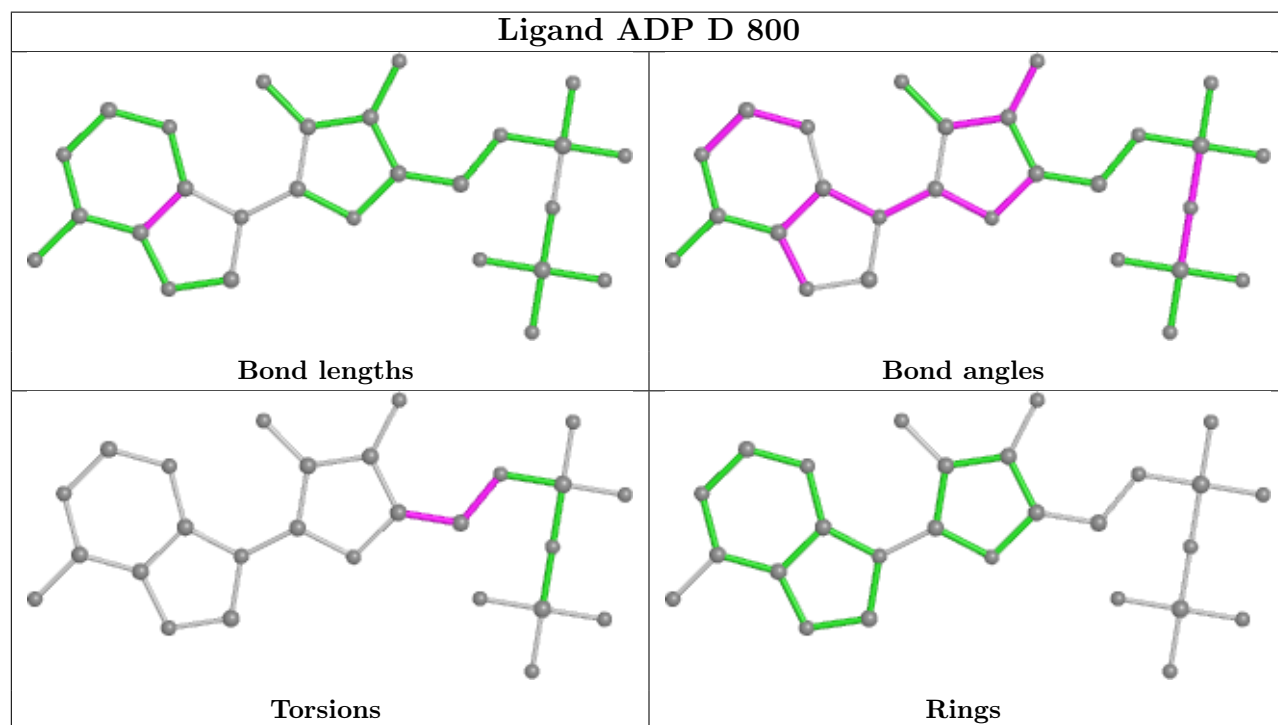
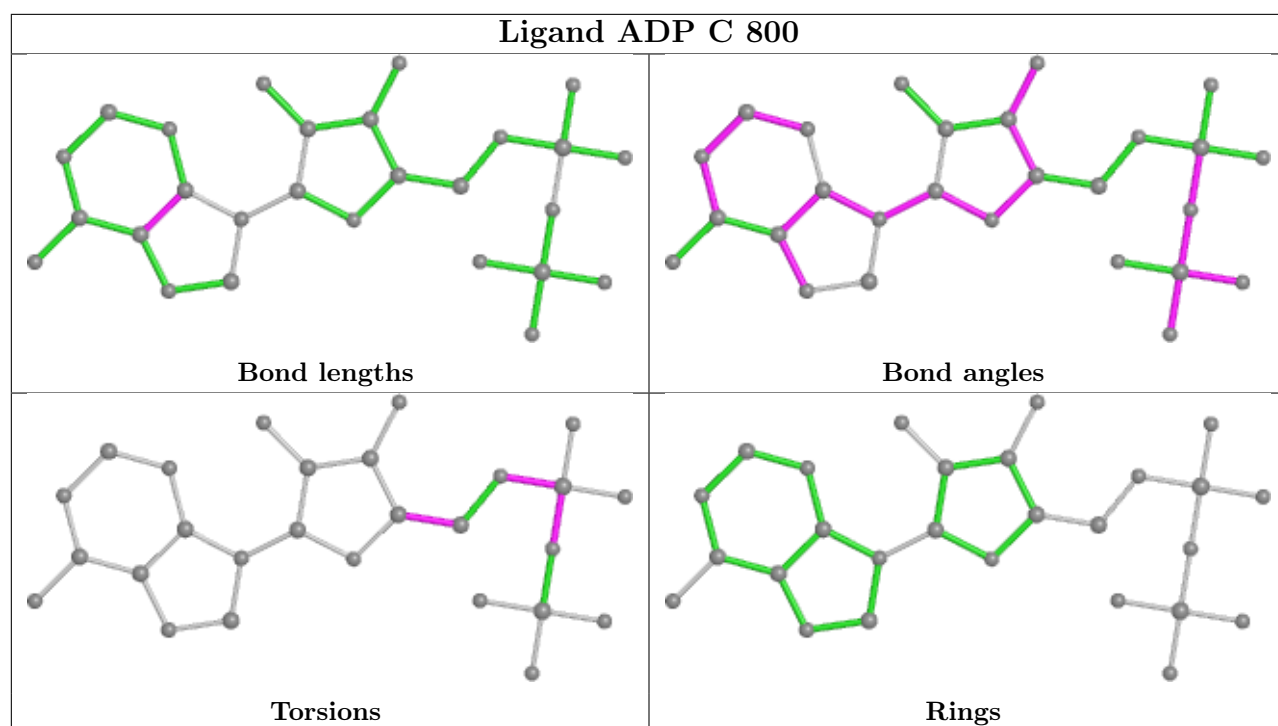
There are no ring outliers.

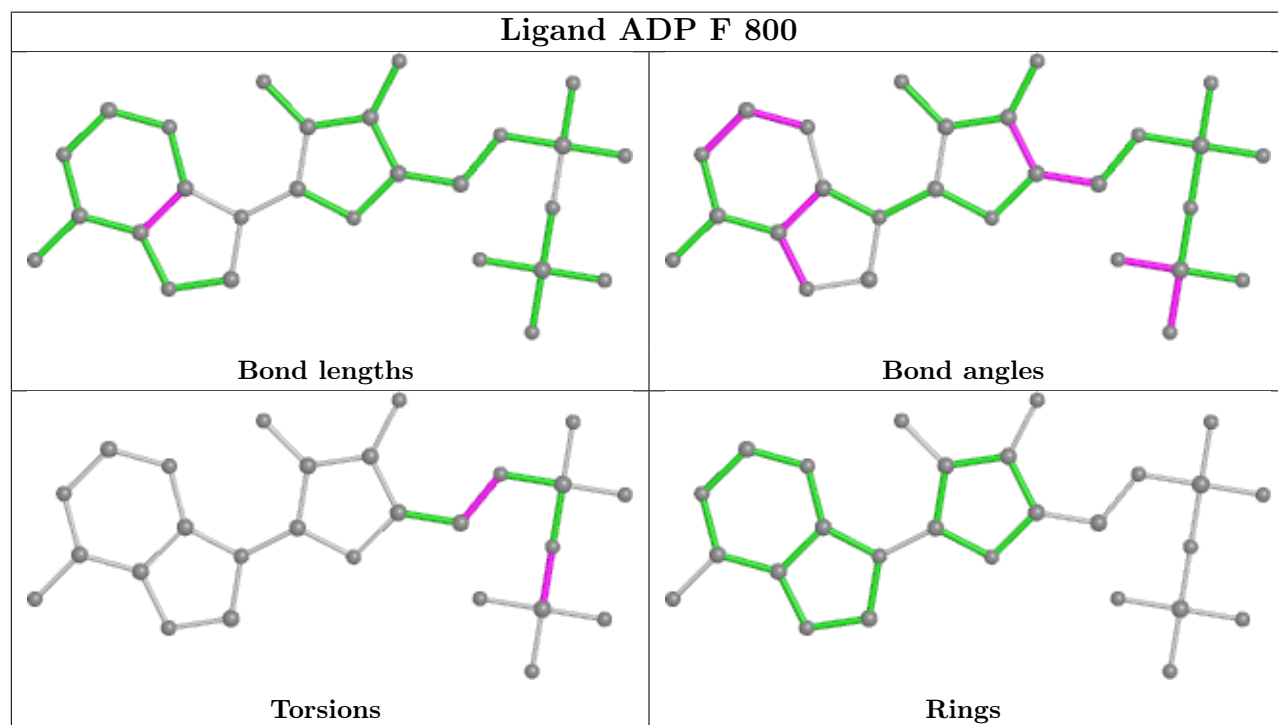
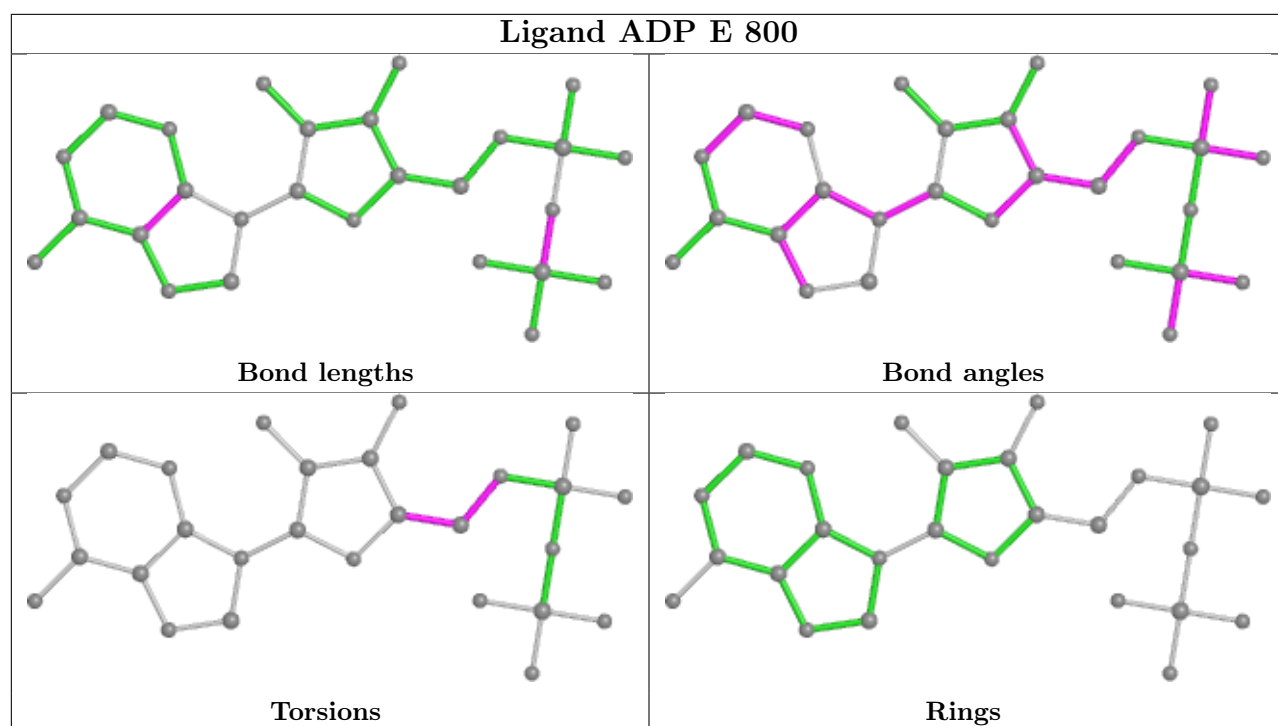
8 monomers are involved in 14 short contacts:

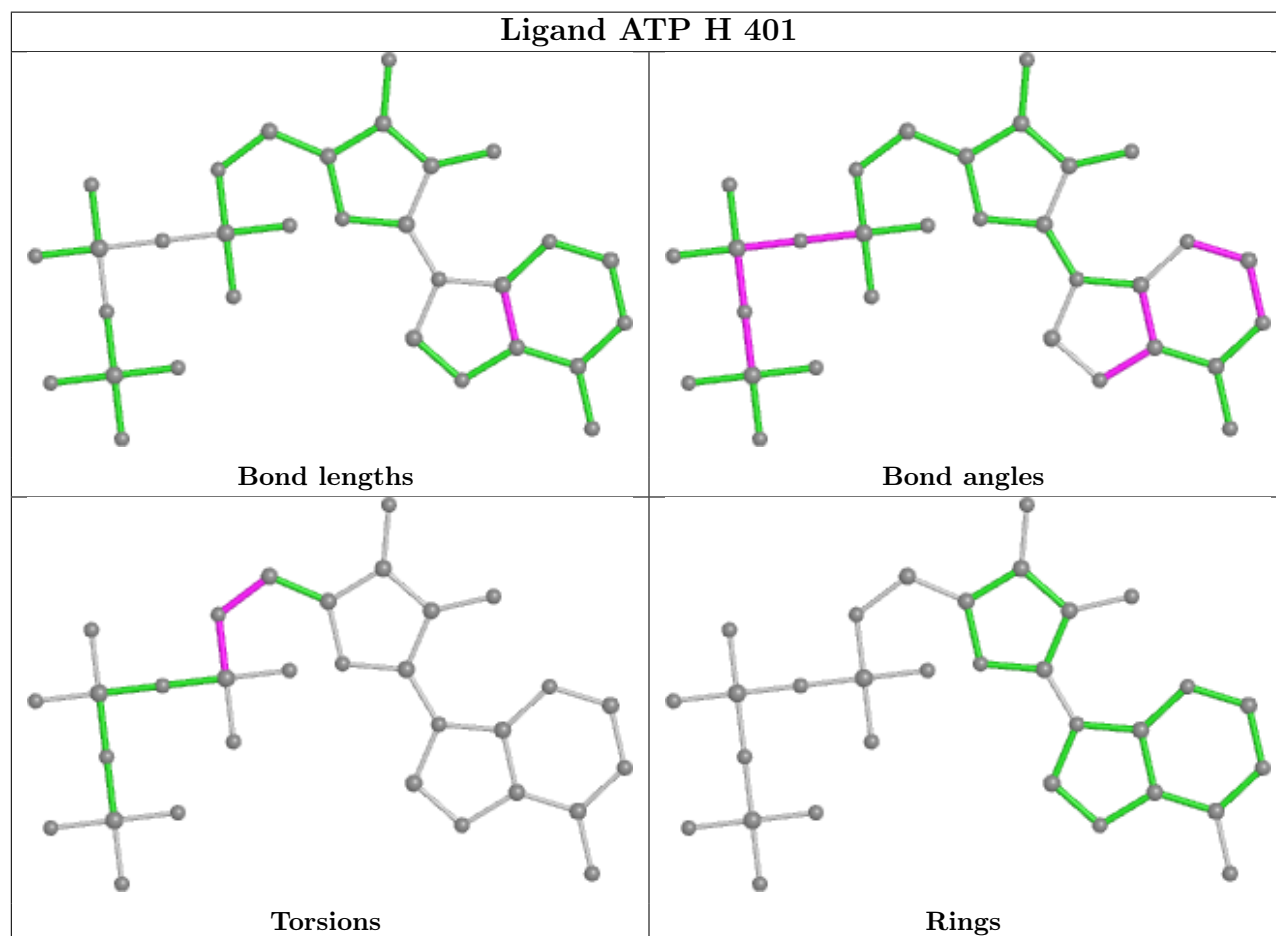
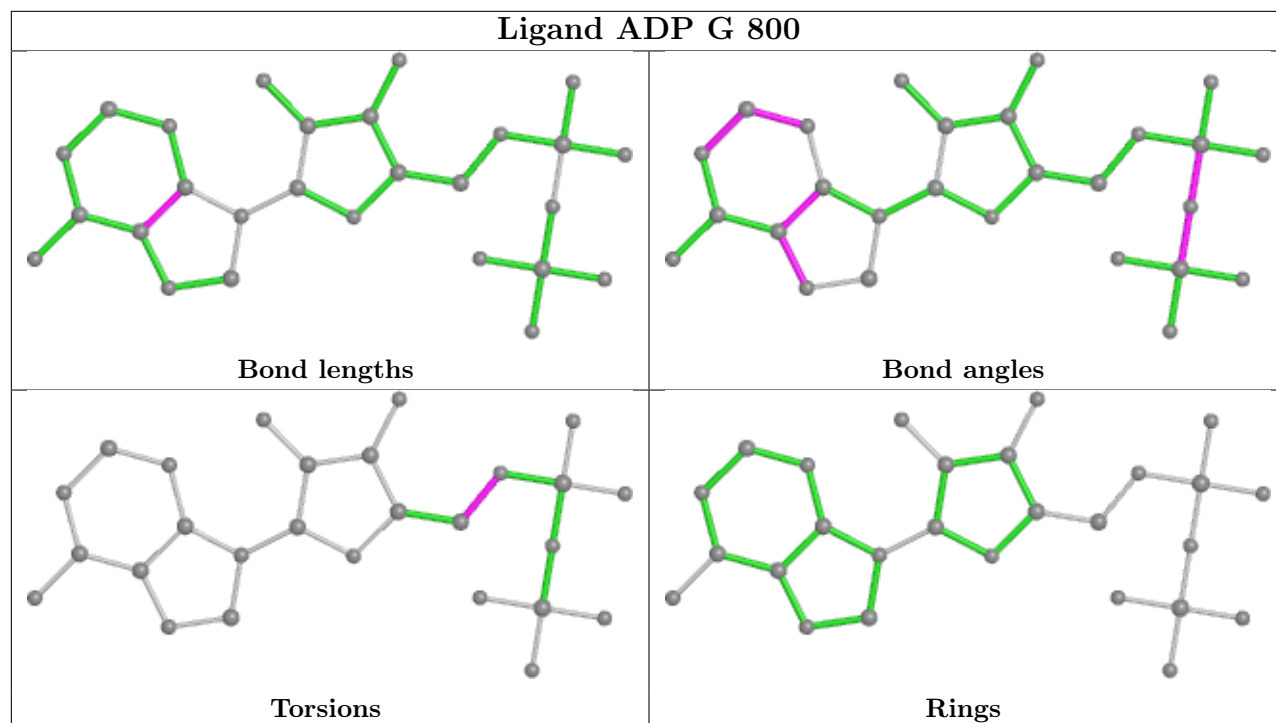
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	800	ADP	1	0
22	B	800	ADP	1	0
22	C	800	ADP	2	0
22	E	800	ADP	1	0
22	F	800	ADP	2	0
22	G	800	ADP	2	0
22	I	800	ADP	1	0
22	J	800	ADP	4	0

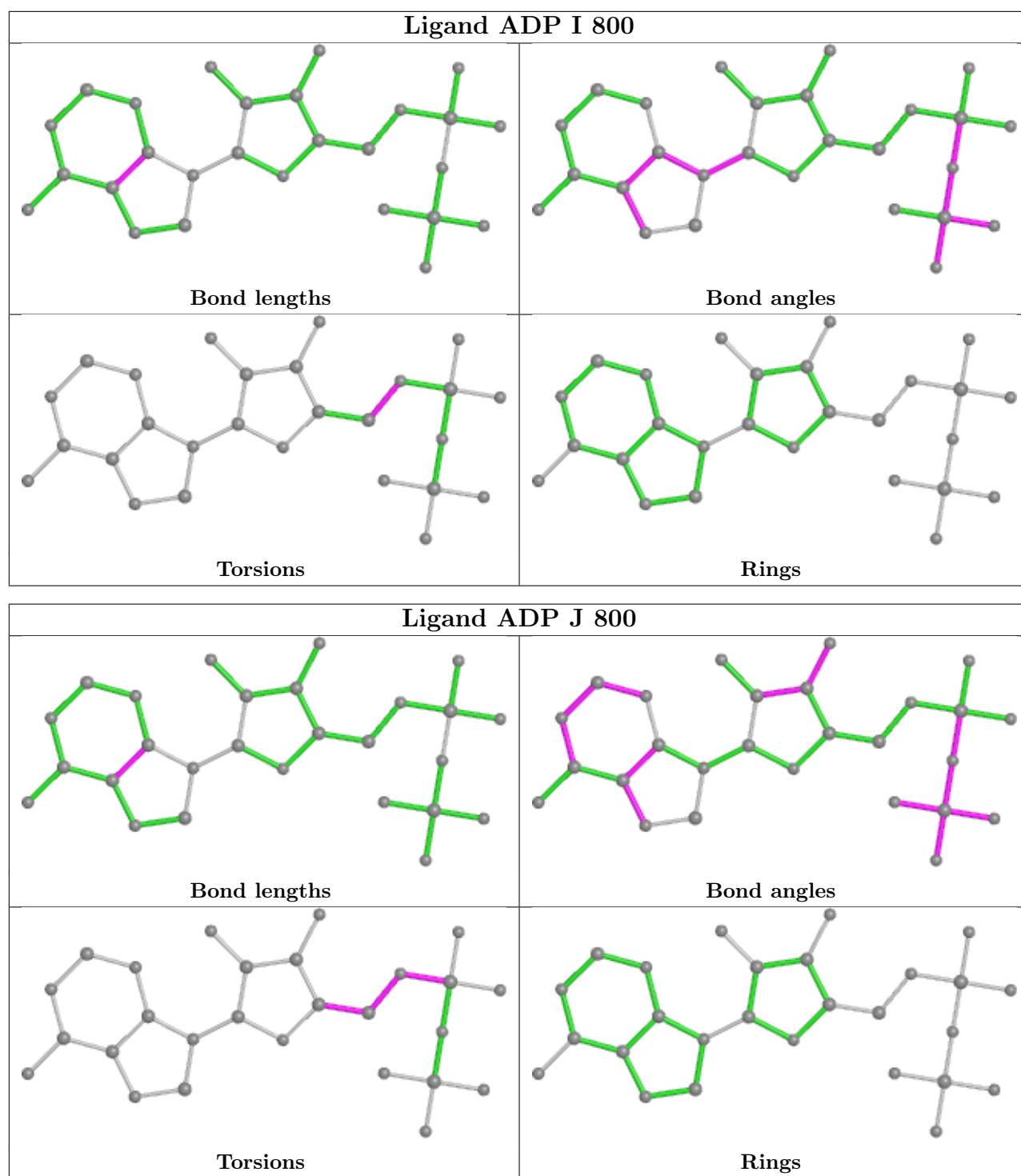
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
12	Y	12
7	N	5
6	M	5
8	P	3
8	O	3
9	Q	2
9	R	2

The worst 5 of 32 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	171:UNK	C	201:UNK	N	103.17
1	N	367:UNK	C	401:UNK	N	94.98
1	M	171:UNK	C	201:UNK	N	93.67
1	M	367:UNK	C	401:UNK	N	83.48
1	N	634:UNK	C	701:UNK	N	69.69